

PREPRINT



# NEW DEAL

**Austrian Research Agenda**

# Table of Contents

<b>04</b>	<b>Preface</b>
<b>06</b>	<b>A New Deal for Industry</b>
<b>16</b>	<b>Manufacturing</b>
<b>82</b>	<b>Sustainability</b>
<b>160</b>	<b>Materials</b>
<b>242</b>	<b>Analytics</b>
<b>360</b>	<b>Keywords Index</b>
<b>368</b>	<b>Authors Index</b>

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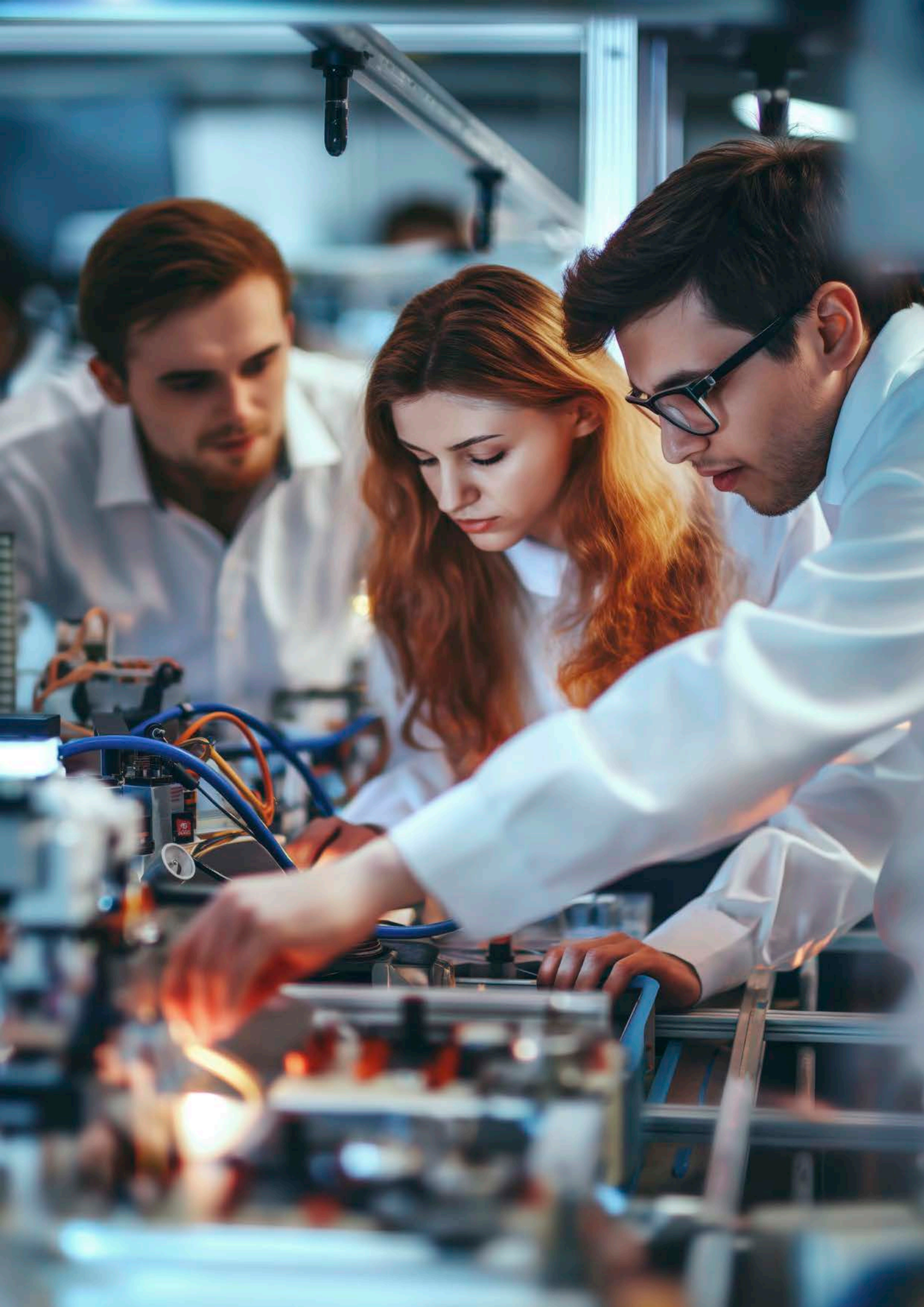
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## Preface

**“A New Deal for Industry: Austrian Research Deal”** is a forward-looking manifesto intended and developed to catalyze the transformation of Austria’s industrial sector. This ambitious strategy envisions a future where Austria leads in sustainability, innovation, and global competitiveness. By addressing key areas such as advanced manufacturing technologies, material science, digital transformation, and circular economy principles, the agenda sets the stage for a new era of industrial excellence. This book aims to provide a comprehensive **overview on these key areas, underlining their significance and the pivotal role of Austria’s scientific community** in driving this transformation.

This **Austrian Research Agenda** provides a comprehensive framework for transforming Austria’s industrial sector into a beacon of sustainability, innovation, and global competitiveness. By focusing on key areas such as sustainability, advanced manufacturing technologies, materials science, digital transformation, and education, the agenda charts a clear path for achieving long-term growth and environmental stewardship. Through collaboration, innovation, and continuous improvement, Austria is poised to lead the global industrial landscape into a prosperous and sustainable future.

The key takeaways are:

- **Sustainability:** Emphasis on circular economy, CO<sub>2</sub> reduction, and sustainable business models.
- **Advanced Technologies:** Integration of 6G, robotics, AI, and IIoT in manufacturing processes.
- **Materials Science:** Development of sustainable materials and the application of ICME.
- **Digital Transformation:** Implementation of digital twins and big data analytics for process optimization.
- **Education:** Establishment of learning factories and continuous competence development programs.
- **Innovation:** Promotion of open innovation and public-private partnerships to drive industrial innovation.

# Sustainability in Industry

## Circular Economy

Central to the Austrian Research Agenda is the target of a circular economy. A transformative approach redefines traditional growth paradigms by prioritizing societal benefits over mere economic gains. The circular economy focuses on eliminating waste and pollution, keeping products and materials in continuous use, and regenerating natural systems. The agenda outlines several strategic initiatives to facilitate this transition, including the development of sustainable materials, the enhancement of recycling technologies, and the promotion of product designs that extend lifecycles.

Transitioning into a circular economy requires a fundamental shift in how products are designed, produced, and consumed. This approach is not solely about waste reduction; it involves creating a sustainable industrial ecosystem where resources are utilized efficiently. Achieving these goals necessitates collaboration across multiple sectors. By fostering an environment that supports circular practices, industries can significantly reduce their environmental footprint while driving innovation in product design and manufacturing processes without ignoring the importance of competitive costs. The agenda emphasizes the importance of a collaborative effort among industries, policymakers, and the scientific community to realize these objectives.

## CO<sub>2</sub> Reduction

The reduction of carbon dioxide (CO<sub>2</sub>) emissions is a critical priority within the agenda. Addressing this issue is essential for mitigating climate change and achieving international climate targets, such as the European Green Deal, which aims for the EU to become climate-neutral by 2050. The agenda highlights various strategies to reduce CO<sub>2</sub> emissions, including adopting cleaner production methods, investing in renewable energy sources, and improving energy efficiency across industrial operations.

Industries are encouraged to integrate CO<sub>2</sub> reduction and management strategies into their core operations through a combination of technological innovations, process optimizations, and behavioral changes. Monitoring and reporting CO<sub>2</sub> emissions are vital components of this strategy, enabling industries to track progress and make data-driven decisions. By prioritizing CO<sub>2</sub> reduction, industries contribute to global climate goals, but this needs to be balanced out with enhancing their operational efficiency and reducing

costs. The agenda underscores the need for the scientific community to develop and implement these innovative solutions, ensuring that Austria remains at the forefront of global environmental stewardship.

## Sustainable Business Models

Sustainable business models are integral to aligning economic growth with environmental and social responsibility. The Austrian Research Agenda promotes the development of business practices that incorporate sustainability into their core strategies. This includes adopting green technologies, enhancing corporate social responsibility initiatives, and integrating sustainability metrics into business performance evaluations.

Sustainable business models extend beyond compliance with environmental regulations. They involve a holistic approach that considers the environmental, social, and economic impacts of business activities. The agenda encourages businesses to innovate and find new ways to create value while minimizing their environmental footprint. This can involve developing new products and services that meet the evolving needs of the market, investing in sustainable supply chains, and engaging with stakeholders to build a sustainable future. The scientific community's role in developing and implementing these models is crucial, ensuring that businesses can thrive while contributing positively to society and the environment.

# Advanced Manufacturing Technologies



### **6G and Wireless Communications**

The advent of 6G technology represents a significant leap forward for the industrial sector. This next-generation wireless communication technology promises ultra-reliable, low-latency networks that are essential for advanced manufacturing processes. The agenda thoroughly explores the potential applications of 6G in industry, emphasizing its role in enabling real-time data exchange, enhancing automation, and improving overall production efficiency.

6G technology is expected to revolutionize industrial communication, supporting a wide range of applications from autonomous vehicles to smart cities. In manufacturing, 6G will enable more responsive and flexible production systems, where machines and devices communicate seamlessly to optimize operations. The agenda highlights the importance of investing in 6G infrastructure and developing applications that leverage its capabilities to enhance industrial productivity. The scientific community is called upon to lead research and development efforts in this area, ensuring that Austria remains at the cutting edge of technological advancements.

### **Robotics and Automation**

Robotics and automation are key components of modern manufacturing processes. The agenda discusses the integration of advanced robotic systems to enhance production efficiency, ensure worker safety, and improve product quality. Robotics technology is rapidly evolving, with new capabilities such as collaborative robots (cobots) that can work alongside humans in shared workspaces.

The use of robotics and automation can significantly increase the efficiency and flexibility of manufacturing operations. Robots can perform repetitive and hazardous tasks with high precision and speed, freeing human workers to focus on more complex and creative activities. The agenda emphasizes the need for industries to adopt robotics and automation technologies to remain competitive and meet the demands of a rapidly changing market. The synergy that can be achieved from both the scientific community and industry play a pivotal role in advancing these technologies, ensuring their successful development and integration into industrial processes.

### **Artificial Intelligence (AI) and the Industrial Internet of Things (IIoT)**

AI and IIoT are transformative technologies that are reshaping the industrial landscape. AI technologies are used for predictive maintenance, process optimization, and real-time decision-making, while IIoT connects machines, sensors, and devices to create a networked production environment.

The integration of AI and IIoT allows industries to move towards smart manufacturing, characterized by highly automated and optimized processes. AI can analyze vast amounts of data to identify patterns and make predictions, enabling proactive maintenance and reducing downtime. IIoT provides the infrastructure for collecting and transmitting data from various sources, creating a connected ecosystem that supports continuous improvement. The agenda highlights the importance of investing in these technologies to drive innovation and enhance industrial performance. The scientific community's expertise is crucial in harnessing the full potential of AI and IIoT, ensuring that Austria's industrial sector remains competitive on a global scale.

# Materials Science and Engineering



### **Sustainable Materials**

Developing and using sustainable materials is a central focus of the research agenda. Sustainable materials are those that have minimal environmental impact throughout their lifecycle—from production to disposal. The agenda emphasizes the need for materials that are renewable, recyclable, and that can be produced on a low carbon footprint.

Research in sustainable materials aims to discover new materials, improve the properties of existing ones or enhance their production efficiency to meet sustainability criteria. This involves exploring alternative raw materials, developing eco-friendly manufacturing processes, and enhancing the recyclability of materials. The agenda also highlights the importance of material innovation in achieving circular economy goals and reducing the environmental impact of industrial activities. The scientific community is tasked with leading these research efforts, ensuring that Austria remains at the forefront of sustainable material development.

### **Integrated Computational Materials Engineering (ICME)**

ICME is an interdisciplinary approach that integrates computational tools and methods to design and optimize materials, processes, and products. The agenda highlights the use of ICME to accelerate the development of new materials and improve manufacturing processes. This approach combines data from experiments, simulations, and literature to create comprehensive models that predict material behavior and performance under various conditions.

ICME enables researchers and engineers to explore a wide range of material compositions and processing conditions in a virtual environment, reducing the need for costly and time-consuming physical experiments. By leveraging advanced computational techniques, ICME can significantly speed up the development of new materials and optimize existing processes. The agenda emphasizes the importance of ICME in speeding up innovation and enhancing the competitiveness of the industrial sector. The scientific community's role in advancing ICME methodologies is vital for maintaining Austria's leadership in materials science.

# Digital Transformation and Data Analytics



### **Digital Twins**

Digital twins are virtual representations of physical objects or systems that can be used to simulate, predict, and optimize performance. The concept of digital twins is pivotal in the digital transformation of industries. By creating digital twins of manufacturing processes, industries can monitor real-time operations, predict failures, and implement improvements without physical interventions, thereby saving time and resources.

Digital twins provide a dynamic and interactive model of industrial systems, allowing for continuous monitoring and optimization. They can be used to simulate different scenarios, evaluate the impact of changes, and identify potential issues before they occur. The agenda highlights the importance of investing in digital twin technology to enhance operational efficiency, reduce downtime, and improve overall performance. The scientific community's expertise in developing and implementing digital twin solutions is essential for achieving these goals.

### **Big Data and Analytics**

Big data analytics is essential for making informed decisions in modern manufacturing environments. The agenda stresses the importance of collecting and analyzing large volumes of data to gain insights into production processes, identify areas for improvement, and enhance overall efficiency. Advanced analytics techniques, including machine learning and AI, are employed to process and interpret this data, enabling predictive maintenance, quality control, and process optimization.

The ability to analyze large datasets allows industries to uncover hidden patterns and correlations that can drive operational improvements. Big data analytics can be used to optimize supply chains, improve product quality, and enhance customer satisfaction. The agenda emphasizes the need for industries to invest in data analytics capabilities to stay competitive and meet the demands of a data-driven market. The scientific community's role in advancing big data analytics is crucial for ensuring that Austria's industrial sector remains innovative and efficient.

# Education and Innovation



### **Learning Factories**

Learning factories are practical training environments where students and professionals can gain hands-on experience with advanced manufacturing technologies. The agenda outlines the establishment of learning factories to bridge the gap between theoretical knowledge and practical skills. These facilities provide opportunities for experimentation, innovation, and collaboration, preparing the workforce for the challenges of Industry 4.0 and beyond.

Learning factories simulate real-world industrial environments, allowing participants to work with the latest technologies and tools. They provide a platform for developing practical skills, testing new ideas, and solving real-world problems. The agenda highlights the importance of learning factories in fostering a skilled and adaptable workforce that can drive industrial innovation and growth. The scientific community is instrumental in designing and implementing these educational initiatives, ensuring that the next generation of workers is well-equipped to lead Austria's industrial future.

### **Competence Development**

Continuous competence development is crucial for maintaining a competitive edge in the industrial sector. The agenda advocates for ongoing training and upskilling of employees to keep pace with technological advancements. This includes offering specialized courses, workshops, and certification programs that cover emerging trends and technologies in manufacturing. Investing in employee development ensures that the workforce remains skilled and knowledgeable about the latest technologies and best practices. Competence development programs can help employees adapt to new roles, improve their productivity, and contribute to the overall success of the organization. The agenda emphasizes the need for industries to prioritize employee development to build a resilient and innovative workforce. The scientific community's role in developing and delivering these training programs is critical for ensuring that Austria's industrial sector remains at the forefront of global innovation.

### **Open Innovation**

Open innovation is a collaborative approach where industries, academia, and research institutions work together to drive innovation. The agenda promotes open innovation as a means to accelerate the development of new technologies and solutions. By fostering a culture of collaboration and knowledge sharing, the agenda aims to create an ecosystem where ideas can be freely exchanged and rapidly translated into practical applications.

Open innovation involves breaking down traditional barriers and encouraging collaboration across different sectors and disciplines. This approach can lead to the development of new products, services, and business models that address complex industrial challenges. The agenda highlights the importance of creating platforms and networks that facilitate collaboration and innovation across the industrial ecosystem. This includes setting up innovation hubs, incubators, and accelerators that bring together researchers, entrepreneurs, and industry experts to work on joint projects and share their insights and expertise. The scientific community's involvement in these collaborative efforts is essential for driving Austria's industrial innovation.

### **Public-Private Partnerships**

Public-private partnerships (PPPs) are highlighted as a strategic tool for achieving research and innovation goals. PPPs leverage the strengths of both the public and private sectors to fund and execute large-scale research projects. The agenda discusses the formation of PPPs to address complex industrial challenges, develop cutting-edge technologies, and drive economic growth.

By addressing these key areas, the Austrian Research Agenda aims to create a resilient, flexible and forward-looking industrial sector that not only meets today's demands but also anticipates and adapts to foreseeable and yet to be seen challenges of the future. The agenda's comprehensive approach ensures that economic growth is aligned with environmental sustainability and social responsibility, setting a strong foundation for a flourishing industrial future.

Alois Ferscha

**Manufacturing**





# Enforcing Innovation for the New Deal of Production

Christian Ramsauer, Hans Peter Schnöll, Matthias Wolf, Maria Hulla

## Vision

The manufacturing sector is of significant importance as it is accounting for around 20% of the gross value added and roughly 25% of employment in Europe (World Bank 2023). For the European Union, innovation is key to compete in the global competition, maintaining technological leadership, enabling economic growth and job creation, and react resiliently to disruption while at the same time addressing environmental and societal challenges (European Commission 2021a). To harness the potential of innovation, European governments, institutions, and businesses need to foster an ecosystem that supports research and development, encourages entrepreneurship, and promotes collaboration between academia and industry, especially in relation to the manufacturing sector.

The future of manufacturing sector, at the same time, is heavily influenced by the so called “twin transition” (World Economic Forum 2022), referring to the ongoing digital and sustainability transformations. While the digital transformation aims at agile production systems and the needed real time data for adaption to disruptive business environment, sustainability efforts are focused on minimizing the ecological footprint of production by reducing waste and circulating materials while enforcing human strengths in creating value. These ideas were adopted by the European Union renamed as the “Industry 5.0” paradigm. As an extension of the Industry 4.0, it also highlights research and innovation as drivers for a transition to a sustainable, human-centric and resilient European industry that captures the value of

new technologies, while respecting planetary boundaries and fostering worker’s wellbeing in a growing economy (European Commission 2021b).

Based on the new paradigms and requirements, the design and operations of product- and factory-life cycles have to be reconsidered focusing on circularity, sustainability and resiliency. To drive this transformation, the Institute of Innovation and Industrial Management at Graz University of Technology focuses on the whole life cycle from product development over eco-efficient production to the evaluation and improvement of environmental impacts, researching and educating the topics of innovation and industrial management along the industrial value chain.

- **Open Innovation**
- **Product Design**
- **(Virtual) Rapid Prototyping**
- **Human-centered**
- **Resource-efficient Production**
- **Competence Development**
- **Learning Factories**

## Approach

For the new deal of production, the Institute of Innovation and Industrial Management of Graz University of technology thus focuses its research and industrial cooperations on four strategic topics of (1) maker movement, (2) product design, (3) efficiency in

production and (4) agility and develops application-oriented trainings to upskill students and executives.

### Innovation as key for fast and sustainable development

The **maker movement as driver for open innovation** is based on the idea that everyone can design, manufacture and distribute own products. With affordable access to digital production technologies, today it is possible for everybody to realize their own product ideas. Furthermore, the trend of making is becoming increasingly important in industry. While the established cooperation of industry and research is a key enabler for innovation in our society, recent developments force several industries to deal with high degrees of uncertainty and volatility leading to shortened innovation-cycles. International studies show, that so-called makers - creative minds, with the intent to develop new products and services - have substantial potential to generate disruptive innovations in such short cycles (Sang and Simpson 2019). New products and services are developed more effectively when creative students and makers, researchers, start-ups, SMEs and established companies meet at the same location and work collaboratively together (Friessnig & Ramsauer 2021). To further exploit innovation for industry, research on how to better integrate makers into the well-established cooperation of industry and scientific research is necessary. For this reason, the project series “Enforcing Innovation across Maker, Industry & Research” (MI&R) was established in 2017 (ongoing). Here students and makers meet research and industry and work together on open innovation (Kohlweiss et al. 2020). In researching the impact of the maker movement on start-ups, SMEs and established firms several cooperation formats, trainings and workshops were developed and are continuously improved to strengthen our innovative industry.

### Product design and fast development through rapid prototyping

enables successful companies to offer the right product at the right time at an appropriate price. As a consequence of accelerated changes in the business environment such as customer requirements or available technologies, it is becoming more and more difficult to fulfill customer needs. Product lifecycles are getting shorter and time is therefore a scarce resource. Furthermore, the complexity of product design and development processes is increasing, e.g. due to the need to integrate mechanical components, electronics and software. Characteristic

examples therefore are cyber-physical systems as part of industry 4.0. To meet upcoming challenges, it is essential to avoid unnecessary external and internal complexity and to minimize unavoidable complexity. Design thinking can be one answer to face those challenges. It is a set of both, mindsets and design-based activities that foster the collaboration required to solve problems in human-centered ways. Thinking like a designer can transform the way organizations develop products, services, processes, and strategy. The Design Thinking approach brings together what is desirable from a human point of view, with what is technologically feasible and economically viable. Its process is based on the intuitive workflow of a designer and based on a deep understanding of the customer (Peng 2022). The new “Schumpeter Laboratory for Innovation”, offers the opportunity to research on product design and work with state-of-the-art rapid prototyping technologies and VR-enhanced design methodologies (Fig. 1) to teach product development for the next generation

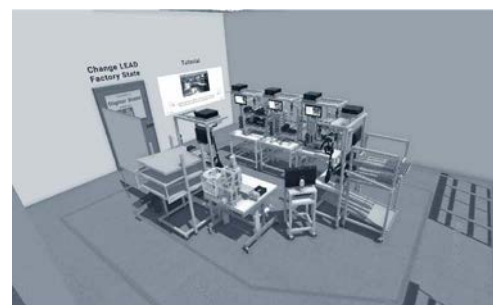


Fig. 1. VR enhanced product and process design

### Industrial management for efficient, sustainable and agile production

Due to technological progress and more volatile working environments, companies have to adapt and change ever quicker. **Digital factories and process optimization** (simulation, virtual reality, etc.) (Fig. 2), the use of disruptive technologies (internet of things, artificial intelligence, etc.) and the design of competitive working environments (collaborative robotics,



Fig. 2. Simulation based factory planning and optimization (created in Technomatix Plant Simulation)



wearables, agile infrastructure) enable the design of the future of human work to be human centered and sustainable. All these new means build the important toolkit for achieving the status of resilience and the condition of remaining robust and successful in always faster and more volatile markets. In order to demonstrate how such sustainable, resilient and agile concepts could look like in production environments, the “LEAD Factory” is constantly advanced (Wolf et al. 2023). In this classical learning factory, which is based on the assembly process of a scooter, virtual factory planning and design tools, human and process simulation software, energy efficiency measurement devices, and several digital transformation tools are installed and researched. The future goal is to link such models with real-time data from cyberphysical production systems, in order to enable real-time control of the factory productivity through so-called “digital twins”.

Increasing competition, demographic changes in the working population and growing efficiency requirements lead to a higher intensity of work for fewer and on average older workers. Going into a higher degree of automation can only counteract this to a limited extent because of technical and economic limits, making it more than ever important to consider the **worker at the center of value creation**. Therefore, our research focuses on collaborative working environments in which humans and machines complement each other’s capabilities. In regard to **human centered work design** research focuses on simulation-based ergonomic design of workplaces (Fig. 3) for prolonged health and safety or for technologies that link the humans and technical systems as real time locating systems (RTLS) to make it more adaptable and inclusive (Wolf et al. 2022).

For example, research is being



Fig. 3. Lead Factory and digital workplace design

conducted on how and when systems for physical support (e.g. exoskeletons) are useful in order to avoid overload and absenteeism (research project “ExoFitStyria”). For the growing amount of information to be processed, worker-guidance systems and extended reality

applications are under investigation. Such technologies connect people with the technical system and provide only the necessary information at the right time, so that the workers become the center of efficiently designed production processes (Hulla et al. 2021). It is important to design such systems in accordance with human requirements and to handle associated personal data with care. In addition to technical development, current research projects are concerned with the acquisition and transfer of necessary skills (research project “LeNuWas” and “VolaDigital”). These competences can in turn be developed in the “LEAD Factory”.

Due to the EU’s goal of ensuring CO<sub>2</sub>-neutral production in Europe by 2050 (European Commission 2022), the **reduction of environmental footprints** will take on a central role for production. Smart production systems offer the opportunity to provide the relevant data as a “by-product”. The relevant emission data, the product footprint (CPF) as well as other sustainability targets can be computed and monitored with high temporal and spatial resolution via smart data acquisition directly at the machines and with the use of networked libraries. This is the basis for controlling the actual situation and finding new potentials of reduction. Further analysis and forecasting tools (e.g. energy flow analysis, energy value stream mapping, energy simulation) can be used to process the data as a decision-making aid or for automated control of the technical systems. Research is being conducted on transparent procedures for determining the relevant emissions for companies (e.g. research project “Transform. Industry”) and trainings for product evaluation (carbon footprinting) and their targeted reduction (energy efficiency training) are developed in the LEAD Factory (Wolf et al. 2023). Regarding environmentally conscious production we follow the objective to create transparent and easy-applicable evaluation and improvement methodologies and tools especially SMEs. We focus the main objective to improve the ecological footprint of companies and products while maintaining productivity and focusing on economically feasible measures.

Increasing market volatility and uncertainty force manufacturing companies to adapt their operating model to a substantially changing environment. For this reason, it is necessary to anticipate uncertainty and deal with its effects on operations proactively. The **agility concept as answer to disruptions and volatile markets** can be seen as a key to thrive

in such a challenging environment (Fig. 4).  
The principal idea is to mitigate

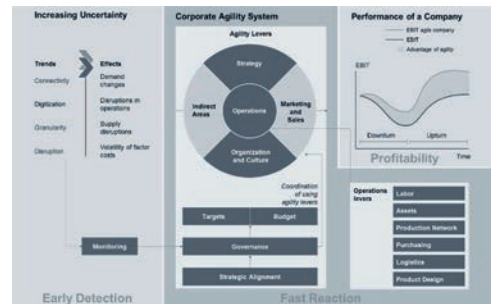


Fig. 4. Agility concept

risk in market downturns and to take advantage of opportunities in upturns to achieve superior long-term corporate performance. Agile manufacturing enables companies to

prepare proactively for uncertainties and to react quickly to changes in order to optimize the economic situation by leveraging the whole value chain. It is essential to consider the organization holistically to assure that agile operations come to life in industrial practice. Research is focused on the identification and implementation of operational agility levers, and organizational structures and behavioral patterns in management (Ramsauer et al. 2017). In addition, the digital modeling of production systems across several factories for the transparent planning of resilient value streams in simulation models is researched in cooperation with industrial partners with the main objective to improve the resiliency of value streams in times of back shoring activities in Europe.

## Impact

Inteaching/training and industrial/research projects, the Institute of Innovation and Industrial Management focuses on the four topics of (1) maker movement, (2) product design, (3) efficiency in production and (4) agility. Well-prepared data, clear depictions or hands-on learning are used to sensitize for the major levers and opportunities for product and process development and improvement. Stakeholders - no matter if they are engineering students or C-level executives - are often surprised how easy and fast effective solutions can be implemented. New designs and concepts can be realized quickly; only hours or days pass from the first idea to the functional prototype. Efficiency improvement measures pay back in just a few months. Emissions and environmental pollution can be significantly reduced with just two or three actions. The institute's "Schumpeter Laboratory of Innovation" currently offers over 1,700 registered users easy access to state-of-the-art production technologies such as 3D printers. In the context of a wide variety of projects, numerous innovative and in some cases patented product solutions and start-ups have been initiated there over the past ten years. In the LEAD Factory, around 750 persons from academia and industry have been trained since 2014. In the field of industrial management, more than 120.000 square meters of shop floor have been successfully planned so far during factory planning projects supported by planning software including discrete-event simulation and VR. Furthermore, carbon emissions at product level have been reduced by at least 40% in all the industrial projects examined up to now. As part of the project, an energy flow analysis was conducted at the two most energy-intensive factories. As a consequence, an energy reduction potential of 11% and 24% were identified for 2020 by implementing tangible actions in the analyzed facilities.

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## Competencies

The researchers at the Institute of Innovation and Industrial Management have extensive experiences in creating innovative products as well as developing strategies for an efficient production of tomorrow using 1,200 m<sup>2</sup> of laboratory space. In two working groups, around 35 persons work together with project partners to investigate current issues in a problem-oriented manner. In the area of teaching, more than 30 courses are offered that cover a broad spectrum but still address very specific subjects and current challenges of the industry. Further information is available on [iim.tugraz.at](http://iim.tugraz.at).

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# Towards Eco-Digital Production Systems

Selim Erol

## Vision and Approach

Eco-digital production systems as we envision it, are systems that have low negative ecological impact (are ecologically sustainable) and have a high degree of digitalization. The order of words is not chosen arbitrarily, while a low ecological impact of production systems is a societal necessity, digitalization is basically a means to achieve economic efficiency gains. Given this prioritization, a frame is set for a future research and education agenda.

At the IIEM and as part of an University of Applied Sciences we favor a research and education approach that is foremost based on practical problems and requirements from regional industry. However, as a research institute we also strive to go beyond existing concepts of production systems and related solutions. The level we focus on (according to the ISA-95 reference model) is on the work-place level and above. Thus, the research object in focus is a workplace, a

production line or cell or the production system of an industrial firm including related subsystems like transport or maintenance systems.

We see production systems as complex socio-technical systems where humans

- **Production**
- **Digitalization**
- **Sustainability**
- **Circular Economy**
- **Engineering Education**

play a vital role, though increasingly are supported by intelligent and networked technical systems. In contrast to a more traditional view, we see these systems in strong relation with their natural and social environment and the impact they have on it (see Fig. 1).

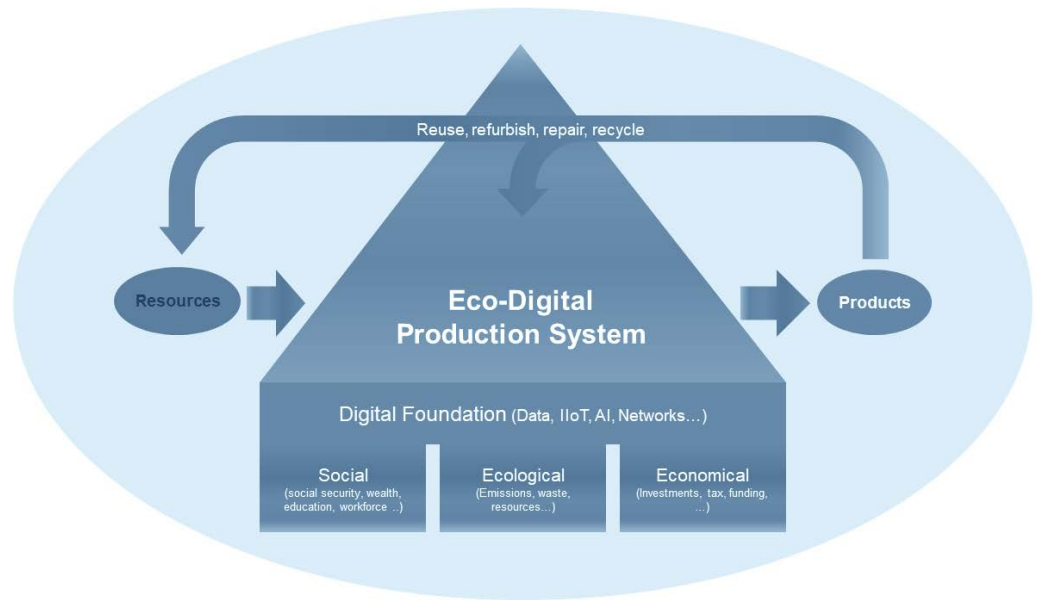


Fig. 1. Eco-digital production systems

## Challenges and Opportunities

According to UN estimates, the world population passed the 8 billion mark in November 2022. In other words, over the past 25 years, the number of people on the planet has increased by one third, or 2.1 billion. The growth in population is mainly confined to low in-come countries, e.g. Africa [1]. This development undoubtedly poses a challenge on economic systems and production capacities. Developing countries struggle to cope with increasing demand for food and energy but also for improved living standards, including a rising need for mobility. These developments inherently pose stress on society and natural resources. The change in climatic conditions is an additional and strongly interlinked development that aggravates the previously mentioned challenges. Recently, global political developments have put established global supply chain networks at risk. Given these global developments and due to its location in Europe as well as its historically-rooted high share of industrial production, Austria faces some particular challenges in the field of manufacturing of goods.

One of these recent challenges are rapidly **increasing costs of production**, due to a rise in energy prices. In addition to increasing costs of labor, industrial firms are struggling to offer **competitive prices for products** in the global market. Austria is commonly known as a high income country with high production costs. Competitiveness is reached through a highly educated work force as well as research and development capacity ensuring high-

quality high-technology products. **Digitalization of production processes** is a means to increase efficiency and productivity but requires engineers with skills and experience in different areas of information technology and automation as well as investments in respective technology. These challenges finally have led to the German “Industrie 4.0” initiative, drawing a vision for a future highly digitalized and reindustrialized Europe. At the same time the need for green production processes and transparent supply chains has arisen. This is due to the increasing demand from customers for products, that are produced in a transparent and responsible manner, as well as the demand from entrepreneurs for resource efficiency. Legal acts like the EU directive on corporate sustainability due diligence [2] and other regulations encouraged by the Circular Economy Strategy drive manufacturing enterprises to (radically) redesign products and production processes both on the technical level and business model level.

The **digitalization and ecologization urge** in the industrial production domain creates manifold opportunities for scientific research and education, especially in the field of engineering and management science. For example, the pace of technological developments and the broad and ambitious vision of “Industrie 4.0” have led to a certain paralysis of industrial enterprises with regard to a proper transformation of their production systems towards fully digitalized “cyber-physical” systems [3]. Here, the opportunity for management science lies in providing empirical evidence

on the state of digitalization and the maturity of industrial enterprises but also the provision of empirically grounded methods to develop sustainable **digital transformation strategies** and measures [4]. The same applies to enterprises' transformation towards circular business models and technologies. Enterprises seek well-founded **guidance to reduce risk** in their transformation endeavors. On the operations level digitalization directly affects the future physical production process. Digitalized work places must be organized differently, e.g. when humans collaborate with robots, or are supported by intelligent assistance systems on the shop floor.

**Applied research** in close cooperation with industry can provide valuable case-studies, best-practices and prototypical implementations to learn from. For engineering science, multiple opportunities can be identified in the field of material, construction and manufacturing technology likewise.

**Circular and eco-friendly products** require new (renewable) materials, new ways of designing and constructing such products, e.g. design for disassembly and repair as well as new energy and material efficient production processes, e.g. decarbonized manufacturing and transport processes. Enterprises in search for additional efficiency gains increasingly drive **digitalization and intelligentization** of their supply chains in a way that certain processes are completely automated (autonomous) and at the same time human work processes are augmented to reduce typical human drawbacks like physical and cognitive fatigue, errors and delays. Intelligent automation of production processes involve a plethora of traditionally independent scientific and technological disciplines. For example, collaborative robotics involves robotics and automation (originally in the mechanical and electrical engineering domain), image processing (originally related to computer engineering domain) and also human factors and ergonomics. The same applies to virtual or augmented reality (VR, AR) applications to support maintenance processes. Use of **algorithms and huge amounts of data** to gain real-time insights in production efficiency, predict future disturbances and improve forecasting are other examples where computer science meets software engineering and production engineering disciplines. The integration of technologies and approaches into an intelligent production system is a key challenge and therefore great scientific opportunity.

The **scientific opportunities** mentioned above require well-educated and highly-skilled engineers that are able and willing to tackle **complex interdisciplinary challenges**. A future engineering education system must provide capable and motivated engineers both in quantity and quality to satisfy an increasing demand from industry. Subsequently, universities and other institutions, will need to develop **education opportunities** that are permeable for interdisciplinary knowledge sharing and development. The ultimate challenge for educating future production engineers is to enable and empower them to engineer eco-friendly, resource-efficient and digitalized production systems, thus eco-digital production systems.

Our **research interest** is particularly on questions regarding how to plan and control production processes on the levels mentioned above in an efficient and sustainable way, thus with no negative impact on the environment. For this purpose we search for new concepts, methods and technical support systems. A **central question** at our attention is, how to make available and use data from different sources (e.g. machines, devices, sensors, human generated data), ensure their quality and quantity, efficiently store and process this data to support both human and machine agents in complex planning and control tasks. We aim at developing practical methods, tools and technical support systems and prototypes hereof together with industrial partners.

The primary **epistemological approach** we follow is an engineering science approach [5]. We employ methods from computer science, management science and industrial engineering science to develop general solution approaches for practical problems in industry. Due to the complex and interdisciplinary nature of research projects in the subject domain, we supplement our own expertise through **collaborations** with other disciplines and respective research institutions. Our research strives to produce tangible and applicable results [6]. To be able to test and validate our research, we make use of **test beds** from industry partners and our own **laboratories**. We operate two laboratories, in sum 1200 sqm, that can be used to emulate near to real-world factory environments, e.g. a small scale semi-automated production line and a full scale job shop environment.

## Impact

The **IEM** has established itself as a **regional education and research institution** in the field of industrial production and logistics. Considerably funded research projects with a focus **on intelligent digitalization of production systems** and promising first projects with a focus on **environmental aspects of production systems** helped to build up respective staff and laboratory infrastructure.

Projects like the establishment of the Innovation Lab Industry 4.0 and the Factory Lab have shown that state-of-the-art infrastructure is vital for research and development projects with regional industry but also for educating the next generation of production engineers.

IEM currently provides its **expertise in the following study programs**: bachelor and master programs of Industrial Engineering and Management, bachelor program Robotics and Mechatronics, bachelor program Sustainable Production and Circular Economy, master program Eco-Design. Both research activities and the joint development of study programs with industry show that upcoming challenges and research opportunities are to be found both in the ecologization of production systems and their intelligentization. Digitalization is a means to achieve these goals and provides even more research and education opportunities.





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## Competencies and Activities

Researchers employed at the IIEM are educated in engineering disciplines and are skilled in multiple methods and tools. Our **competencies** are in the analysis, modelling, simulation and optimization of production systems, the design and development of methods, tools and technical solutions for planning and control problems on the workplace level, the production line level and the production system level. The skillset spans from conceptual and mathematical modelling, simulation methods and tools, optimization methods, manufacturing technology, computer-aided engineering methods, and last but not least software engineering methods with a strong focus on data analytics and artificial intelligence applications.

The **Institute of Industrial Engineering (IIEM)** as a regional research institution in Lower Austria has a relatively short history, reaching back to 2012. Originally a sub unit of the study program Industrial Engineering and Management, it had developed a teaching portfolio that mainly covered subjects in management science. Since 2020, the focus was expanded to cover as well production engineering subjects, e.g. **manufacturing engineering, automation engineering, software engineering, data analytics and simulation**. The emphasis on digital competencies in industrial engineering education enables our students to contribute to an increasing number of digitalization projects brought in from industrial firms, e.g. in the course of theses.

The acquisition of a substantial three-year grant from public EU and national funds to build a large (1100 sqm) **fabrication lab** ("Innovation Lab Industry 4.0", [7, 8]) for prototyping and accompanying research activities have laid ground for establishing a fruitful and long lasting cooperation with regional industry. Opened in 2021, the lab is now an open space for collaborative **engineering of smart products and prototyping**. Today it hosts a wide range of manufacturing machinery and computer workstations that enable seamless digital product engineering and prototyping. Meanwhile students from various study programs, private makers as well as

regional small to large industrial firms and start-ups use the lab for their development and training activities. Our staff supports and trains industrial firms in using different manufacturing technologies ranging from CNC milling, turning to additive printing and laser cutting technology. The project was accompanied by research activities that identified user requirements and developed best-practices for university operated open fabrication labs. Another research activity aimed at the development of a virtual space (digital tools and platforms) in addition to the physical lab space to augment typical innovation activities.

A recently obtained grant within the COIN capacity building program from Austrian Research Promotion Agency (FFG) enables us to further develop our scientific competency in the field of **practical artificial intelligence (AI) applications in the production planning and control domain**. As part of a of a three-year project we will systematically identify potential use-cases for AI supported planning and control. Together with industrial partners we will develop methodological guidance in the identification and application of proper AI methods for specific **planning and control tasks in highly variable production scenarios**. Preliminary results from a wide range of qualitative interviews with industrial firms reveals a deep uncertainty regarding the expected benefit, the use-cases and the practical implementation although in most studied firms AI related projects have already been started in some way. The results from this ground laying study will later lead to the development of two demonstrators. The **demonstrators**, implemented in our two labs, will show how selected planning and control tasks on different levels of a production system can be augmented **to significantly improve key performance indicators of a production system**. Especially targeted at small to medium sized firms (SME), the demonstrators will enable us to showcase AI applications for SME and together develop solutions for practical planning and control tasks. First prototypes have already been developed for the use-case of real-time workpiece tracking, surface color detection under varying light conditions [9] and assembly progress

and quality tracking. These prototypes **showcase how low-cost and open source technologies** can be used in an automated production line for batch production.

In the course of an INTERREG exchange project with Czech and Austrian universities and the Austrian Industry 4.0 Platform for Smart Production we set up a **network of testbeds for research and education projects in the field of digitalization**. Similarly, a EU grant from EIT Manufacturing Learning Factories Network enabled us to develop a training offer for practitioners in industrial automation and AI application based on our

laboratory infrastructure.

A recent project, also publicly funded by the Austrian Research Promotion Agency (FFG), is targeted on the development of circular product-service systems for a very important and traditional industry in Austria – the furniture and interiors industry. Together with experts in the field and five industry partners we developed a training program to learn principles of design and engineering for circular products and related services. Originally targeted at a particular industry, the training program will be rolled out to other industries in the future.

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# Production Ecosystems and Marketplaces

Deepak Dhungana

## Vision

The process of manufacturing goods involves many different stages and activities and requires the involvement of a complex ecosystem of different players. No matter whether it is the customers, suppliers, factory operators, distributors, retailers, product designers, logistics companies, financial institutions or regulators, each player in the ecosystem plays a crucial role in the manufacturing process, and their contributions are essential to the success of the entire system. Traditionally, these stakeholders interact and contribute to the overall process in a peer-to-peer fashion and the implications of the decisions are not transparent. This makes it incredibly difficult to understand a company's sustainability practices and their impact on society and the environment. Metrics related to factors such as greenhouse gas emissions, energy and water usage, waste management, labor practices, diversity and inclusion, and risk management should be traceable and transparent to provide stakeholders with information about the sustainability performance of products and services. Arguably, the notion of products and services should therefore consider not just the final consumable, rather the overall trace from the initial raw materials all the way through the design and production processes to the end consumers.

To achieve the desired transparency, a digital backbone is required to capture and store data about the production process, from raw material sourcing to the final product. This data should be easily accessible and shared with stakeholders in the ecosystem, allowing for greater transparency and accountability. This

vision statement proposes research on manufacturing ecosystems, composed of a collaborative network of relevant stakeholders and a digital infrastructure to manage and maintain the interactions in order to **(i)** enable consumers to define the production requirements under the consideration of sustainability performance factors **(ii)** create flexible and optimal manufacturing consortia to fulfill the production requirements **(iii)** consider the role of both humans and machines during production **(iv)** monitor and ensure that both customer and regulatory requirements are met **(v)** improve traceability of manufacturing chains to ensure compliance with regulations and standards related to environmental, social, and governance (ESG) issues.

- **Manufacturing Ecosystems**
- **Traceability of Products and Production**
- **Production Consortia**
- **Factory as a Service**

Our goal is to develop and provide essential technologies that enable and support this vision, in particular, this requires methods and tools for **(i)** modeling factories as production services, and products as production requirements **(ii)** automated analysis of production capabilities to generate multi-factory production plans, enabling collaborative production **(iii)** automated configuration and re-configuration of factories based on the product specifications **(iv)** consideration of humans in the loop and safety requirements while

generating production plans (v) monitoring infrastructure for the production processes and their supply chains, making them transparent to the stakeholders in terms of sustainability parameters such as energy consumption and CO<sub>2</sub> footprints.

## Marketplace

In recent years, there has been a surge in research on flexible production processes due to the growing demand for customized products. As a result, new techniques have emerged that can handle the adaptability of production facilities and related intelligent procedures. Various initiatives, such as the Smart Manufacturing Leadership Coalition<sup>1</sup>, the Industrial Internet Consortium<sup>2</sup>, and Industrie 4.0<sup>3</sup>, are working towards revolutionizing the future of industrial manufacturing. To address the flexibility requirements, factories are shifting from the traditional „machine park operation“ approach to a „production as a service“ or „manufacturing as a service“ model, as described by Lu et al. 2014. Our approach is based on the notion of a factory and its production capabilities being “production services” offered through a **marketplace** that brings the different stakeholders together (Dhungana et.al C-2018).

The term “marketplace” in this context denotes a digital infrastructure component, where demand and supply

are matched. Such marketplaces serve not only to create economic value for buyers, sellers, market intermediaries, but also to monitor, and ensure that the ESG measures are correctly recorded and reported. Production facilities showcase their abilities to potential customers and offer their services in the marketplace. The product owners, such as designers and sellers, can then match their production needs with the capabilities of the factories. In turn, the factory owners can reconfigure their existing facilities to meet the specific requirements of the products to be manufactured. Such interactions in the marketplace not only consider the features of the products to be manufactured, but also the metrics relevant to ESG practices. This allows the propagation of consequences of product requirements in the planning of the production process, and the propagation of consequences of production process in the planning decisions toward the product design phase.

**Smart Factory (Factory Operators)** are seen as **more** than just manufacturing facilities that have integrated advanced digital technologies such as the Internet of Things (IoT), artificial intelligence (AI), and machine learning (ML) into their operations to increase efficiency, productivity, and automation. In the context of production ecosystems, these are production facilities that have adopted the notion of “any-time-anywhere production”, whose production services are offered

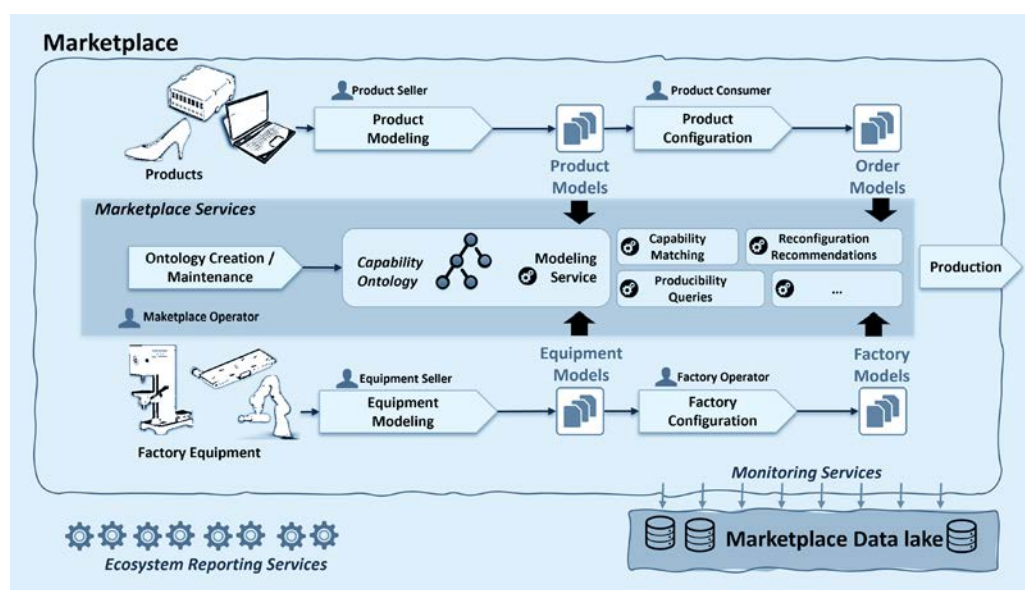


Fig. 1. Overview of a marketplace for production ecosystems (adapted from Dhungana et.al. C-2018)

<sup>1</sup> smlconsortium.org

<sup>2</sup> iiconsortium.org

<sup>3</sup> plattformindustrie40.at



through a marketplace, and which have incorporated automated configuration and re-configuration of devices and workflow based on the product specifications. In this context, it is crucial to consider Adaptive Task Sharing (ATS) methods to combine the strengths of automation and human skills to provide flexible and resilient factories (Dhungana et.al. C-2021).

#### **Smart Product (Product Designers)**

are called smart because they are aware of their own production process (Dhungana et.al. S-2015). This means, in the future, the designer of products must also consider associated manufacturing steps - an integrated engineering approach is necessary, that considers both the required production capabilities and the product features. To model products as a set of production requirements, it is important that a common ontology is established between the designers of both products and production facilities. Product variability and factory variability go hand in hand (Dhungana et.al. E-2017) and thus, product designers bridge the gap through common modeling practices (Dhungana et.al. S-2015).

**Smart Customer (Product Buyers)** are consumers who are well-informed and knowledgeable about the products and services they buy. In the context of production ecosystems, their role is gradually gaining importance as the trend towards “customized products”, and lot-size-one orders is gaining momentum. By defining the product features, consumers implicitly define the production requirements, which must be considered by the production facilities. Additionally, consumers are getting more and more aware of the sustainability performance indicators of the products and thus make more informed decisions not only based on the product features but also the performance of the production environments and supply chains.

## Marketplace Services

**Modeling Services:** Products and production services in the marketplace are modelled and offered through a shared infrastructure. This means, a common ontology or a mark-up language is needed to “standardize” product and factory descriptions. This is a key step in providing other services through the marketplace. With advancement in AI, the modeling activities could be envisioned to be automated. As depicted in Figure 1, modeling services are at the core of the marketplace and different models are used to share information and transfer responsibilities.

**Matchmaking Services** are services provided by the marketplace to factory operators and product sellers, enabling them to answer two basic queries.

**Q1:** Given a configured product, find all the factories that can manufacture the product.

**Q2:** Given a factory, find all products that can be manufactured in that factory. One of the key services required for producibility tests is the Skill Matching Service which can be used to semantically identify matches and gaps between services provided by the factories/ equipment and capabilities required for manufacturing a product. It is getting increasingly difficult for factories to provide the required flexibility to support lot-size-one production orders. Therefore, collaboration is especially important for manufacturing companies to ensure that they do not lose manufacturing contracts because they can only partially fulfill the requirements of their customers (*Dhungana et.al. E-2020*). It is therefore equally important to generate production plans across multiple factories, so that the production requirements for a given product can be met through collaboration with other factories (*Dhungana et.al. S-2015*).

**Monitoring Services** enable collection of relevant data among all the ecosystem participants and in all relevant interactions (*e.g., Dhungana et.al. J-2021*). The importance of making use of market data, user behavior data and product usage data for better performance of recommendation engines, better user experience for users of the configurators and for increasing developer productivity throughout all stages of the application development lifecycle by offering good tool support and agile development should be studied in more detail. With novel approaches in this direction, it should be possible for factory vendors, factory operators, product owners/sellers to organize and manage market data for better pricing and analytics and in the long run for better exploitation of data generated by different ecosystem participants.

For example,

- (i)** Better market segmentation and product portfolio management targeted to the market segments,
- (ii)** Transparency in stakeholder interactions and ecosystem processes,
- (iii)** Contextual personalization of marketing strategy and product placement. Transparency also allows customers to make informed decisions, regulatory to enforce policies (*e.g., Dhungana et.al. S-2022*), and it supports overall Quality control and assurance.



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## **Summary and Outlook**

Ecosystems are not controllable, just like markets, these highly dynamic environments are likely to be influenced by a multitude of factors, not controllable by individual organizations. Future research in smart production ecosystems can nevertheless identify the factors responsible for a healthy ecosystem and foster these. The distributed nature of knowledge in the ecosystem and the managerial independence of the involved parties poses huge challenges in collaboration. In many cases, there are technical problems to be solved (e.g., distributed modeling, redundancy modeling, SLA modeling, etc). In other cases, there are still many organizational and process issues to be addressed (e.g., quality management, change management, vendor interoperability etc).

One of the open issues in this field is fostering Open Innovation across multiple participants. In the smart production ecosystem, this process is best driven by the customers. By allowing customers to create real and virtual products, companies can use customers as marketers and co-creators this is often referred to as open innovation. This means, novel approaches are required to combine (company and factory) internal and external ideas to advance the development of new technologies.

Future research in this area also need to consider privacy-preserving ways of modeling the information, so that the intellectual property rights are preserved but enough information is shared. Special audit methods can be adopted to ensure the production of intellectual property developed specially for one customer. Some other examples of items in the research agenda are: (i) Encrypted sharing of models and other entities in the ecosystem and analysis operations on encrypted models (without having to decrypt), (ii) Tools and techniques for detecting violation of digital rights management based on the analysis of published models of products, factories, and factory components. Privacy Preserving Ecosystem Interactions will be crucial for the success of such a marketplace, as product design specifications, factory capabilities and details of factory components typically represent crucial intellectual properties of their owners (product sellers, factory operators, factory vendors). Due to the crucial nature of the information, voluntary sharing of such models and information is very unlikely.

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# Collaborative Manufacturing

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## Vision

Increasing customer demands for individualized products push manufacturing companies towards agile and modularized production processes. Digitalization enables them to efficiently connect with other companies in order to build up **collaboration networks** and to overcome inefficiencies by sharing resources among each other. It is well known that collaborative or joint planning and orchestration of plans can yield considerable cost savings [1,2,3].

So far, research mainly focused on centrally planned frameworks, where collaboration partners are forced to reveal critical information. This assumption can be seen as a barrier since manufacturers might be reluctant to enter such a collaboration. To overcome this issue, decentralized mechanisms are to be developed. In case of multi-level **lot sizing decisions**, for instance, extremely complex coordination problems can arise. However, also for the centralized case, efficient solution approaches are needed in order to solve problems of realistic size and under real-world settings.

In decentralized systems, decision makers hold private information like costs or capacities [1]. On the interface between **Operations Research** and **Game Theory**, the challenge is to design efficient and effective coordination schemes based on mathematical programming models, where as little as possible information has to be shared. Collaborative planning is more than just a coordination. It is jointly organized coordination of adaptations in an effort to improve plans for all collaborating players.

The problem occurs in horizontal collaborations, where producers are acting on the stage within a supply chain, as well as in vertical collaborations, where producers are in a supplier-customer relationship. While the huge majority of studies addresses the problem under the assumption of centralized planning, only little is known about efficient **mechanisms**, in case that a fully decision maker does not exist. This is particularly true if dynamic stochastic problems are to be considered. Hence, we face a

- **Shared Resources**
- **Additive Manufacturing**
- **Joint Lot Sizing**
- **Optimisation**
- **Cloud Manufacturing**
- **Auctions**

clear research gap in the application of decentralized mechanisms on joint lot sizing problems.

In its easiest form, joint lot sizing is performed by two companies, i.e., a supplier and a producer or a buyer and a seller. In real-world setting, however, joint lot sizing is more effective if several participants within a network orchestrate their production and ordering plans. Further complexity is added if production lead times or **transportation** has to be considered as well. Also, customer demand should be assumed to be **dynamic** and **stochastic**.

Generally, not all manufacturing technologies are suitable for sharing resources. One of the most promising technologies for collaborative planning



that has appeared in the last decade is **Additive Manufacturing** (AM). AM, also known as **3D printing**, is a manufacturing technology that produces the needed product layer-by-layer directly. In contrast to conventional technologies, no costly tools, moulds or punches are required for the production process. Furthermore, the manufacturing production process is digitally streamlined and produces neglectable production quality deviations. Hence, this technology makes it easy to share or exchange production jobs between plants or machines/agents [6]. This aspect can also help tackle the current environmental problems. As one can move production locations close to the customer, **CO<sub>2</sub> emissions** due to transport could be reduced.

However, to enable and ease the barriers of collaborative planning, suitable technologies are needed. Since [6] introduced the **Cloud Manufacturing** paradigm, scholars have studied this novel approach and found that it may play a vital role in shared manufacturing and collaborative planning [7]. The core idea of is to provide **Manufacturing-as-a-Service** over cloud applications. This connects suppliers, who share their production resources, with customers who have parts which need to be produced [8].

Our vision proposes research to enable the application of **collaborative planning** in the context of the **Sharing Economy** in order to considerably increase efficiency in manufacturing. This paradigm has a **technological** (e.g., suitable digital platforms), an **economical** (e.g., functional exchange mechanism and reasonable profit sharing), and a **legal** (e.g., data protection, antitrust and norms) component.

We aim at the design **key enabling mechanisms** allowing for the implementation of sharing resources concepts in real-world manufacturing settings. This included **centralized** and **decentralized** approaches with appropriate solution techniques for each of them. For both of them, sophisticated methods to share profits in a perceived fair way are key to ensure stability of the proposed mechanism. Also, incentive compatibility (i.e., truthful behavior) has to be taken into account.

## Approach

To leverage the benefits of **collaborative planning** in particular in the field of additive manufacturing, service matching and scheduling are essential in cloud manufacturing. In the past, researchers primarily focused on centralized additive manufacturing planning methods. Such approaches can produce globally better **solutions** which, however, struggle to efficiently generate schedules in **dynamic** cloud manufacturing environments. Multi-agent technologies are promising methods for overcoming these problems in cloud manufacturing. **Autonomous agents** can be modelled with objectives and preferences such that schedules are created in cooperation, coordination, and **negotiation** suggests that game theory approaches could be suitable tools when designing decentralized systems.

Among the research challenges in the field is to develop (i) suitable **mechanisms** for decentralized decision making and (ii) **efficient** solution approaches for the underlying decision problems in both the centralized and the decentralized settings. We propose to use the full range of (data-driven) **optimization method** in order to cope with the problem-inherent complexity. These include mathematical programming, heuristics, and (Math)heuristics. In order to cope with desirable properties regarding **game theoretical** aspects, research on appropriate **profit sharing** mechanisms and **incentives** is needed.

## Impact

From an economic point of view, the developed mechanisms will lead to an increase in cost **efficiency**.

The use of efficient planning during the reallocation process and the integration of fair group decision methods will reduce inefficiencies.

This will improve **the economic situation** of participants. Fair and transparent mechanisms to share profits and to prevent players from cheating, will increase the willingness to enter collaborations.

Increased efficiency leads to decreased resource, e.g., energy **consumption** or capacity utilization.

Hence, the society can benefit from efficient and therefore more **sustainable** manufacturing processes.



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## Competencies

The proposing research group is leading several research projects funded by highly competitive agencies, including **FWF** and **FFG**. Currently, the project EMIL (Exchange Mechanisms in Logistics) is led by Margaretha Gansterer, the department head. The group has expertise in **optimization methods** for challenging decision problems. They are experts in **auction-based** transport **collaborations**, which enable service providers to reduce inefficiencies in their manufacturing or delivery plans. In their research, both the game theoretical aspects and the **computational complexity** of these mechanisms are addressed.

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# Next Level Industrial Design

Mario Zeppetzauer, Elke Bachlmair, Florian Nimmervoll

## Vision

On the one hand, design reflects the movements of the market. On the other hand, it also actively influences societal trends and needs. Therefore, industrial design, by designing artifacts that combine physical and digital attributes, carries a multi-dimensional responsibility to actively contribute to a more sustainable future.

The goal of research through design is to use the act of designing as a way to generate insights and knowledge. It is often applied in interdisciplinary research projects.

With a human- and life-centered approach in mind, the development of the next 'thing' has to measure up to many needs. This demands a pluralistic pool of divergent and convergent design methods which must fit the demands of the problem space.



Fig. 1. Examples of previous projects  
1: B. Hierner (2018): redesign of a wearable brain-computer interface  
2: A. Radlak (2021): Haptic design in communication and therapy  
3: A. Podverbni (2019): Public interactive light installation

Hence, five core values define the Industrial Design Linz approach to innovation:

### (i) Holistic and multidisciplinary approach to creating products and services

At its core, our understanding of industrial design represents a fundamental shift in the way we approach the design of products, services and systems, moving away from a narrow focus on individual consumption and economic growth towards a holistic understanding of societal and environmental factors. This approach recognizes that design decisions have far-reaching consequences, and as such, demands

- Industrial Design
- Design Thinking
- User Interaction Design
- User Interface Design
- Human Computing Interface
- User Experience,
- Physical/Digital Prototyping
- Immersive Simulation
- Ergonomics
- Universal Design
- Mixed Reality

a defined ethical and responsible approach to design that prioritizes the well-being of people and the planet over short-term gains. As a matter of fact, only by bringing together individuals with a well selected range of skills and knowledge, multi-disciplinary product development teams can foster creativity, innovation, and problem-solving.

By incorporating partners from applied sciences, academia and industry, design students and design researchers are able to develop products for the complex and evolving needs of users and society.

### **(ii) Problem-solving and sustainable solutions**

A life-centered design approach acknowledges the importance of equity and social justice, recognizing that many of the world's most pressing challenges, such as poverty, inequality, and climate change, are the result of systemic injustices that must also be addressed in the design process (SDGs).

Designers are challenged to move beyond traditional design methodology, and instead, adopt a more collaborative, participatory, and iterative approach that incorporates diverse perspectives and stakeholder inputs.

### **(iii) Universal and accessible P2C (product to customer) interaction**

Iterative testing of products and design concepts is an essential part of an inclusive product development process.

Mixed-reality simulations empower design teams to effectively test products on different user groups.

Thus, collaboration with diverse stakeholders is obligatory - for example, including people with disabilities, to ensure that design decisions are informed by their lived experiences and needs. Incorporating mixed-reality methods reduces the need for physical prototypes, enabling designers to rapidly iterate and test ideas at a lower cost and with less environmental impact.

### **(iv) Meaningful products and services**

Products, services, and environments can become societal enablers when accessibility and usability for the widest possible range of people, regardless of age, ability, or background is given.

Meaningful products and services provide value beyond their basic function or purpose. They often have the ability to handle complex problems and create strong connections with their users (by empowerment).

Thus, research through design emphasizes the importance of experimentation, iteration, and collaboration in the design process, and encourages designers to take risks and explore new possibilities in their work. Hence, the utilization of new technologies must show benefits to people and society. E.g. studying force patterns in an alpine ski boot (2021), redesign of a wearable brain-computer interface (2018), sensoric white cane (2017), security check terminal (2021).

### **(v) Next level industrial design process utilizing multiple methods of digital-analog prototyping and mixed-reality simulation**

The discourse on Human-Centered Design is well established, and customization, specialized small-batch production, circularity, sustainability, and transformation are central topics in the international design discourse.

Nonetheless, more often than before, current methods and tools along the design process are no longer congruent with current and future requirements of innovative new product development.

Mixed reality offers the potential to transform the act of designing by enabling designers to create and test prototypes in virtual environments. This technology allows designers to visualize and manipulate 3D models in real-time, facilitating a deeper understanding of a product and its utilization.

As technology continues to evolve, designers will play an increasingly important role in shaping the way we interact with it. Immersive mixed-reality methods facilitate product interaction, testing and evaluation in earlier development stages.

In this connection, investigating perceptual criteria during product interaction offers new insights for design and product interaction research. A context-related environment under reproducible laboratory conditions is intended to meet the demand for excellence in user research. Therefore, a fully immersive mixed-reality testing environment (e.g., sample of study-related population) helps cut lab-biased behavior of subjects dramatically.

Furthermore, by using generative design, where algorithms and machine learning tools generate a wide range of design possibilities, designers can quickly identify the most promising concepts. This approach can help to streamline the design process and uncover innovative solutions that may not have been considered otherwise.



Industrial Design Linz has outstanding, state-of-the-art laboratory equipment and experimental infrastructures, e.g., the Co.Lab Perception (pre-launch) and Co.Lab Mixed Reality (Varjo XR-3, HTC, Oculus, etc.)

## Approach

50 years of industrial design education in Linz show a long-term perspective on industrial design with an emphasis on developing a deep understanding of the process of designing products, systems, or environments. Hence, state-of-the-art industrial design methodology is the result of changes in perspective and paradigm shifts in society, science and education.

With an emphasis on functionality, aesthetics, and user experience, students refine their skills by participating in interdisciplinary real-world projects and through extended academic supervision. A holistic approach strongly supports empathizing with the intended user groups. This comprises the consideration of constraints in product interaction (e.g., elderly people) as well as the investigation of emotional effects in product perception.

This demands systematic approaches to guide and support designers and stakeholders during a period of environmental, societal and economic upheaval as environmental constraints demand a shift in objectives to a new qualitative renaissance in design nowadays. Therefore, models, methods, tools and techniques to guide designers in creating products and services have to be adapted, developed and tested. Moreover, the advent of big data and artificial intelligence has brought new opportunities, but it has also given rise to novel ethical considerations. In recent decades, the focus of the design community has undergone a notable shift, moving away from a focus on physical product design towards the creation of user experiences. This shift has also seen a move from designing individual services to the development of areas within interconnected systems, while the traditional model of mass production has given way to more agile and individualized manufacturing possibilities. E.g., the global 3D printing market size was valued at USD 16.75 billion in 2022 and is projected to grow at a compound annual growth rate (CAGR) of 23.3% from 2023 to 2030 (Grand View Research) .

After all, the playing field of industrial product design looks very different

today than it did ten years ago and a myriad of challenges, such as resource depletion, pollution, and overconsumption, among others, describe the present.

Almost everything is in the process of being digitized. Physical products, virtual worlds, production lines and product concepts of product individualization are dependent on the digital environment we have created. In addition, machine learning and artificial intelligence are expanding this environment at a breathtaking speed and on a gigantic scale. New products and services are capable of creating new markets and young designers need not only an understanding of modern design language but also of user-oriented product development methods. Designers are shaping interactions, analyzing data, and making increasingly complex system and product structures accessible to users. Also, global teams become more common in the workplace, there is a greater emphasis on collaborative design methods that allow designers to work together in real-time, regardless of their location. This involves the use of cloud-based design tools, virtual whiteboards, and other collaborative technologies.

## Impact

In the Industrial Design domain by design research, applied industry-related research, applied design and advanced design visions:

Industrial design has a significant impact on the global economy, as the design of products and services is a critical factor in driving innovation, competitiveness, and growth in many industries.

Design research as well as applied design assume a pivotal role by introducing technological and social innovations that challenge and transform the existing paradigms.

Our applied research activities incorporate studying user needs and preferences, usability testing, understanding design trends, and exploring new materials and manufacturing processes. These subject areas focus on ensuring that products are accessible, efficient, and environmentally responsible, and that they meet the needs of diverse user groups. These are crucial prerequisites that enable future designers to actively contribute to a sustainable society and provide innovative links within corporations.

Industrial design has a significant impact on a wide range of fields, including product design, transportation design, furniture design, interior design, and consumer electronics. Consequently, Industrial Design Linz is an established research partner for many international companies.

Main fields of applied design work in the bachelor and master programs are healthcare, life sciences, machinery, sports & recreation, transportation, safety, renewable energy and circularity. The top US industries for employment of industrial designers are consumer electronics, medical products, and furniture (Source: IDSA). Here, applied research comprises ergonomics, human factors, sustainability, usability, product perception, product aesthetics and gender dependencies among others.

In the Mixed Reality in Design domain exploring visualization and interaction with physical-digital 3D models in real-time:

Virtual and augmented reality technologies have already begun to make their mark in the industrial design field, allowing designers to create and test products in a virtual environment before bringing them to life. The global market for mixed reality in industrial applications is projected to grow from \$829 million in 2020 to \$4.4 billion by 2026, at a CAGR of 31.3% (Source: MarketsandMarkets). This affects costs and time spent on physical prototypes and provides an accurate representation of the product to stakeholders. Incorporating immersive mixed-reality technologies in our design toolkit – for simulating and creating excellent person-product and person-context interaction – makes Industrial Design Linz a versatile and effective partner in many areas of product development. Products, parts, assemblies are created, modified, visualized and simulated efficiently and support interdisciplinary nonlinear project team work.

In the Perception in Design domain, perception plays a critical role as it helps understand how people interact with products and how they experience them. This can be classified into (i) people (disabled, different culture and social background etc.), (ii) specific use cases (iii), people-to-product interactions, and (iv) environments.

This involves user interviews, surveys, observations and use case simulations.



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## **Competencies**

Industrial design is an ever-evolving field, and new technologies and methods are constantly developed to improve the design process and enhance product functionality, usability, and aesthetics. Industrial Design Linz demonstrates competency having developed and applied these methods for over five decades. Design is playing an increasingly important role in shaping the future, as it has the power to influence the way we interact with technology, services, or each other. For example, Industrial Design Linz contributes to in-depth product pre-development in the fields of renewable energy (Solpol solar energy technologies based on polymeric materials) and investment goods (Andritz Hydro). Main fields of applied research are found in product perception and interaction, mixed-reality design methods, product enhancement and optimization through embedded systems, circular product design, new product development methods and user research.

Distinct work areas: Industrial Design, Design Thinking, User Interface Design, User Experience, HMI, VR, AR, Digital/Physical Prototyping, Model Making, CMF Design, Generative Design, Design and Innovation Management, Usability Testing, Mixed Reality in Design, et cetera.

Successfully carried out cooperations and projects with small to large companies, startups, organizations, academic and research partners.  
In the fields of investment goods, consumer goods, healthcare and life sciences, sport goods, mobility design, furniture etc.:

Andritz, Austrian Power Grid, Austroflamm, Biocomfort, BMW, Borealis, Doing Circular GmbH, EADS, Energie AG, Engel, FESTO AG, Friepess, FRONIUS, Greiner, Greiner bio-one, g.tec, Internorm, KAPPA, Kapsch, KISKA, KTC, LCM Linz Center of Mechatronic, Linz AG, Loxone, Lumapod, Madame WU, MKW, Mühlböck, Neudoerfler, Nexx, ÖBB, ÖWF, Palfinger, PCE, Planttech, Pöttinger, RICO, Rieder Beton, Robart, Roomle, SBM, Schiedel, Schneeberger, Schwarz, Sennheiser, Siemens, Skidata, Solpol, Starlim Sterner, STIWA, Teufel, Topic, Trumpf, Vaude, Veritas Verlag, Voestalpine - Böhler, Wacker Neuson, Wintersteiger, Zorn (JUZO).



Fig. 2. Examples of previous projects

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- 5: F. Westermeier et al. (2020): Conceptual public transport app
- 6: M. Zeppetzauer et al. (2014): Sensitive surface demonstrator
- 7: J. Haider (2021): Security check terminal
- 8: P. Mühlbacher (2017): Sensoric white cane
- 9: S. Koessler et al. (2020): ÖBB Momo
- 10: C. Picco (2018): Music interaction device
- 11: M. Dorfer (2021): Design of an autonomously driving, electrically powered triplex-spindle lawn mower for flat sport fields

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Example of sensor-based interaction research and published fundamental analysis for future product development:

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# Human-Computer Interaction

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## Vision

The field of smart manufacturing has witnessed a significant transformation in recent years, with the advent of advanced technologies like the Internet of Things, artificial intelligence, and machine learning (Lu, 2017). These technologies have revolutionized the way humans interact with machines and systems, paving the way for a new era of **human-computer interaction (HCI)** in the manufacturing industry. The vision of HCI in smart manufacturing is to create an environment where humans and machines work together seamlessly, leveraging the strengths of both to improve productivity, quality, and safety (Leitão et al., 2016).

Human-computer interaction (HCI) is a multidisciplinary field that focuses on the design, development, and evaluation of **interactive systems** that enable effective and efficient communication and **collaboration between humans and machines**. In the context of smart manufacturing, HCI aims to create a seamless and intuitive interface between humans and machines, leveraging the strengths of each to enhance productivity, quality, and safety (Preece, 1995). HCI in smart manufacturing involves the integration of various technologies such as robotics, augmented reality/virtual reality (AR/VR), Internet of Things (IoT), and artificial intelligence (AI) to create intuitive, user-friendly interfaces that facilitate safe, productive, and flexible human-machine interactions. It encompasses a wide range of applications, including human-robot collaboration, gesture-based interfaces, voice-enabled interactions, and wearable devices, among others (Kumar & Lee, 2022).

One of the key challenges of HCI in **smart manufacturing** is to design systems that are easy to learn and use, and that can adapt to the changing needs and preferences of users. This requires a deep understanding of the cognitive, perceptual, and physical capabilities and limitations of humans, as well as the technical and operational characteristics of the manufacturing environment. Additionally, HCI in smart

- **Human-Computer Interaction**
- **Smart Manufacturing**
- **Visual Analytics**
- **Immersive Media Technologies**
- **Production Planning & Control**

manufacturing must consider ethical and social issues such as privacy, data security, and the impact of technology on job displacement and skill requirements (Krupitzer et al., 2020).



## Approach

The rise of Industry 4.0 and cyber-physical systems has led to an abundance of large amounts of data, particularly in the manufacturing industry. **Visualization** and **Visual Analytics (VA)** play essential roles in harnessing this data. They have already been acknowledged as being among the key enabling technologies in the fourth industrial revolution. **Visual Analytics**, “the science of analytical reasoning facilitated by interactive visual interfaces” (Cook & Thomas, 2005), is a comparably young research field. A major tenet of Visual Analytics (VA) is that analytical reasoning is not a routine activity that can be automated completely (Wegner, 1997). Instead, it depends heavily on analysts’ initiative and domain experience. Visual interfaces, especially Information Visualizations (InfoVis), are high bandwidth gateways for perception of structures, patterns, or connections hidden in the data. Interaction is “at the heart” of InfoVis (Spence, 2014) and allows the analytical reasoning process to be flexible and react to unexpected insights. Furthermore, Visual Analytics involves automated analysis methods, which perform computational activities on potentially large volumes of data and thus complement human cognition. From the perspective of data, time-oriented data has unique characteristics and plays an important role in tasks such as exploring trends, patterns, or cycles. The approach of using **immersive media technologies** as HCI for smart manufacturing involves the use of virtual and **augmented reality (VR/AR) technologies** to enhance the human-machine interaction in the manufacturing process (Baroroh et al., 2021). Immersive media refers to the technology that allows users to enter a simulated environment, which can be either completely virtual or augmented with the real world. In the context of smart manufacturing, immersive media can be used to create virtual workspaces that allow workers to interact with machines and production processes in a more intuitive and immersive way. For example, workers can use AR-enabled glasses to receive real-time information and guidance on how to perform manufacturing tasks or use VR simulations to train on new equipment or processes in a safe and controlled environment. The benefits of using immersive media as HCI technology in smart manufacturing include: (1) Enhanced learning and training: Immersive media can provide workers with a realistic and interactive training experience that enables them to learn new skills and perform

tasks more effectively; (2) Improved safety: AR-enabled glasses can provide workers with real-time safety alerts and warnings, reducing the risk of accidents in the manufacturing environment.; (3) Increased efficiency: Immersive media can help workers perform tasks more efficiently by providing them with real-time information and guidance on how to operate machines and complete manufacturing processes; (4) Reduced downtime: AR-enabled glasses can enable workers to quickly diagnose and resolve equipment issues, reducing the time required for maintenance and repair; and (5) Increased flexibility: Immersive media can enable workers to switch between tasks more easily, reducing the need for physical reconfiguration of machines or production lines. In summary, the use of immersive media as HCI technology for smart manufacturing has significant potential to improve worker safety, increase efficiency and productivity, and enhance the overall human-machine interaction in the manufacturing process (Moser et al., 2019).

Due to substantial changes that can currently be observed in the field of industry common methods of **production planning and control** are no longer suitable and employees need additional support to control and interact with the production system. New circumstances like the shortages of resources, rising electricity prices, new regulations for greenhouse gas emissions and skilled workers shortage are new challenges for companies and their employees. The previous mentioned problems lead to an increasing level of complexity that workforce and managers must face both in terms of their internal processes and external logistical requirements. Currently, strategical, tactical, and operational planning is performed based on empirical data with the support of enterprise resource planning (ERP) systems. The planning approaches are static and non-resilient to changes of the environment (e.g., energy prices, availability of (raw)-materials, changing delivery information, etc.). However, an essential success factor for resource-efficient production is the **semi-automated adjustment of the production system** to match the new requirements. In a static system the daily routine of manufacturing companies is characterized by the management of acute problems. The focus of the employees lies on the treatment of the symptoms without solving the real causes. Therefore, models of Operations Research must be extended on strategical, tactical

an operational level to meet energy and sustainability requirements (Biel & Glock, 2016). The supply chain members should share trustworthy information in real-time to identify supply chain problems immediately and set appropriate countermeasures (Altendorfer & Felberbauer, 2023). The solution procedures must be robust to generate production or project plans to account for the randomness of the production system (Felberbauer et al., 2019). Those innovative systems must

be integrated within the IT landscape of the companies so that the employees get easy access to the developed decision support systems. Additionally, the interactive decision support system also supports less qualified employees by a good representation of the relevant data. In summary, the use of digital technologies has significant potential to increase efficiency and productivity and enhance the competitiveness of companies on the global market.

## Impact

HCI has significant **scientific impact** on smart manufacturing, as it enables more effective and efficient human-machine interactions in the manufacturing environment. Here are some specific ways in which HCI has impacted smart manufacturing:

- Improved **productivity**: Innovative systems can help workers operate machines more effectively, reducing energy costs, production errors and improving throughput. This can result in higher productivity and lower costs for manufacturers.
- Enhanced **safety**: By designing interfaces that are easy to use and understand, HCI can help reduce the risk of accidents in the manufacturing environment. Additionally, technologies such as human-robot collaboration and wearable devices can help workers avoid hazardous tasks.
- Better **quality control**: HCI can help workers monitor and control production processes more effectively, improving the quality of manufactured goods. For example, AR/VR can be used to provide real-time feedback on the status of production processes, allowing workers to adjust as needed.
- Increased **flexibility**: HCI can help workers adapt to changing manufacturing requirements more quickly and efficiently. For example, gesture-based interfaces can enable workers to control machines without the need for physical buttons or switches, allowing them to switch between tasks more easily.
- New opportunities for innovation: HCI is enabling new forms of human-machine collaboration, such as the use of augmented reality to provide workers with real-time information and guidance. This opens up new opportunities for innovation in manufacturing processes and products.

HCI has significant **potential for industrial and commercial opportunities** in smart manufacturing. Here are some specific ways in which HCI can create new opportunities for manufacturers:

- Increased **efficiency**: By designing interfaces that are easy to use and understand, HCI can help workers operate machines more efficiently, reducing the time required to complete manufacturing tasks. This can result in cost savings for manufacturers, as well as faster turnaround times for customers.
- Improved **quality control**: HCI can help workers monitor and control production processes more effectively, improving the quality of manufactured goods. This can lead to increased

customer satisfaction and repeat business for manufacturers.

- Enhanced **safety**: By designing interfaces that are easy to use and understand, HCI can help reduce the risk of accidents in the manufacturing environment. This can lead to lower insurance costs for manufacturers and a safer working environment for employees.
- Greater **flexibility**: HCI can help workers adapt to changing manufacturing requirements more quickly and efficiently. For example, gesture-based interfaces can enable workers to control machines without the need for physical buttons or switches, allowing them to switch between tasks more easily. This can lead to greater agility and responsiveness for manufacturers.
- **New revenue streams**: HCI is enabling new forms of human-machine collaboration, such as the use of augmented reality to provide workers with real-time information and guidance. This opens new opportunities for innovation in manufacturing processes and products, as well as the development of new products and services based on HCI technologies.

HCI has significant **potential for societal impact and opportunities** in smart manufacturing. Here are some specific ways in which HCI can create new opportunities and benefits for society:

- **Improved working conditions**: HCI can help reduce the risk of accidents in the manufacturing environment, creating a safer working environment for employees. Additionally, technologies such as human-robot collaboration and wearable devices can help workers avoid hazardous tasks.
- Enhanced **training and skill development**: HCI can provide workers with real-time information and guidance, enabling them to learn new skills and adapt to new manufacturing processes more quickly and efficiently. This can lead to increased job satisfaction and career opportunities for workers.
- Increased **accessibility**: HCI can make manufacturing jobs more accessible to a wider range of people, including those with physical disabilities or limited mobility. For example, gesture-based interfaces can enable workers to control machines without the need for physical buttons or switches, making it easier for people with disabilities to perform manufacturing tasks.
- **Environmental benefits**: HCI can help manufacturers reduce their environmental impact by optimizing manufacturing processes and reducing waste. For example, by providing workers with real-time feedback on energy consumption and resource usage, HCI can help manufacturers reduce their carbon footprint.
- **Economic benefits**: HCI can create new jobs and industries, as well as contribute to economic growth through increased productivity and efficiency in manufacturing. Additionally, by enabling manufacturers to produce higher quality goods more efficiently, HCI can help companies remain competitive and innovative, which can lead to increased economic opportunities and benefits for society.

Overall, HCI has significant scientific impact on smart manufacturing by enabling **more effective and efficient human-machine interactions**. As manufacturing becomes increasingly complex and automated, HCI will continue to play a critical role in enabling workers to operate machines safely and efficiently. Additionally, HCI has significant potential for industrial and commercial opportunities in smart manufacturing.

By enabling more effective and efficient human-machine interactions, HCI can create new value for manufacturers and customers alike. As manufacturing continues to evolve and become increasingly automated, HCI will continue to play a critical role in enabling manufacturers to stay competitive and innovative.

By improving working conditions, enhancing training and skill development, increasing accessibility, promoting environmental sustainability, and driving economic growth, HCI can create new opportunities and benefits for individuals, communities, and society as a whole.



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## Competencies

Research has a high priority at St. Pölten University of Applied Sciences: Around 100 researchers, together with national and international partners from industry and science, carry out projects on application-oriented issues, covering the entire innovation chain from basic research, technology development and prototyping to innovation transfer in the form of business cooperations, spin-offs and start-ups.

St. Pölten University of Applied Sciences is part of the European University Alliance E<sup>3</sup>UDRES<sup>2</sup>. Our university leads this network, which includes a total of 9 higher education institutions from all over Europe. Together as E<sup>3</sup>UDRES<sup>2</sup>, the alliance works closely to make a significant contribution in the areas of higher education, research and innovation. E<sup>3</sup>UDRES<sup>2</sup> stands for “Engaged and Entrepreneurial European University as Driver for Smart and Sustainable European Regions” and promotes the development of small and medium-sized cities and their rural environments into smart and sustainable European regions, and also explore how universities will work in the future. E<sup>3</sup>UDRES<sup>2</sup> integrates challenge-based education, mission-oriented research, human-centered innovation as well as open and engaged knowledge exchange as interrelated core areas and aims to establish an exemplary multi-university campus across Europe.

The Institute of Creative\Media/Technologies (IC\M/T) conducts human-centered, interdisciplinary research on media and interactive technologies, with a view to strengthening the university’s academic programs and achieving scientific advances. The institute consists of four research groups with a team of 40+ researchers: Media Computing, Media Creation, Digital Technologies and Media Business. We perform basic and applied research, as well as carrying out contract research and implementing consulting projects. Our academic and industry network includes highly specialized regional SMEs, as well as global industrial players and top-ranked international universities. Our R&D projects cover all aspects of design science research, a problem-solving approach involving the systematic analysis, design, creation and evaluation of digital artefacts. Unlike empirical research, it is not restricted to description, explanation and prediction. Instead, it aims to change the world, improve it and create new worlds. This includes developing novel artefacts, and generating knowledge about them and their use, sphere of application and impact. We create digital artefacts to fulfil people’s needs and desires, overcome their problems and take advantage of new opportunities.

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# Context-specific, Human-centred Support Technologies

Robert Weidner, Katharina Schmermbeck

## Vision

### **Individual, context-specific technologies allow effective support**

while neither overruling nor replacing the worker performing their task [1].

Depending on the support system and its characteristics, it can alleviate cognitive and physical stress and **reduce the risk of occupational illnesses** such as musculoskeletal disorders. Exoskeletons, which have been initially used for military, rehabilitation, and assistive purposes, are becoming increasingly important for physical support in work contexts.

An exoskeleton is a wearable system, which depending on its morphology, functional design, and applied principles of control, enables, enhances, facilitates, or stabilizes the user's movement or posture [2]. Albeit strong interest from research and industry over the past decade, it is a persisting challenge to meet the strict requirements on temporal as well as spatial alignment between exoskeletons and humans.

Through its research and projects, the Chair for Production Technology at the University of Innsbruck strives to tackle today's challenges of support technologies including exoskeletons. Addressing them from an **interdisciplinary and holistic perspective** enables to create novel functionalities and mechanical designs, methods for development, evaluation, and industrial implementation as well as further insights into the biomechanical effects of exoskeletons in different work situations.

## Context

During the last decade industrial production, logistics, and maintenance processes have become increasingly shaped by using data from interconnected machines and devices. It can enhance production efficiency and productivity while reducing error rates and machine downtimes. Driven by pressing requirements for sustainability, highly flexible processes for smallest batch sizes, as

- **Context-specific Support Technologies**
- **Human-centered**
- **Wearable Technologies**
- **Human-Machine-Interaction**

well as demographic changes, there has been a shift towards **human-centered workplaces and process chains**. In paradigm of industry 5.0, manufacturing, logistics, and other work processes will leverage the unique cognitive capabilities of the human worker in their decision-making, creativity and flexibility while assigning repetitive, heavy tasks to machinery. This, however, **requires new forms of human-machine collaboration and innovative solutions** for processes where deployment of smart machines is either unprofitable or infeasible. Particularly in the context of an ageing workforce and remaining manual activities, such as repetitive assembly tasks in, e.g., awkward postures or carrying heavy loads in field construction sites, employers need to take actions to ensure the health and safety of workers.

## Approach

Due to the manifold of application fields and users, a **universal solution for a generalized support does not exist**. Nevertheless, to avoid single non-transferable solutions, the systems need to be **designed and built for maximum adaptability**. More specifically, the form and triggers for the adaptation depend on the support context including the human user with their individual capabilities, the support technology with its morphological features, and the task with its characteristics to be performed [3], as depicted in figure 1.

Achieving the necessary adaptability to the support context requires a deep and thorough understanding of the environment, in particular the ongoing processes, common activities, and tasks. **Models and frameworks** developed to describe the environment and overarching aspects take into account well-established concepts such as ergonomic principles for the **design of work systems** and national as well as international safety regulations [4]. Building on the obtained

knowledge, suitable **measurements for workplace improvements**, e.g., the use of exoskeletons and cobots, are investigated and tested in the laboratory or field prior to their final technical realization and implementation into the industry. A test course specifically developed for these purposes enables the recreation of typical work scenarios from logistics to field construction work in a well-controlled laboratory setting [5]. Moreover, it enables to include different measurement methods, such as motion capture and electromyography, to investigate **quantitative biomechanical and ergonomic effects** as well as **qualitative effects** regarding acceptance and usability.

**According to identified tasks, environment, and user characteristics**, it is aimed to either **further qualify support technologies by functionally or morphologically adapting the systems or to develop new approaches**. Functional aspects mainly focus on the adaptation of support characteristics, i.e., applied task- and posture-dependent support torques, by, e.g., analyzing retrieved

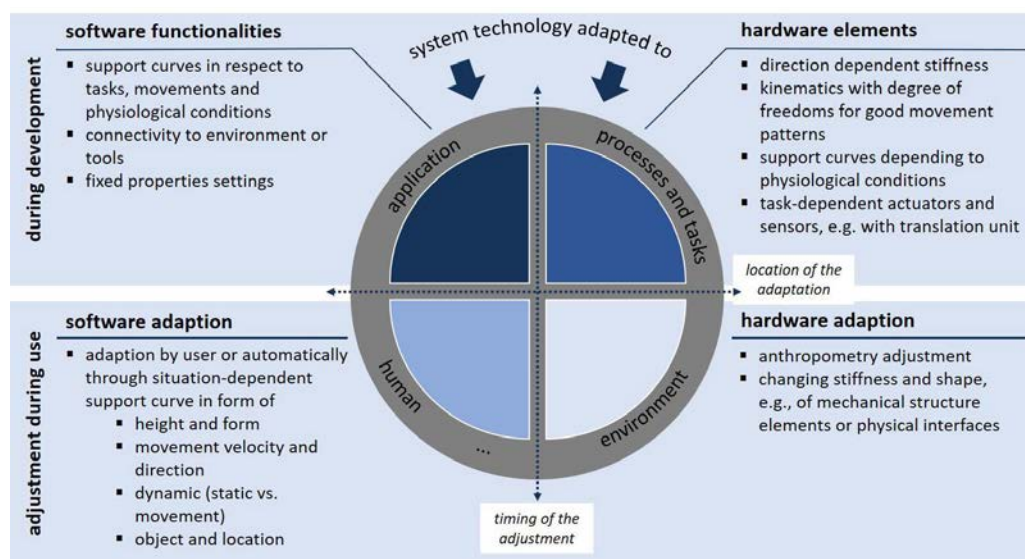


Fig. 1. Possible adaptations of support technologies [3]

sensor data with different statistical methods including machine learning approaches. The morphological adaptation of the exoskeleton to its user is realized by applying state-of-the-art manufacturing methods as well as different simulations approaches and frameworks for human-centered technology development [6]. Figure 2 shows a selection of exoskeletons which have been developed within the working group. Moreover, the development of novel sensors, such as [7], and interactions concepts and support theories [2] contribute to general advances in the field of human-machine interaction. This holistic approach unites the expertise of different disciplines while keeping the needs and requirements of users in its focus (figure 2).

To bridge the gap to the successful implementation of the developed support technologies, the institute maintains an intensive and regular **exchange with industrial and**

**scientific partners** and representatives from various industrial sectors in Austria as well as Europe. Building on this dialog and experience in technology development the working group is able to identify user needs and requirements from the working environment, processes, and activities. Moreover, different human-centered frameworks for the successful implementation of support technologies, such as exoskeletons, have been created and deployed in various projects and industry sectors [8],[9]. Moreover, frameworks and concepts are continuously included into standardization processes in different organizations, e.g., DIN, VDI, to ensure a successful knowledge transfer into the industry. This is also reflected by a comprehensive practical guideline for the implementation and evaluation of exoskeleton, which has been developed with the Institute for Occupational Safety and Health of the German Social Accident Insurance [4].

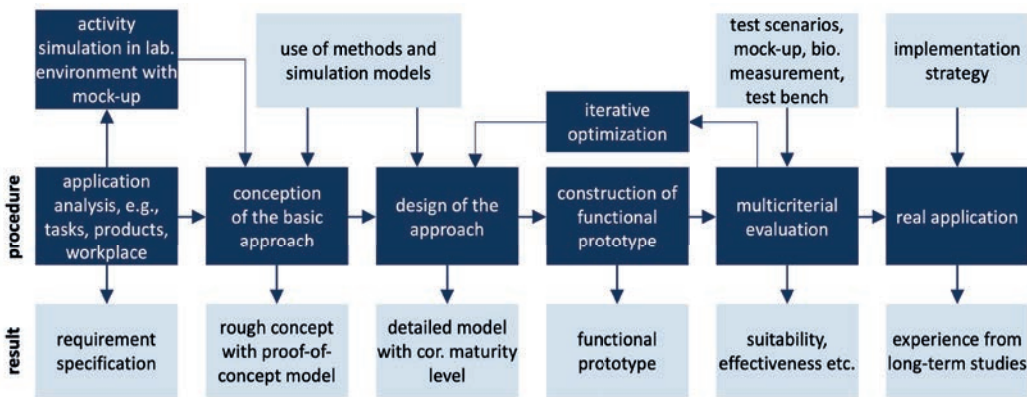


Fig. 2. Methodological approach of the working group for development human-centred technologies



Fig. 3-5. Examples of developed exoskeletons

## Impact

By applying a **holistic, human-centered approach**, the research not only contributes to the advances of support technologies but shapes the future of workplaces by better understanding how humans and technologies can successfully collaborate in closest proximity to leverage their respective advantages while alleviating weaknesses. Successful developments will therefore have a great influence on various stakeholders, sectors as well as society in general.

**Advancing workplaces with adaptable and context-specific support technologies** will lower the risk for musculoskeletal diseases of workers by reducing physical stress. This does not only contribute to solve one of the major challenges regarding occupational health identified by the European Union and reduces the number of sickness days. More importantly, it advances people's Good Health and Well-Being, which is one of the Sustainable Development Goals (SDGs) of the United Nations Agenda 2030.

Reaching **different industry sectors and fields of application** will **improve the safety and health of workplaces**. Moreover, it will lead to **higher productivity, lower error rates, and more flexibility of processes** by focusing on human capabilities to take reasonable fast decisions even in unknown and complex environments.



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## **Competencies**

The working group has been participating and leading numerous publicly as well as industry-funded projects since its foundation, e.g., developing support technology and development methods (smartASSIST, BMBF – Federal Ministry of Education and Research, Germany), frameworks for industrialization and adaptivity (FFG project A2P), development environment for designing and evaluating exoskeletons (EVO-MTI, funded by dtec.bw – Digitalization and Technology Research Center of the Bundeswehr which is funded by the European Union – NextGenerationEU), innovation camp including 28 Austrian companies into the scientific progress regarding exoskeletons for manual workplaces (FFG project exoATwork), ExoMePT funded by DFG (Deutsche Forschungsgemeinschaft), AutoPro funded by BMWi (Federal Ministry of Economic Affairs and Energy Germany), lower body exosuit to support ankle dorsiflexion (AktivOrthese) funded by BMWi, back exoskeleton to support care workers (KIKU) funded by dtec.bw, exo@work, funded by BGHW as well as several industry funded projects for the development specialized support technology as well as evaluation and optimization of workplaces.

The Chair of Production Technology has a state-of-the-art laboratory for various manufacturing processes. Additionally, the experimental laboratory has equipment for a variety of different movement studies (Motion Capture – Xsens MVN Awinda, Vicon Nexus, Biosignal Sensors – EMG, NIRS, Ergospirometry, Ergonomic Assessment Tool – Scalefit, force and pressure sensors – AMTI, etc.). The Chair also have a great variety of different commercially available exoskeletons for the support of different body regions, e.g., shoulder, hand, back.

Weidner is also member of different scientific communities, e.g., ÖWGP (Austrian Scientific Society of Production Technology) - currently as first Vice President -, the WGMHI (Wissenschaftliche Gesellschaft für Montage, Handhabung und Industrierobotik) and board member of the GfA (Gesellschaft für Arbeitswissenschaft) as well as managing partner of the exoIQ GmbH (part of the TTS Group with companies like Festool GmbH, Shaper GmbH, Saw Stop GmbH and Tanos GmbH).



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# Production Activities of the FH Campus Wien

Bernhard Mingler, Sebastian Geyer, Heimo Hirner, Gernot Korak, Christoph Mehofer

## Research and Education Competencies of the FH Campus Wien in the Field of Production

With more than 8,000 students, FH Campus Wien is Austria's largest university of applied sciences and makes a significant contribution to Austria's research competence and education in production and manufacturing.

The FH Campus Wien network includes approximately 150 domestic and foreign universities and colleges as well as industrial enterprises, companies, associations, public institutions, and schools. R&D projects are conducted as part of courses, as funded research projects, and as external research contracts. In 2021 FH Campus Wien became the first University of Applied Sciences in Austria to establish its own **ethics commission** and it is, as a founding member of the Sustainable Universities Cooperative, committed to **sustainability**. Study programs that deal intensively with the subject of production at FH Campus Wien are '**High Tech Manufacturing**' Bachelor and Master.

Focus of the **Bachelor's program** is to meet the needs of production and manufacturing companies for **highly qualified employees**. Highly qualified in this context means the ability to think and act in an **interdisciplinary** manner, to understand the functioning of partial and complete systems and to develop system solutions. This is achieved through targeted subject-specific education in the field of technology and all production processes, as well as a complementary generalist education with a focus on interdisciplinary projects and entrepreneurial thinking.

The **Master's program** is characterised by the required combination of engineering and management topics, with a clear emphasis on engineering. Production-related topics such as "**additive manufacturing**", "**digitalisation**", "**simulation**" and "**entrepreneurship**" dominate the curriculum and the research projects.

Other important production-relevant topics in the Department of Engineering are **IT, IT-Security, Internet of Things (Industry 4.0), Electronics, Technical Management, Safety, Artificial Intelligence, and Medical Technology**. In addition, the topic of production also plays a major role in the Departments Building and Design and Applied Life Sciences.

- **Interdisciplinary Research**
- **Future-Oriented Education**
- **Additive Manufacturing**
- **Digital Photonic Production**
- **Virtual and Augmented Simulations**

In our **application-oriented research** and development the high diversity of courses gives us powerful leverage when implementing **cross-disciplinary projects**. This sets us apart from other universities and makes us a pioneer in forging networks between the disciplines and their subject-specific competencies. Lifelong learning has become a necessity in our knowledge-based society and should be made

available to everyone. The Campus Wien Academy is facing up to this challenge and offers **innovative learning programmes** that deal with the topic of production, among other things, and are tailored to the needs of the job market and society.

Our research results flow directly into teaching and ensure that our training programmes are always forward-looking and trendsetting. We see this, among many other aspects, as an important part of **practice-oriented education**. As part of their Bachelor's and Master's theses, students already work on R&D issues from companies in the production industry and develop solutions for them. Our graduates therefore stand for a **practical and future-oriented academic education** that guarantees a high degree of employability. Companies and organisations that are interested in posting job offers and getting in touch with our students and graduates can become members of our campus network.

The funding of our research projects and thus the **transfer of knowledge** between teaching and business is ensured by the excellent cooperation with companies and funders such as the Austrian Research Promotion Agency, the Austrian Science Fund, the Vienna Business Agency and MA 23 - Wiener Fachhochschulförderung. In addition, students, alumni, and employees of FH Campus Wien who wish to start a business can use office space and an infrastructure for smart production via a free one-year funding scheme provided by the **in-house start-up service**.

## Research Interests and ongoing Projects in the Field of Production

Changes in many of our areas of life, such as communication, work, education, business, industry, and public administration, have never been as rapid as they are today. These changes are significantly caused by **digitalisation** - a **transformation process** made possible by technological innovations and developments. Research on the interdisciplinary topic of digitalisation is therefore also of great importance in the context of production, where it enables innovations in areas such as artificial intelligence, industry 4.0 & automation, e-government, digital health, smart cities, sustainability, digital inclusion and e-Learning. This strengthens the skills needed for the

intensifying **digital transformation** among our researchers and students and secures Austria as a location for innovation and development. In this context, the High Tech Manufacturing degree program at FH Campus Wien, as a member of the **Mechatronics Platform**, is the organiser of the 2023 annual conference with the main theme of "Digital Manufacturing and Sustainable Development".

### Additive Manufacturing Science and Education Lab - AMSEL

**Additive manufacturing (AM)** technologies are leading to a rethink of traditional production in many industries and make it possible to produce even small series in a cost- and material-efficient way. The targeted use of materials in the manufacturing processes enables resource-conserving and sustainable use of primary raw materials. In the further development in this area, an increased commitment to teaching is also an important aspect. The focus of AMSEL is on improving the quality of teaching through the implementation of an **education laboratory for AM** at the FH Campus Wien. As part of the current curriculum of the Bachelor's and Master's degree program High Tech Manufacturing, students learn about additive manufacturing technologies primarily from a theoretical perspective. Since the High Tech Manufacturing degree program currently mainly has industrial AM equipment (**SLS - Selective Laser Sintering, FDM – Fused Deposition Modeling and Hot Lithography**), for which training courses lasting several weeks would be necessary, the students can hardly gain any practical experience in this area in the corresponding exercises. The implementation of AMSEL closes this gap between theory and practice and, following its successful establishment in teaching in the Master's degree program High Tech Manufacturing, will be available in future for teaching in all degree programs at FH Campus Wien. The technological focus in this laboratory is on low-threshold AM technologies such as **Fused Layer Modeling (FLM), Digital Light Processing (DLP) and Masked-Stereolithography (MSLA)**. The operation of these machines is easy to learn in exercises and workshops.

### Concrete 3D Printed Objects - C3PO

C3PO is a joint project of the Departments of Engineering and 'Building and Design'. For the construction industry, additive manufacturing processes of building elements, for example **structural concrete components**, can be of great ecological and economic benefit in structural and civil engineering and

open completely new possibilities. C3PO conducts application-oriented research into the **3D printing of concrete objects** and components and aims to expand the range of applications in the **construction industry**. The researchers focus on targeted, efficient material application, which leads to reduced use of concrete. This should contribute to the **conservation of primary resources** and reduce the ecological footprint of concrete components. The optimisation of cross-section topologies also brings about a significant reduction in the dead weight of concrete structures, which should make it possible to use slimmer load-bearing elements - for example, also for special structures - during construction projects. Within the framework of the project, an additive manufacturing system for concrete and mortar with and without fibre reinforcement is being developed and set up. **Optimised cross-sections** are produced with high design accuracy, even with small component dimensions. Further steps envisaged could include the **integration of sensor technology** for the constructive further development of the components and **predictive maintenance**.

#### PhD program “Digital Photonic Production” - Digiphot

FH Campus Wien offers support in initiating and handling doctoral/ PhD studies in cooperation with other universities. The first doctoral cooperation is currently underway with the Vienna University of Technology. In the joint doctoral college **Digital Photonic Production** (Digiphot), TU Wien and FH Campus Wien aim to clarify important questions about 3D printing and make additive manufacturing more practical.

Additive manufacturing technologies and their achievements have attracted a lot of attention in recent years. However, to exploit the great potential of these technologies on a broad scale, there is still some progress and development to be made. These include, for example, the development of appropriate design tools to help designers take advantage of the possibilities of additive manufacturing (e.g. **great design flexibility, consumer and patient-specific designs, digital materials**, etc.). In addition, the materials used, and the workpiece properties obtained must meet the high requirements of the applications, e.g., medical or industrial (thermomechanical properties, reproducibility, cost, etc.). To achieve this, advanced methods for characterising nanostructured

materials for additive manufacturing, novel tools for generative design of additively manufactured parts, methods for online monitoring of **laser-based additive manufacturing processes and process simulation of selective laser melting** are being developed and applied.

In addition to the expected scientific progress, the **doctoral college** is also intended to strengthen the cooperation between TU Wien and FH Campus Wien and to serve as a model for cooperation between universities and universities of applied sciences. Furthermore, the status of Austria and the city of Vienna as an international hotspot for materials research should also be further consolidated.

#### Example of joint projects with industrial partners, Fronius company on the topic of integration of virtual / augmented simulation and real welding

Welding is a demanding activity that requires a lot of practice. **Welding simulators** are therefore increasingly being used in training and for training purposes. The company Fronius is in the process of optimising its welding training system to make it more efficient and user oriented. The FH Campus Wien is conducting joint research with Fronius on the implementation of **virtual or augmented simulations**. As part of the projects, concepts and demonstrators of **position detection** and **tracking solutions** suitable for welding training systems are developed.

#### Further Projects

In cooperation with the degree program 'Applied Electronics and Technical Informatics', projects are being carried out that deal with **printed electronics and a newly acquired sputtering and thermal evaporator system for coatings**. **Cross-disciplinary projects** are used to develop and implement sensors, for which the materials science components as well as the functionality must be considered.

FH Campus Wien offers students the unique opportunity to become part of **interdisciplinary student teams** - the Os.Car Racing Team, the Res. QBots Team, the Cyber Security Team or the newly founded Cosmic Coaster Team. While developing and building a racing car for the Formula Student, a rescue robot or a rocket, students gain important skills about many aspects of the production process in theory and

practice.

Together with Siemens Mobility Austria, the FH Campus Wien offers a **training-integrated degree program** that combines a skilled worker intensive training with a Bachelor's degree. During the training, students not only receive theoretical background knowledge, but can also put this into practice directly at Siemens Mobility's production site in Vienna. In this way, they gain valuable work experience in production and can apply what they have learned in seminar papers and theses as well as in their later professional lives.





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## Summary

Building on extensive experience in **interdisciplinary research** and **future-oriented education**, the FH Campus Wien is very well positioned to meet the challenges in the field of production. Our focus is currently on **additive manufacturing**, but we are basically open to all production-related topics and look forward to exciting new topics and projects.



# Intelligent Digital Twins

Martin Gebser

## Vision

Driven by the vision of **Industry 4.0**, a central, present endeavor in business and industries aims at increasing the degree of automation, efficiency and integration of processes and systems. Beyond direct economical advantages like shorter production cycles and reduced costs, the development and dispersal of modern high-performance technologies is of global environmental and societal importance, as urgent climate goals call for more efficient resource and energy utilization. The roll-out of sensor technology, edge computing devices and digital infrastructure is expected to raise the **demand for semiconductor wafers** by 56% from 2020 to 2030, amounting to a production capacity increase from 19 to more than 29 million wafers per month (semiconductors.org/wp-content/uploads/2020/09/Government-Incentives-and-US-Competitiveness-in-Semiconductor-Manufacturing-Sep-2020.pdf). However, setting up new production facilities is very costly as, e.g., cutting-edge lithography equipment can account for prices up to \$200 million (<https://www.cnbc.com/2022/03/23/inside-asml-the-company-advanced-chipmakers-use-for-euv-lithography.html>). But more importantly, a **reduction of global greenhouse gas emissions** by 43% is required between 2022 and 2030 to meet the 1.5 °C target (un.org/sustainabledevelopment/progress-report). That is, raising production volumes by duplicating the current practices, resources and processes would be in stark contrast to sustainable development goals, which call for new concepts and better efficiency.

Complex production and logistics processes, with the semiconductor industry as a prominent example, drastically exceed the limits of human cognition, so that their efficient

management cannot be accomplished without automated planning support. To this end, the two complementary categories of Artificial Intelligence (AI) techniques, referred to as **model-** and **data-driven AI**, approach challenging computational tasks from orthogonal perspectives. For applying model-driven AI methods, the **knowledge** about a problem domain is formalized in a machine-processible way, e.g., one may try to feed traffic regulations into the board computer of a car in order to make autonomous driving safe(r). Vice versa, data-driven AI methods work by training statistical frameworks to extrapolate **patterns** from sample inputs, which would for autonomous driving mean that a large amount of car rides are analyzed to extract policies mimicking the operations of human drivers. Arguably, neither of these two approaches can be expected to bring about any silver-bullet solution, as the road traffic is too complex to gather rules or data anticipating all possible

- **Production and Logistics Systems**
- **Simulation Models**
- **AI Planning and Dispatching**
- **Semiconductor Manufacturing**
- **Robotics**

driving situations and AI systems lack common sense needed to appropriately react to unforeseen circumstances. The same complications apply to complex production and logistics processes as in semiconductor manufacturing, where variable operation durations, success rates and sudden disruptions obstruct exact domain models and the sparsity

of real-world data logged in the running production precludes any meaningful analysis by statistical learning methods. In order to bridge the gap and harness modern AI technologies for more efficient and less resource-consuming production management, the development and proliferation of **digital twins** must be promoted to supply large-scale simulation and experimentation environments.

On the one hand, digital models detach the generation and analysis of sample data from the running production, and a respective switch from historical to simulation data already gave a tremendous boost to Google's AlphaZero game-playing agent, which with comparably modest training efforts beats the best humans in two-player games ([deepmind.com/blog/alphazero-shedding-new-light-on-chess-shogi-and-go](https://deepmind.com/blog/alphazero-shedding-new-light-on-chess-shogi-and-go)). Making such remarkable advances of data-driven AI technology accessible for production industries crucially relies on the availability of digital twins to perform **extensive training runs** independently of the running production. As a second utility, simulation runs with a digital twin generate information about the performance parameters of a production system, such as characteristic operation durations, success or disruption rates, which can in turn be supplied to model-driven AI methods for **optimizing the production planning**. With this background knowledge at hand, powerful optimization methods are available to improve the efficiency and resilience of production and logistics as, e.g., also adopted recently by Chile's health administration for planning countermeasures against the COVID-19 pandemic ([businesswire.com/news/home/20220426005980/en/Chile-Receives-Franz-Edelman-Award-for-COVID-19-Research-Supported-by-Gurobi](https://businesswire.com/news/home/20220426005980/en/Chile-Receives-Franz-Edelman-Award-for-COVID-19-Research-Supported-by-Gurobi)). In conclusion, digital twins of production facilities promote the application of modern AI technologies for optimizing the economic and ecological efficiency likewise, where higher degrees of automation and less manual intervention into the simulated processes are advantageous and desirable for enabling accurate models.

## Approach

While simulating production processes by digital twins is an established methodology in the semiconductor industry to forecast the yield, plan tool dedications or manage maintenance operations, the common practice consists in the use of commercial simulation software that is vendor-

specific, closed-source and barely customizable by third parties. In order to provide a framework for the conception of and experimentation with AI approaches in a uniform setting, we have developed an **open-source event-based simulator** of real-world scale semiconductor fabs [1]. The simulator provides interfaces for plugging in **dispatching agents** that inspect the work in progress for making decisions about the production operations to process and the resources to allocate, where agents implementing classical dispatching rules like First-In-First-Out (FIFO) or applying Reinforcement Learning (RL) to adapt advanced dispatching policies are two common approaches [2]. By instantiating the framework with an RL agent to prioritize the production operations competing for the same resources, we achieved substantial improvements of the **lots completed on-time**, i.e., their production processes are completed at given target dates, in comparison to classical dispatching rules [3]. The latter strictly prioritize lots by predefined categories called "super-hot", "hot" and "regular", which yields a constant handicap for regular lots at each of the several hundred production steps and makes their on-time completion almost impossible, while the RL agent incorporates target dates and supplies a fairer dispatching policy.

Albeit statistical and, in particular, deep learning methods have emerged as very promising and successful data-driven AI approaches, the downside is that they generate uninterpretable and thus unexplainable black-box solutions, which can obstruct their acceptance in practice. For instance, an online-shopping platform may make recommendations to customers without need to understand and justify the reasons, but a medical assistance tool proposing drug therapies without giving specific information about the positive and contra indications would not be trustworthy, and corresponding considerations apply to production management in the semiconductor industry. To reconcile **empirical efficiency and transparent explainability**, we have applied genetic programming to optimize interpretable dispatching rules to the different characteristics of machine groups [4]. While the principles for deciding about operations to process and resources to allocate are similar to classical dispatching rules by relying on transparent decision criteria, the optimization by AI methods investigates a vast amount of promising settings that by far exceed human expert knowledge as well as manual exploration capacities. Digital twins

are again the key asset enabling the application of automated AI optimization means, driving the rapid experimentation and exploration of opportunities that would otherwise be limited to best guesses by human experts on how to manage production processes.

Model-driven AI approaches provide powerful means to perform **optimization at global scale**, e.g., scheduling a whole sports season at once rather than assigning fixtures from the first to the last match day. Particular challenges in semiconductor manufacturing lie in the high number of processing steps per lot that stretch over several weeks in the real world as well as variable process durations, success rates and disruptions that cannot be accurately predicted in advance. However, in a pioneering case study we modeled the specific processes in semiconductor manufacturing and experimentally evaluated the feasibility and limits of global optimization methods [5]. So far these experiments were performed offline, i.e., the optimized schedules are not yet utilized to adjust dispatching by the digital twin and validate the impact on performance parameters like the lots completed on-time. In the future, integrating AI methods for global planning in advance and reactive dispatching on the fly has high potential for combining the strengths of orthogonal AI approaches and making more effective use of the experimentation environment provided by a digital twin. Similar opportunities are encountered in the field of robotics, where control routines are usually prototyped and assessed in simulation before transferring them to physical robots, giving the advantage that AI methods for complex task and collaboration planning can be developed and evaluated on digital models [6].



## Impact

The remarkable advances and success stories of both model- and data-driven AI techniques in the last three decades are mainly owed to the increasing availability of powerful computing hardware as well as comprehensive data collections, while the basic methodologies did not change fundamentally. As a consequence, it appears unlikely that any new technologies will emerge and integrate into real-life environments as, e.g., faced in autonomous driving and industrial settings without significant engineering efforts.

The major bottlenecks remain sparsity of real-world data, limited accuracy and predictability as well as lacking experimentation and exploration opportunities. To bridge the gap between the real and the AI world, digital twins provide crucial means for developing and validating novel computational methods rapidly and without physical limitations. Once they are established and properly evaluated, AI developments can be transferred into the real-life environment, such as a semiconductor fab, yet without claiming absolute perfection but rather to provide **assistance and support for performing complex planning and management tasks** more effectively than doable by experts alone.

A central research goal lies in the development of pioneering system architectures for the integration and cross-fertilization of state-of-the-art model- and data-driven AI technologies on top of digital twins. This methodology goes beyond the current industry practice to use simulation methods mainly for reproducing and analyzing production and logistics processes in a trial-and-error fashion, yet without readjusting and optimizing them. The latter task is to be taken over by AI techniques, whose “intelligence” refers to a high degree of automation and applicability to diverse target domains, so that developments made in the semiconductor manufacturing and robotics fields can be adopted in other contexts as well.

Insights about the correlation between input parameters and the effectiveness of AI methods to improve performance indicators, gained on the basis of digital twins, provide important information regarding the data that should be systematically collected and evaluated for real production and logistics facilities, which can in turn be harnessed to streamline the layout of physical equipment and processes. Beyond the scientific interest and direct economical advantages, the AI research aims at a **more efficient resource and energy utilization** by production and logistics systems, going in line with urgent global climate goals.



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## Competencies

My research units (AAU Department of Artificial Intelligence and Cybersecurity, TUG Institute of Software Technology) have pronounced expertise on AI methods and their applications in industrial and real-life domains. In joint research with Infineon Technologies Austria AG, performed in the context of my endowed professorship, we develop simulation models for semiconductor factoring along with intelligent resource allocation and production scheduling strategies. The collaborative FFG project **Swarm Intelligence and Combinatorial Optimization for Energy Efficient and Adaptive Industry 4.0**, led by Lakeside Labs GmbH, amplifies our research on integrated AI approaches by linking swarm intelligence algorithms for bottom-up optimization with global optimization by means of constraint solving techniques. Graz University of Technology's Autonomous Intelligent Systems Lab is internationally renowned for pioneering research on AI planning and control methodologies in the robotics field. A variety of collaborative projects, including the FFG projects **AI-based Cooperative Air and Ground Robotics for Support of Emergency Services in Crisis Situations, Enabling and Assessing Trust when Cooperating with Robots in Disaster Response, Off-road Navigation for Robotic Platforms, ROBOTic 3D-Mapping, Orientation and Localization for Subsurface Emergency Applications** and **Simulation of Autonomous Vehicle Control based on Passive Localization**, focus on specific robot navigation and cooperation challenges. Moreover, innovative robotic platforms and control software architectures developed at the Autonomous Intelligent Systems Lab were awarded prizes at several international robotic research competitions, such as the RoboCup Logistics League and the European Land Robot Trial.

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# Additive Manufacturing in general and for the UAV Market in special

Christian Schmid, Mario Döllner

## Vision

During the past 3 years the development of Austrian economy reveals basic issues of supply chain approach. A situation characterized by long distance transports of products, raw materials and semi-finished products, highly diversified production-facilities located worldwide.

Many European companies relocated their manufacturing capabilities towards low personnel cost countries like China, Vietnam, etc.. The effect on CO<sub>2</sub> production rises with longer transportation distances but also the availability of different goods becomes more problematical, especially during COVID-19. Production lines stuck due to a lack of special parts needed for finishing the production process of various products like cars, electronic articles etc.. Effects that generates a negative impact on growth of economy and higher CO<sub>2</sub> emissions. Besides that, whole branches in our and foreign economies change form “produce then sell” to the other way round – “sell then produce”. Customized products, lot sizes of 1 are asked for from the market. Traditional manufacturing approaches with sequently driven processes, where the productive part of the whole process is low and the logistical part plays the main role in lead time and cost structure does not support this new demand of developing and producing more individually designed products.

Traditional manufacturing processes like casting, cutting, forming, joining are the dominant technologies which either reduce any kind of raw material by subtracting parts of it in form of chips, or need fixtures, forms and molds to produce serial parts with no opportunity to change the product

without adopting the tools. Additive manufacturing technologies waive forms or unnecessary material. Material is used in the specific amount and form needed to realize a product. No extra molds or fixtures are used for manufacturing a workpiece with additive manufacturing technologies. 7 principles of additive manufacturing technologies are standardized in ISO 52900-2015. Additive manufacturing, also known as 3D printing, is a rapidly evolving field that has seen numerous breakthroughs and advancements in recent years [1, 2]. Due to broad research activities in diverse domains, additive manufacturing has received many innovative achievements. In the following, a short vision of novel fields is given.

**Metal 3D printing:** One of the biggest recent achievements in additive manufacturing is the development of metal 3D printing technology. This allows for the creation of complex metal parts that would be difficult or impossible to manufacture using traditional methods. Metal 3D printing

- **Additive Manufacturing**
- **UAV**

has already been used to create aerospace parts, medical implants, and other high-performance components.

**Bioprinting:** Another area of significant progress in additive manufacturing is bioprinting, which involves printing living tissues and organs. Scientists have successfully printed functional tissues such as skin, cartilage, and blood vessels. While the technology is still

in its early stages, bioprinting has the potential to revolutionize the medical industry by enabling the creation of patient-specific organs for transplant.

#### **Large-scale 3D printing:**

Advancements in large-scale 3D printing have made it possible to print entire buildings and other large structures. This technology is already being used to construct low-cost housing in developing countries and to create emergency shelters in disaster zones.

**Multi-material printing:** Another recent development in additive manufacturing is the ability to print with multiple materials at once. This allows for the creation of complex, multi-functional parts that can perform multiple tasks simultaneously. For example, a 3D-printed part could contain both electrical wiring and mechanical components.

**Rapid prototyping:** Finally, additive manufacturing has significantly improved the speed and efficiency of the prototyping process. Companies can now quickly iterate and test new product designs, which has accelerated the development of new products and reduced time-to-market. Hybrid production, the combination of traditional and additive manufacturing has a high potential to create a synergic impact on manufacturing processes and in production due to higher flexibility regarding different processes and materials, reduction of transportation and jigs and tools. Overall, additive manufacturing continues to push the boundaries of what's possible in manufacturing, and these recent achievements are just the beginning. One additional interesting field of application, which we will focus on for a moment, is the UAV market. One of the key advantages of additive manufacturing for the UAV market is the ability to create complex parts with intricate geometries that would be difficult or impossible to produce using traditional manufacturing methods. This allows for the creation of lightweight, high-performance parts that can improve the performance of UAVs. Additionally, additive manufacturing allows for rapid prototyping and iterative design, which can significantly reduce the time and cost of developing new UAVs. This is particularly important in the fast-paced UAV industry, where new technologies and applications are constantly emerging. Furthermore, additive manufacturing enables the creation of custom and on-demand parts, which is ideal for the UAV market. UAVs often have unique requirements and specifications, and additive

manufacturing can be used to create customized parts that meet these specific needs.

Finally, additive manufacturing can also be used to produce UAVs themselves. Large-scale 3D printing technology has already been used to print entire UAVs, which can significantly reduce the time and cost of manufacturing compared to traditional methods. Overall, additive manufacturing has the potential to revolutionize the UAV market by enabling the creation of lightweight, high-performance parts and the rapid development of new UAV technologies. As the technology continues to evolve, we can expect to see even more exciting developments in the UAV industry.

## **Approach**

The concept of additive manufacturing dates back to the 1980s, when Chuck Hull invented stereolithography (SLA), which uses a laser to solidify layers of resin to create 3D objects. However, it wasn't until the 1990s that the term "additive manufacturing" was coined to describe the process of building parts by adding material layer-by-layer [4].

In the following decades, additive manufacturing technologies continued to evolve and improve. In the early 2000s, selective laser sintering (SLS) and fused deposition modeling (FDM) were developed, which allowed for the use of a wider range of materials, including plastics and metals. By the mid-2000s, additive manufacturing had begun to make significant inroads into industries such as aerospace, automotive, and healthcare. Companies were using 3D printing to create prototype parts and even final products.

In the years since then, additive manufacturing has continued to advance, with the development of new technologies such as metal 3D printing, bioprinting, and large-scale printing. These advancements have opened up new possibilities for manufacturing and are leading to new applications in areas such as personalized medicine, space exploration, and more. In fact, the following research aims can be summarized:

- 1. Materials development:** Additive manufacturing has led to the development of new materials and the improvement of existing ones. Researchers are working to develop new metal alloys, ceramics, and composites that can be used in 3D printing, as well as to optimize



existing materials for additive manufacturing processes.

2. **Process optimization:** Researchers are working to optimize the 3D printing process itself, including factors such as print speed, temperature control, and the use of support structures. By improving the printing process, it is possible to create more accurate and reliable parts.
3. **Design for additive manufacturing:** There is a growing focus on designing parts specifically for additive manufacturing, rather than adapting traditional designs. Researchers are exploring new design principles and software tools that can help designers create parts that are optimized for 3D printing.
4. **Post-processing:** After parts are printed, they often require post-processing to improve their mechanical properties or surface finish. Researchers are exploring new post-processing techniques, such as chemical treatments and heat treatments, to improve the properties of 3D printed parts.
5. **Quality control:** As additive manufacturing moves from prototyping to production, there is a growing need for quality control measures to ensure that parts meet the required specifications. Researchers are developing new methods for measuring the quality of 3D printed parts, including non-destructive testing techniques.

Overall, the research in additive manufacturing is focused on improving the quality, reliability, and efficiency of the 3D printing process, as well as expanding the range of materials and applications for additive manufacturing. These research results have the potential to transform many industries, from aerospace.

In Europe, research activities have been supported by the FP7 and the new Horizon program. As an overview, there are several EU-funded projects focused on additive manufacturing.

- AMable<sup>1</sup>: This project aims to help small and medium-sized enterprises (SMEs) in Europe adopt additive manufacturing technologies. It provides funding and support for SMEs to collaborate with experts in additive manufacturing and develop new products and services.
- AM-motion<sup>2</sup>: This project is focused on developing a strategic roadmap for additive manufacturing

in Europe. It brings together stakeholders from industry, academia, and government to identify the key challenges and opportunities for additive manufacturing in Europe.

- SYMBIONICA<sup>3</sup>: This project is focused on developing new technologies for medical applications. It aims to create a new generation of custom-made, 3D printed implants and prosthetics that are tailored to the individual needs of patients.

These projects are just a few examples of the many EU-funded initiatives focused on additive manufacturing. They demonstrate the growing importance of additive manufacturing in Europe and the potential for this technology to transform many different industries.

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<sup>1</sup> [cordis.europa.eu/project/id/768775](https://cordis.europa.eu/project/id/768775)

<sup>2</sup> [cordis.europa.eu/project/id/723560](https://cordis.europa.eu/project/id/723560)

<sup>3</sup> [cordis.europa.eu/project/id/678144](https://cordis.europa.eu/project/id/678144)

## Impact

Additive manufacturing has a significant impact on many industries, including aerospace, healthcare, automotive, and consumer goods. Here are some of the key impacts and benefits that additive manufacturing has had on industry.

**Faster prototyping:** With additive manufacturing, it is possible to quickly create prototypes of new designs and test them for functionality. This has helped to speed up the product development process and reduce time-to-market.

**Customization:** Additive manufacturing allows for the creation of highly customized products that are tailored to the specific needs of individual customers. This has led to the development of new business models that rely on mass customization rather than mass production.

**Lightweighting:** Additive manufacturing can be used to create lightweight components for aerospace and automotive applications, which can help to improve fuel efficiency and reduce emissions.

**Reduced waste and save resources:** Additive manufacturing can produce parts with a high level of precision, which reduces waste and makes the manufacturing process more efficient.

**Distributed manufacturing:** Additive manufacturing allows for decentralized manufacturing, which can reduce the need for large centralized factories and transportation costs.

**Improved supply chain:** Additive manufacturing can help to simplify supply chains and reduce lead times, as parts can be produced on demand rather than being stored in inventory.

**New design possibilities:** Additive manufacturing allows for the creation of complex geometries and internal structures that would be difficult or impossible to produce using traditional manufacturing methods. This has led to the development of new products with improved performance and functionality.

Overall, additive manufacturing has had already a transformative impact on industry, offering new opportunities for innovation, customization, and efficiency. As the technology continues to improve and expand, it is likely that its impact will only continue to grow in the years to come. New potential is given by combined process in one workstation setup using traditional and additive processes.



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## Competencies

Our research unit at the University of Applied Sciences has established applied research initiatives on national as well as international levels. In addition, PhD cooperations are held with the University Passau and TU Clausthal as well as with the University of Rostock.

Some of the recent research initiatives in the context of additive manufacturing are development of a low cost large scale Wire and Arc Additive Manufacturing system which allows the users to also produce small to midsize lots of welded products without skilled welders (grant Tyrol). Related to this topic, design guidelines are developed for WAAM-3D-Printing [5, 6]. Another approach is the use of prefabricated plates, tubes or profiles combined with 3D-printed geometries like fixtures, hinges or connectors and seals [7, 8, 9]. Meanwhile our research group is turning out experiments with solder alloys in an integrated casting process during Material Extrusion processes.

The development of 3D-Printing customized ski-shoe liners from the smartphone app to the personalized infill structure for adopting the liners with different comfort zones were researched and developed using FFF Fused Filament Fabrication-3D-printing processes with different materials, infill structures and densities [10]. Additive manufacturing processes are fully digitized processes. Still 3D-printing processes like FFF, but also metal welding driven processes like Wire and Arc Additive Manufacturing WAAM have issues with layer adhesion, lack of material or shape imperfections. Our scientists are working on different thermographic, sensor driven or computer vision methods to detect and control these effects [11, 12].

In the context of UAV research, our group is on the development of a novel hydrogen drone (K-Regio grant Tyrol), where especially a new tank design for hydrogen on drones is in the focus. Furthermore, drone swarm research is considered in order to integrate the hydrogen drone in search and rescue missions. Furthermore we are developing large size rapid production layup-forms and molds for UAV together with industrial partners. The integration of additive manufacturing techniques in the context of developing a sensor-based system for the detection of dangerous goods has been evaluated in an EU regional grant (KUUSK Drohnenkompetenzzentrum).

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# Chair of Ferrous Metallurgy

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## Vision

Steel is the most used metallic material of our time and is the basis for modern society. Due to the social and economic development of the world population, steel production has been more than doubled worldwide since the turn of the millennium. In 2022, world steel production amounted to nearly 2 billion tons. It has caused 7 to 8 % of CO<sub>2</sub> emissions worldwide, making the steel industry one of the largest greenhouse gas (GHG) emitters in the industrial sector. Climate protection is one of the biggest challenges facing the steel industry today. [1]

Steel is a readily available, sustainable material that can be recycled repeatedly. Due to its many advantages, such as strength and ease of machining, steel is used in a wide range of applications. It is the most excellent material for society's infrastructure, a material that supports people's lives and overall economic development.

The Paris Agreement adopted in 2015 defines global targets for reducing GHG emissions. The global steel industry expressed its commitment to reducing the CO<sub>2</sub> footprint from its operations and the use of its products, including by-products. The World Steel Association defined three main elements for the implementation:

- Reducing the impact of steel production
- Efficiency and the circular economy
- Developing advanced steel products to enable societal transformations [2]

The EU, responsible for 10 % of global GHG emissions, aims to act as a global leader in the transition toward a net-zero greenhouse gas emissions economy. In December 2019, the European Commission announced the EU Green Deal, which has the objective that Europe become the first climate-neutral continent by 2050. Greenhouse-gas emissions should be reduced through a socially fair transition and an overall better quality of life.

The European steel industry has founded the clean steel partnership (CSP), a public-private partnership coordinated by the European Steel Technology Platform ESTEP and the European Steel Association EUROFER. In its Strategic Research and Innovation Agenda (SRIA), for which the EU Green Deal is one fundamental pillar, the CSP's vision is to establish steelmaking processes with -50% CO<sub>2</sub> by 2030 and to reach net-zero CO<sub>2</sub> emission from production by 2050. [3]

- **Steel-Making**
- **CO<sub>2</sub> Reduction**
- **Sustainability**
- **Steel Quality**
- **Circular Economy**

The forthcoming transformation towards climate neutrality of our society can only succeed with steel as a key enabler. It is indispensable to build up new CO<sub>2</sub>-free energy generation and supply infrastructure. The same applies to the transformation toward climate neutrality of sectors for transport, building infrastructure and energy-intensive industrial processes, including the steel industry itself.



The Chair of Ferrous Metallurgy (CFM) regards itself as a scientific partner of the Austrian and European steel industry for the transformation process of the production sites towards climate neutrality and more sustainable use of steel as material. We have a well-developed key competence in fundamental-oriented and applied research for iron- and steel production. The vision is to further strengthen this for CO<sub>2</sub>-free steel production, enhanced efficiency of the processes by increasing digitalisation, and superior steel product qualities. Closely linked to the research activities is the academic education of metallurgical engineers with research-led teaching at the Montanuniversität Leoben. The students of the bachelor and master study programs “Metallurgy and Metals Recycling” and the master study program “Sustainable Materials” should be prepared during their study for their future professional challenges.

## Approach

The CFM research and teaching expertise covers all technological process steps in the steel production chain, from primary and secondary raw materials to the casted semi-products. The research is organised into three groups focusing on primary metallurgy, inclusion metallurgy and casting processes.

The primary metallurgical processes group researches ironmaking and crude steel production processes. One focus is improving and optimising the dominating ironmaking technology, the blast furnace with the sinter and coking plant. Strong competence is available for alternative ironmaking technologies, i.e. direct and smelting technologies. In the last years, the use of hydrogen to avoid CO<sub>2</sub> emission from fossil energy carriers for steelmaking was intensively explored for the production of direct reduced iron (DRI) from fine-grained iron ores with fluidised bed reactor technologies. DRI is a metallic iron input material for crude steel production in electric arc furnaces and LD converter. CFM was the scientific partner of Primetals, voestalpine and K1-MET for the development of the HYFOR technology. An HYFOR pilot plant was built at the voestalpine Donawitz site.

The technology of hydrogen plasma for smelting reduction of iron ores to produce crude steel is another emerging breakthrough technology for CO<sub>2</sub>-free crude steel production, which has been examined at the CFM since

the 1990s. Based on that, a bench-scale plant for SuSteel (sustainable steel) was constructed on the voestalpine Donawitz site and is currently operated with the development partners K1-MET and voestalpine Donawitz and Linz. In addition to the use of hydrogen, research is also being conducted on hydrogen production. For two years, research has been conducted on a basic research topic on the production of hydrogen and high-grade carbon by pyrolysis of methane using thermal plasma.

Solid carbon will be indispensable in the production chain of steel production. Carbon is the most important alloying element for steel, and the most efficient alloying procedure is adding solid carbon. Solid carbon is also hard to replace in the electric arc furnace (EAF) for slag foaming. The research at CFM is to explore the behaviour of solid carbon carriers from bioenergy resources regarding carbon yield during alloying and slag foaming efficiency in the EAF.

The circularity of steel and steelmaking by-products is another topic in the research at CFM. Steel scrap is an important secondary raw material for steelmaking. Various chemical elements introduced into the molten steel by scrap are considered undesirable trace elements. These are often difficult or impossible to remove metallurgically, such as copper and molybdenum. A research focus at the CFM is on the behaviour of these elements in the steel melt as well as their effects on the finished product. They cause problems in the casting process due to lowered liquidus temperatures as well as changed interfacial properties, which influence the behaviour of non-metallic inclusions in the system steel-slag-refractory material. The development of new steel grades that are more tolerant to trace elements is a central research task.

A particular focus is also laid on indirect sustainability, significantly strengthening the further improvement of steels needed for renewable energy production and electromobility. In the course of fundamental changes in production technologies to reduce the CO<sub>2</sub> footprint, maintaining or even optimising the final steel quality is a crucial research task. Combining the fundamental metallurgical process expertise with interdisciplinary fields like artificial intelligence as well as new analytical techniques opens innovative possibilities for process control and development.

For casting processes, developing

smart quality prediction systems by combining physical and numerical simulation, thermodynamic modelling, and process data analysis is part of ongoing projects. Physical modelling here involves experimental simulation of crack formation during and after the solidification of steel with worldwide unique experimental setups. Behind the experiments stand numerical models for solidification simulation and microstructure evolution. High-temperature confocal microscopy results are used to assess microstructure and phase transformation kinetics and serve for the indirect parametrisation of precipitation models. Thermal boundary conditions for the simulations come from a nozzle measuring stand and voluminous data from advanced sensors in steel plants, such as fiber-bragg instrumented moulds. Besides classical numerical simulation and experimental work, also machine learning approaches have become increasingly important for the connection of quality data and process data. CFM's contribution to newly proposed European projects claims the development of new strategies for quality prediction.

Another recently developed research field is high-temperature oxidation of steel, being now and in future of highest interest: Changes in raw materials mix for steel production, e.g. an increasing scrap rate will result in the more complex control of residual elements in steel production, involving Cu, Sn, Sb, As and many others. These elements show a certain tendency to enrich along grain boundaries in an oxidising atmosphere, resulting in so-called liquid metal embrittlement. As a final consequence, cracks may start to form during casting, reheating and rolling. Thermo-gravimetric analysis with water steam supply and mass spectrometer here allows to simulate nearly all industrial processes relevant for steel production and processing. Hydrogen burners in industrial furnaces and their impact on surface quality may be a further field of research in the future.

Another way of saving CO<sub>2</sub> emissions is the direct connection of the casting and rolling process. The so-called endless strip-production (Arvedi-ESP) process is one of the most promising worldwide applied processes. The continuous extension of the product mix to new steel grades, such as advanced high-strength steel, demands the careful adjustment of process parameters, the adjustment of quality prediction systems and the detailed investigation of surface oxidation and

descaling. These activities are part of a recently started project.

The sustainable use and recycling of metallurgical slags is a further topic which was explored at the CFM in recent years. In cooperation with other Chairs at the Montanuniversität Leoben, research institutes and industrial partners, the stability of Cr and V compounds for leaching conditions from steelmaking slags was researched. The research work included the treatment of slags to enhance the stability of these elements.

## Impact

Steel, as the number one structural material, will continue to play a significant role in the development and well-being of our society. The research activities of CFM should help the Austrian and European steel industries to continue operating their production sites competitively. It should stimulate investments in breakthrough technologies which will be a unique selling proposition for the steel producers, and the development of new steel grades to enhance the recycling rate of steel scrap.

The research activities of the CFM strongly depend on third-party funding. The national funding agency FFG (Austrian Research Promotion Agency) is the main source for the financing of research projects with industrial partners.

The national programme COMET (Competence Centers for Excellent Technologies) is an important funding instrument for CFM. The fundamental motivation behind COMET is to develop new expertise and encourage greater internationalisation to promote excellent cooperative research between industry and academics. CFM has been a university partner since 2006 in the COMET centre programmes K1-MET, "Competence Center for Excellent Technologies in Advanced Metallurgical and Environmental Process Development", and IC-MPPE "Integrated Computational Materials, Process and Product Engineering". In the case of K1-MET, CFM is allocated with the highest portion of the research budget of all academic partners. Univ. Prof. Johannes Schenk, head of CFM, is one of the General Managers of K1-MET GmbH and is the Chief Scientific Officer (CSO).

The CD Laboratory for Inclusion Metallurgy in Advanced Steelmaking is currently running at the CFM under the lead of Univ.Prof. Susanne Michelic. Here, non-metallic inclusions, their formation and modification in various steel production processes are being researched. A special focus lies on secondary metallurgical treatments to control the final steel cleanliness. The results will be available to industrial partners for their process improvement and product development. At the same time, basic knowledge on the research topic for CFM is being built up in the CD laboratory.

Another important financial basis for research projects is EU funding programs for industrial research, namely Horizon 2020 and RFCS. In these projects, CFM is closely cooperating with universities, research institutes and company partners of the EU.

PhD and master thesis are financed and executed through third-party funded projects. That contributes to the research-led teaching of young academic talents. The supervision of PhD and master thesis is also done for students employed at K1-MET.



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## Competencies

The research at CFM is executed predominantly in projects with close cooperation with partners in the steel producing industry, metallurgical plant builders and refractory suppliers. The methods applied are experimental investigations, mathematical modelling and simulations, as well as advanced analytics.

The CFM staff currently consists of 49 employees: three professors, one emeritus professor, three postdocs, 14 PhD students, 13 student workers, two lecturers and 13 technicians and administrative persons. The proportion of women is 25%. CFM operates two medium size technical laboratory centres, two small experimental laboratories, one metallography laboratory and one workshop. These centres and laboratories are equipped with several furnaces, microscopes, metallographic devices and measuring instruments.

CFM is well recognised as a competent academic institution in Austria and the EU. However, in the last decades, an international network in all continents comprising companies, research institutes and universities has also been built. Proof of this is the stay of scientists, especially from Asia (China, Korea, Japan and India) as visiting researchers in the last two decades. In the field of teaching, there have been student exchanges with China and Brazil in the same period.

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**Sustainability**



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ZERO**



# Enabling Circular Streams in Chemical Engineering

Karin Kloiber, Christian Paulik

## Vision

“CHASE is dedicated to driving the twin transition in the chemical process industries by enabling sustainable and efficient processes through science-based, pre-competitive research in process industries in Austria and Europe, with a focus on the research areas Process Digitalization, Process Intensification, and Circular Process Streams. Our emphasis is on cross-linking analytics, process engineering, process modeling, and data science to (re)engineer chemical systems. Our mission is to increase the long-term international industrial competitiveness of national industries by building and leveraging scientific competencies and raising technological synergies in our collaborative partnerships with the industry.

We actively respond to market requirements expressed by industrial partners and socio-economic backgrounds and innovation pressures, while we support challenging targets given by the EU Green Deal and Sustainable Development Goals formulated by the UN. With a focus on continuous improvement and co-creation, we strive to be a trusted partner for our clients, employees, and stakeholders, and a leading force in shaping a more sustainable future for the chemical process industries.”

## Approach

**The Digital Knowledge Twin:** The transformation toward green & digital processes is disruptive and, above all, inevitable. It is also hard to achieve. The pivotal point to a successful transformation is the ability to turn the multitude of existing data into actionable information and knowledge.

This is commonly captured by the notion of the digital twin (DT), i.e., the (synchronized) duality between a digital and a physical counterpart, where the digital instantiation mimics the physical entity with a granularity that is adequate for the intended purpose. Dechema describe DT as the main enabler for capturing, deploying, and managing knowledge along the different value chains by the use of large volumes of data<sup>4</sup>. Typically, one thinks of DT as purely data-driven instances that can predict failure, control processes, and deliver hitherto invisible information, in particular where processes are little understood and cannot be modeled on physical grounds.

- **Chemical Systems Engineering**
- **Circular Economy**
- **Digital Twin**
- **Twin Transition**
- **Sustainable Business Models**

However, ‘**Digital Data Twins**’ capture neither physical principles nor the often-implicit domain knowledge, and they are not necessarily well suited to perform well outside of their learned domains. They are also not a priori explainable which may impede acceptance by users. More importantly, actionable big data in the chemical industries are typically hard to get by, mainly for two reasons: abundant process data inform solely on a limited space of process conditions and cannot generally be interpreted from a causal perspective. On the other hand, while systematic experimental data

covers a larger design space, it is often sparsely populated, owing to time and cost constraints. This poses a severe obstacle in particular to SMEs which (remarkably enough) constitute 96% of European chemical companies and are pivotal to achieving resilience on a European level<sup>3</sup>. Therefore, the reality in the chemical industries dictates new generic approaches to digitalization as well as tailored solutions.

At CHASE, we understand that addressing these complex challenges requires a multifaceted approach. This entails a computational strategy that focuses on data availability, process modeling, and the development of generalizable workflows for process digitalization. Our goal is to make data more accessible and usable, leveraging novel machine learning methods to infer root causes from non-interventional production data. This contributes to unlocking the power of large volumes of data that have, to this day, not delivered robust actionable insights. It also includes the use of machine learning (ML) and deep learning (DL) for data generation and augmentation where (experimental) data are sparse. We also place great emphasis on improving process observability using process analytical technologies (PAT), to ensure that our partners have access to accurate and high-quality real-time information about their processes. Indeed, the combined multimodal analysis of production and PAT data holds great promise to improve process monitoring and control. Overall, we prioritize data availability and usability in our efforts to drive digital transformation development.

In addition to this, we firmly believe that for building suitable accurate, and robust process models, data must be put into the context of domain knowledge. The integration of domain-specific know-how into what we call **Digital Knowledge Twins** is at the very heart of CHASE projects and represents the Center's USP. Knowledge comes in many flavors, e.g., laws of nature (conservation laws, continuity equations) that are captured in physical simulations, or as empirical concepts that can be cast as mathematical statements (e.g., kinetic equations). Additionally, knowledge can also be based on the expertise and experience of individuals or organizations, often intangible, not easily quantifiable, and particularly difficult to capture. At the same time, digitization of organizational knowledge is an important asset in operations, in particular when adequate data are not (yet) available, or the predictive potential is unclear.

It supports the initiation of digital transformation projects and enhances knowledge transfer and management. Notably, it may reduce barriers to the adoption of digital technologies where broad acceptance is still lacking, serve as a contact point between domain experts and data scientists, and helps meet FAT (fairness, accountability, transparency) objectives of algorithmic decision-making. The inclusion of domain knowledge into computational models is considered one of the 'Grand Challenges' of machine learning<sup>5</sup> and is generally far from trivial. Our system of industry partners, however, provides us with a number of opportunities to implement and explore hybrid data- and knowledge-driven solutions, for instance by the deployment of hybrid modeling techniques, and through the contextualization of operational knowledge and data-derived insights. In our sector, hybrid models are particularly valuable in (mechanistic) model transfer, or where physical models need to go online. We speak of a 'Digital Knowledge Twin' if data and knowledge have been optimally combined for superior performance of models and smart devices that derive from it.

**The Data Sharing Bottleneck:** For a digitalization project to succeed, the foremost prerequisite is the availability of sufficient high-quality data. With the notion that processes cannot be meaningfully optimized in isolation (at least from a sustainability perspective), this condition represents a severe bottleneck, as the sharing of data is far from established routine between industry partners. What's more, it is often unclear which data need to be shared and how much, and while several important projects are underway that tackle material provenance and faith along value chains in the form of product passes, few efforts have been made to explicitly analyze and evaluate its entire material and process history together. The benefits of data sharing, however, are potentially enormous. For instance, the sharing and the analysis of comprehensive data along a recycling value chain can provide insight into an optimal recycling strategy. In particular, a (downstream) application-guided identification of critical quality attributes and critical process parameters enables optimized sampling schemes, parsimonious process monitoring, as well as informed decisions on how to guide material streams and the corresponding process parameters - such that a maximum amount of waste is steered toward its optimal fate. Secure data-sharing strategies can be realized based on

homomorphic encryption, secure multiparty computing techniques, or distributed ledger technologies that guarantee (statistical) data privacy, and also authenticity. While these techniques offer promising solutions, they ultimately rely on sophisticated algorithms, and their wider adoption depends on improved scalability (i.e., increased compute power), the generation of sufficient expertise to implement them as well as on the trust of the involved parties. Thus, we believe it is also necessary to assess and point out the scope and limitations of these techniques to the non-experts that actually drive such projects, concerning in particular an imminent trade-off between privacy, compute power, and guarantee to deliver. With this in mind, CHASE assesses different strategies toward efficient data sharing, with the foremost goals to (a) showcase the potential of secure, authentic, and governance-respecting data and information exchange, and (b) to enable the actual assessment of process chains not only from a technological but also from a **sustainability perspective**.

#### **Methods for circular process design:**

Closing the loop in the chemical industry involves designing and implementing sustainable processes that reduce waste, recycle materials, and minimize the use of non-renewable resources. CHASE adopts a strategic position in the context of several waste-to-value approaches where chemists, engineers, biologists, and data scientists collaborate in the fields of carbon upcycling and (microbial) CCU (carbon capture and utilization). In particular, we research selective CO<sub>2</sub> activation on heterogeneous catalyst surfaces for the conversion to valuable carbon building blocks, replacing classical synthesis routes based on crude oil. The idea is to screen and evaluate a range of catalysis systems for their effectiveness, performance, and selectivity and subsequently upscale the synthesis of the most promising candidates for conversion to a range of chemical precursors. A systematic evaluation of performance on various scales represents a valuable knowledge base for efficient continuous processing.

The use of microbes to convert CO<sub>2</sub> or industrial waste is an emerging technology that holds promise for reducing greenhouse gas emissions and sustainable sourcing of commodities. However, major challenges arise from the fluctuations in microbe metabolism due to aging and environmental conditions, as well as the inherent variability of the input streams. These factors make it exceedingly difficult to maintain a stable and efficient

operation of microbe cultures. Thus, scaling up these technologies to meet global demand will be a significant challenge that requires scientific research and the development of infrastructure and supply chains. At CHASE we investigate the microbial conversion of waste streams to valuable compounds using advanced sensing technology and computer-aided approaches. For instance, we use a mechanistic approach to model the conversion of saline wastewater into higher carbon compounds or apply a physics-informed approach (computational fluid dynamics modeling) to reactor design for archaea in an H<sub>2</sub> conversion reactor. The models inform on parameters that impact the performance of the system, such as the efficiency of mixing or gas-liquid mass transfer, and represent an invaluable tool for intensification and upscaling of methane production. These examples illustrate two different entry points for the computational optimization and robustification of biological processes, i.e., process design and process control.

One of the most prominently researched aspects of waste management in CHASE is the recycling of plastics. For instance, we want to advance the reintroduction of polymers in food contact applications, a field with high potential for increasing the recycling rate, yet highly regulated: currently, only polyethylene terephthalate can be recycled for food contact, but no closed loop scenario for polyolefin food packaging materials has been established yet, due to strict regulations and safety requirements. Polyolefin recycling is challenging due to the material's tendency to adsorb and retain odors, release additives or degradation products, and ensuing challenges in the sorting and cleaning processes. Also, little is known about which contaminations can be effectively removed by the subsequent recycling step, to what extent, and under what conditions. A systematic assessment of the effectiveness of mechanical recycling for decontamination could speed up the development of regulations and certified procedures for the use of recycled polyolefins in food contact applications. CHASE aims to address these challenges by developing a structured approach to contamination, the corresponding analytics, and a data-driven approach toward the recycling process, to systematically assess the decontamination performance of mechanical recycling, in alignment with EU and US guidelines.

#### **A Process Systems Engineering (PSE) Approach:** A PSE approach

covers essentially three tiers of design & optimization; the (isolated) process; the connected processes including material streams; and ultimately the environmental and social impact of the system. Similarly, while the scientific and technical aspects of our projects are prerequisites for optimization and intensification, we see this as only the first part of the bigger picture of technology impact assessment. We have learned from our continuous dialogue with experts that despite the growing importance and interest in a holistic approach, this is a maturing field that faces severe challenges on several levels. In particular life cycle assessment (LCA) results depend on the predefined scope, system boundaries, and the methods and standards used, and are severely hampered by missing

knowledge on certain environmental impacts and data gaps. This amounts to a level of subjectivity that often precludes a meaningful interpretation of the results. In addition, LCA is typically performed on existing processes, but it would be of tremendous importance to evaluate emerging technologies before implementing them. We believe that with our approaches we can contribute to the mitigation of some of these problems and have initiated a strategic collaboration with academic partners with the goal to provide experimental and in-silico life cycle inventory (LCI) data, advance coupled LCI-Process simulations, and work toward ex-ante methods for informed design decisions for upscaling or before deploying novel technologies to the markets.



## Impact

Digital technologies are driving sustainable market opportunities, and the majority of successful businesses in this space do leverage digital tools<sup>2</sup>. The integration of digitalization and sustainability has significant scientific implications, ranging from advances in material design and process understanding to the biologization of chemistry and polymer recycling. We expect in the near future to see important methodological developments in FAIR (Findable, Accessible, Interoperable, Reusable) data management, secure data-sharing, and the digitization of organizational knowledge. These advancements will enable more efficient and flexible production processes, compliance with regulations, and improved decision-making through the use of smart assistance systems. With a comprehensive view of the value chain, best practices emerge for steering complex material streams through their value chain and a body of evidence will be generated which improves accurate impact assessment. Ultimately, the CHASE projects are designed to support the twin transition of companies by building knowledge through bottom-up, collaborative projects that prioritize the actual needs and requirements of industries.

The creation and application of comprehensive digital knowledge twins have the potential to significantly impact the core business models of companies and research institutions. The extent and speed of the industrial transformation and related market opportunities are widely discussed and reflected in numerous high-level publications, events, and discussion groups. For instance, the Business and Sustainable Development Commission estimated in 2018 that achieving the global goals could create an economic prize of at least US\$12 trillion by 2030 for the private sector (and potentially 2-3 times more). More recently, the Royal Chemical Society organized an industry-academia conclave in 2022 to develop a sustainability & digitalization roadmap for the chemical industry, which included a showcase session on emerging technologies and start-ups driving the sustainability and digitalization agenda. The world's largest chemical industry fair,ACHEMA, also opened in the same year with an event on climate-neutral chemical industry, featuring a green innovation zone with digital hubs and digital labs. In a recent survey by EY, digitalization emerged as the second-most prominent capital issue for chemical businesses, with 65% of CEOs expecting it to have a significant impact on their businesses. Moreover, four out of every 10 chemical businesses prioritize digitalization to fulfill their sustainability goals, according to their CEOs.



Our program is dedicated to driving the digital transformation and innovation in the chemical industry, with the aim of enabling more efficient and sustainable processes, while reducing the industry's environmental footprint. As customer preferences shift and regulations become more rigorous, it's becoming increasingly essential for chemical companies to prioritize sustainability. The latest EU CEO outlook survey (2023) reveals that over 80% of chemical industry leaders now consider environmental, social, and governance factors to be just as important as revenue growth. This is a remarkable shift, demonstrating that sustainability can be a value-driven proposition that pays dividends, rather than a mere risk management exercise - a shift that aligns with our principles and efforts. By working alongside the industry to develop more efficient, sustainable, and profitable processes, we will contribute to reducing the sector's environmental footprint, support its transition to a more circular economy, and toward the industry's continued progress in the years to come.



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## Motivation

In 2017, two years after the announcement of the 17 SDGs by the UN and in response to the global financial crisis of 2008, the Business and Sustainable Development Commission claimed<sup>1</sup> that “our current model of [business] development is deeply flawed” and urged business leaders to adopt more sustainable, socially oriented business models. With this, they addressed the increasing inequalities in wealth and demanded that society take action to build an inclusive, just, and environmentally sustainable economy, in line with the global development goals.

The chemical industry, due to its scale and diversity, is considered a central lever in the **green & digital (twin) transition**: Its production processes span essentially all modern manufacturing industries from transportation and construction to food and medicine. Cross-industrial production networks encompass hundreds of chemical processes generating a myriad of valuable products from a variety of raw materials and intermediates. In fact, over 95% of goods are in contact with the chemical sector value chain at some point in their life cycle<sup>2</sup>. In particular, the EU-27 is the second largest chemicals producer in the world, and, while tremendous progress in GHG emissions and energy consumption has been made since the 1990s, it is still its third biggest carbon emitter<sup>3</sup>.

Modern integrated production networks are highly interconnected, with a complex flow of mass, energy, and information. However, their structures are the result of decades of opportunistic growth, predicated on the constant availability of resources and energy, predictable regional economic frameworks, and stable global market development. Traditionally, little effort has been invested in making this industry sustainable. Even today, with SDGs on every company's agenda, chemical and pharmaceutical processes consume large amounts of energy and resources and emit numerous substances and materials into the ecosystem, making them unsustainable in the long run.

Recent years have impressively demonstrated the vulnerability and the lack of adaptability of the European chemical and the connected manufacturing industries to

- The disruption of energy and material supply chains by multiple crises as well as the depletion of resources facilitated by growing demand in Southeast Asian countries,
- The transformation of financing frameworks triggered by EU taxonomy, which redirects money toward sustainable projects in order to make European economies, businesses, and societies more resilient against climate and environmental shocks, and
- A change of regulatory frameworks by political action plans such as the Plan for Circular Economy of the EU, which has sparked the definition of carbon neutrality targets and regulations that potentially compromise the performance of industrial processes.

This demand for sustainability comes with remarkable business opportunities and revenue potential, as has been highlighted by the World Business Council for Sustainable Development, who claim that the SDGs constitute a framework that permits smart, progressive, and profit-oriented business models – and pointed out that the market opportunities are seized predominantly by businesses that are built on digital technologies<sup>2</sup>. The chemical industry is at a crossroads. Whether we continue to cling to outdated systems and processes or embrace the digital revolution, transforming our industry to thrive in the face of rapid change - the choice is ours to make, and the stakes couldn't be higher. **We believe that**

**digitalization is not an option – it is a prerequisite to survive.**

Notably, while (linear) chemical industries are complex in the first place, the quest for circularity adds another layer of complexity regarding efficiency, novel materials, and novel pathways. The changing industrial production reality confers (as of yet) unmet technological needs that call for immediate action. Changing a complex system first and foremost requires a systemic approach, in order to understand and consequently optimize the processes, and the associated energy and material streams, in particular, if processes and operations need to be rethought at a grander scale. Consequently, the strong change request toward efficient, flexible, and resilient production processes is ultimately a quest to go **digital** while maintaining a **holistic perspective**. The large amounts of data that are being generated by the industries support this view, but much of it remains unused or underutilized, representing a significant untapped resource for improving sustainability and driving innovation. We believe that the primary challenge to a successful transformation is the ability to turn the multitude of existing data into actionable information and knowledge.

At CHASE, we assume a process systems engineering approach to enable the efficient use of resources and sustainable and reliable processes. In particular, we work toward comprehensive virtual instances of processes and process chains that permit meaningful design decisions, optimization and control, and maximization of insight.

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# Sustainable Chemical Process Engineering

Mark W. Hlawitschka

## Vision

Addressing **today's and tomorrow's global challenges** is a primary concern for the **socio-economic** and **environmental system**. By 2050, the world's population is expected to reach 9 billion. Despite overall improvements in living standards, socio-economic disparities still persist, making it crucial for individuals, communities, businesses, and nations to collaborate in tackling interconnected global challenges. This involves ensuring that every person has access to **water, food, energy, and housing** in an economically and environmentally sustainable manner.

**Chemical sciences** are **driving innovation** in various technologies, such as **water purification membranes, drought-resistant crops, antibiotics, batteries** and their **recycling**, and **prevention and reversal of environmentally harmful impacts**. Additionally, **digitalization** and the use of **digital twins** are becoming increasingly **important tools in chemical engineering**.

Through virtual models of chemical processes and products, chemical engineers can optimize their designs and significantly reduce costs, time, waste, and emissions. One of the most important challenges stays the water scarcity. It has significant impact due to competition, conflict, and negative impacts on human health and the environment. The growing population and increasing demand for water for drinking, cooking, sanitation, agriculture, and industrial processes are leading to overuse of limited water resources. The aging society is also a major concern for the chemical industry, as many experienced workers are retiring without enough skilled

replacements. To address this issue, chemical companies need to invest in training programs and partnerships with educational institutions to attract and develop the next generation of chemical engineers. Moreover, chemical engineers are focusing on sustainability by considering the entire lifecycle of their products and processes, from raw material extraction to disposal or recycling. New regulatory requirements on chemical safety, emissions reduction, and waste management are driving the chemical industry in the following years. By working collaboratively, we can help to create a more sustainable and prosperous future for all.

The Institute of Process Engineering at Johannes Kepler University (Institut für Verfahrenstechnik, IVT) aims to achieve this by providing profound knowledge through education and developing state-of-the-art methodologies for better process routes, energy savings, and water protection. Key enabling technologies such as CO<sub>2</sub> to methane

- **Sustainable Chemistry**
- **Energy**
- **Water Treatment**
- **Digital Twin**
- **Process Optimization**
- **Battery Recycling**

by archaea which can be further used as a chemical feedstock or as energy supply, water purification by membrane distillation crystallization as well as new recycling strategies for the black material in batteries are driving our current research.

These goals are in line with the goals of the European union further reported in the the green deal, the transition pathway for the chemical industry as well as the Masterplan for a Competitive Transformation of EU Energy-intensive Industries Enabling a Climate-neutral, Circular Economy by 2050

*“The chemical industry, the fourth largest industry in the EU, plays a key role in the European twin transition. Chemicals are present in about 95% of manufactured goods and are at the basis of Europe’s major value chains.”*

*“Climate change and environmental degradation are an existential threat to Europe and the world. To overcome these challenges, the European Green Deal will transform the EU into a modern, resource-efficient and competitive economy, ensuring:*

- *no net emissions of greenhouse gases by 2050*
- *economic growth decoupled from resource use*
- *no person and no place left behind”*

and find its pathway to the current Horizon Europe Research calls.

## Approach

The Institute of Process Engineering is at the forefront regarding **Computational Fluid Dynamics** for multiphase fluidic apparatuses, the **derivation of simplified models** for obtaining a **digital twin** and integrating these ones into a **real system** by integrating **online data** to the control strategy. By combining the newest computational models with experimental insights, uncertainties can be closed and a reliable **scale-up** of chemical apparatuses can be obtained, leading to energy as well as resources efficient apparatus designs. Further research however is required to identify reliable models for complex multiphase flows [1] and the occurrence of Mulm and foaming. A keyplayer thereby are the optical **measurement techniques** to determine the **particle size** in- and online in the process [2]. This procedure of combining numerical and experimental studies can also be adopted to the current research approaches and serve as a basis for better apparatus design, the isolation of single effects and the generation of digital twins. The work is further extended to **machine learning** and **AI**, to enable a data driven development of models and industrial designs. As an example, coalescence of droplets and bubbles is omnipresent in chemical

apparatuses, but hardly understood, leading to overestimation of the apparatuses. This can be overcome by providing a mini-scale coalescence investigation cell and data driven modelling.

The **recycling of black mass** is becoming increasingly relevant due to the growing demand for lithium-ion batteries and the limited availability of raw materials. Black mass resulting from spent lithium-ion batteries, a mixture of lithium, cobalt, nickel, and copper oxides contains valuable metals that can be recycled. Recycling of black mass not only reduces the demand for virgin raw materials but also reduces the environmental impact of battery production. However, the separation of these metals from black mass is a challenging task due to the complex mixture of substances. This is where the need for efficient separation processes arises, and various methods such as acid/alkaline leaching, precipitation, solvent extraction, and/or the use of ion exchange resins can be used individually or in combination to achieve efficient separation. The use of advanced processes such as extraction columns [3], membrane reactors, and electrochemical methods offers smart possibilities to increase the efficiency of separation processes. Therefore, in-depth research activities are performed to develop robust tailor-made (reactive) extraction methods and equipment technology to enable powerful and efficient separation of complex mixtures of substances in the future.

**Membrane distillation crystallization** (MDC) is a promising technology for the separation and purification of salts and other substances [4]. MDC offers a more energy-efficient and cost-effective alternative to traditional thermal desalination and crystallization processes, which require high temperatures and pressures, leading to high energy consumption and operational costs. MDC operates at low temperatures and pressures, which reduces the energy consumption required for the process. It is also highly scalable, making it suitable for a wide range of applications, from small-scale treatment of brackish water to large-scale industrial operations. With its ability to operate with high salinity feed solutions, MDC is an effective solution for treating brackish or highly saline water sources, as well as wastewater and other contaminated water sources. Based on the current pilot plant, an efficient container plant design is currently discussed to purify industrial and municipal wastewater. Based on our ongoing research, MDC has the potential to become an important

technology for sustainable water management in Europe, helping to address the pressing issue of water scarcity and ensure that the region's water resources are used efficiently and effectively.

Methane is relevant for the chemical industry because it is the primary component of natural gas, which is a widely used feedstock for the production of a variety of chemicals and materials. One example of the importance of methane in the chemical industry is the production of methanol, which is an important intermediate chemical used in the manufacture of a variety of products such as plastics, adhesives, and fuels. In two research projects, we are focusing on the hydrodynamic influence to the methanation [5,6] and on the replacement of the catalyst by archaea, respectively. Methanation using archaea is a process that involves the **conversion of carbon dioxide** ( $\text{CO}_2$ ) and hydrogen ( $\text{H}_2$ ) into methane ( $\text{CH}_4$ ) using microorganisms called archaea.

**Archaea** are single-celled organisms that are similar to bacteria but have distinct genetic and **biochemical** properties. They are able to perform methanation reactions using  $\text{CO}_2$  and  $\text{H}_2$  as a source of energy. The use of bubbly flows in methanation processes can be beneficial because it provides a large interfacial area between the gas and liquid phases, which enhances mass transfer and reaction rates. Compared to a conventional stirred-tank reactor, a **bubbly flow** reactor with a high gas-liquid interfacial area results in a higher methane yield. By using archaea instead of catalyst, the process can be operated at lower pressure and temperature. Additionally, methanation can provide a means of storing excess renewable energy. By converting excess energy into hydrogen gas and subsequently into methane, the energy can be stored and used when needed. This can help to address the issue of intermittent energy supply from renewable sources such as wind and solar. Ground breaking research is required to scale-up the apparatuses from lab to pilot and industrial scale. A deep focus has to be made on the complex interactions of the bubbles with the archaea and the surrounding liquid and also applies to the conventional methanation using a catalyst to finally come to a cost efficient, competitive and stable operation.

Further industrial related projects tackle the recycling of polymers and the reduction of energy demands using heat pumps.

The IVT guides therefore highly relevant

processes from the lab towards the pilot scale. State-of-the-art as well as newly developed measurement and simulation techniques give further insights to the complex interactions and enable a derivation of a digital twin. The research is thereby not limited to the named three examples, but they highlight the complexity of process engineering and apparatus optimization and design.



## Impact

The **sustainable research** performed at IVT is expected to create a high scientific **impact** on the **society** and **chemical industry**, now, in the near future and by long term investigations. A better understanding of the fundamental principles behind the apparatuses will be gained bridging the scales from molecular investigations towards full scaled pilot plants.

The application of machine learning and AI will enhance the design procedure, ranging from new chemicals, new synthesis routes, towards **new apparatus designs**, as well as their combinations and integrations. **Smaller measurement sensors**, and better sensors to justify the multiphase flow will make a significant impact to the design and optimization of current and newly operated equipment. The use of computational fluid dynamics models for multiphase fluidic systems, optical measurement techniques, and the integration of digital twins into real systems helps to achieve reliable scale-up of chemical apparatuses, resulting in energy and resource-efficient apparatus designs for sustainable and efficient chemical production.

Recycling of black mass reduces the demand for raw materials and the environmental impact of battery production, while membrane distillation crystallization technology offers a more **energy-efficient** and **cost-effective** alternative to traditional desalination and crystallization processes, with potential to become an important technology for sustainable water management in Europe. Methanation can help reduce greenhouse gas emissions and store excess renewable energy, providing a solution for intermittent energy supply from renewable sources such as wind and solar.

By providing sustainable process engineering research at the forefront, we are not only providing a significant impact on the industry, but also provide the students and operator of tomorrow with the necessary **toolboxes** to enable an **energy** and **resource transition**.



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## Competencies

We have a long-term knowledge on chemical fluid process technology, ranging from solvent extraction, absorption and chemisorption towards membrane separations. The combination of the development of new measurement techniques, computational fluid dynamics and hydrodynamics investigations made it possible to develop digital twins also for complex systems. The frequent connection to **local** and **transnational industry partners** gives an impact to industry and academia and a frequent exchange of challenges and solutions for the industry and environment of today and tomorrow. The involvement in the **European Federation of Chemical Engineering** (group fluid separation), Prometia (international non-profit association promoting innovation in mineral processing and extractive metallurgy for mining and recycling of raw materials) as well as Dechema Wanted Technology enables a development of strategies for the future.

The Institute of Process Engineering is located at the campus of JKU and enables a perfect exchange between different institutes due to the **crossdisciplinarity** of the topics ranging from **measurement, simulation, chemistry, physics, informatics, law**, etc. Therefore, we operate in our labs and pilot plant hall (in total 750m<sup>2</sup>) TOC analyzer, ICP-OS, Osmometer, titration apparatus, Electronic noses (Aromascan, Airtsense), Viscosimeter, density meter and technical apparatuses such as Bubble columns of various dimensions, RO system 160 bar, Nanofiltration systems (0.5 to 1m<sup>2</sup>), different membrane test cells, Microfiltration / ultrafiltration systems from 1 to 20 m<sup>2</sup>, laboratory centrifuges plate separator, Centrifugal separator Filter press up to 3 m<sup>2</sup> surface, Extraction (mixer-settler, pulsed sieve tray column) up to 200 l extraction medium, DN 32 extraction column, DN 150 separator, absorption columns (packed glass column), distillation / rectification (packed glass column / packed column), Pump test system 20 kW. Besides that, a high-speed camera system with at least 4000 fps at full resolution is focusing on fast processes and helps to identify uncertainties in process design and operation. Furthermore, the system enables a characterization of flow fields (particle image velocimetry) and particle sizes in combination with optical probes.

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# Sustainable Production and Logistics

Sebastian Schlund

## Vision

The manufacturing sector in Europe still holds significant importance. Within the European Union's (EU) non-financial business economy, manufacturing industry accounts for around 29.7 per cent of the **gross value added** and 23.1 per cent of the **employment** (Eurostat 2021). For Austria, the number of employees in industry is even expected to increase over the upcoming five years (Patsch et al. 2021).

The future of manufacturing industry will be deeply influenced by the ongoing developments towards fundamentally improved impact on **sustainability** and further **digital transformation** of the industry. This so-called **twin transition** enforces innovation stakeholders across industry and academia towards the following two directions: i) to redirect value creation towards more circular processes and an entirely reduced ecological footprint and ii) to equip manufacturing systems with real-time capable sensor systems in order to optimize and to adapt to frequent changes and unpredictable conditions. Against this background manufacturing design, operations and improvement has to be rethought in order to become more resilient and more sustainable. Within the Center of Sustainable Production and Logistics at Fraunhofer Austria Research GmbH and the Research Area Industrial Engineering at TU Wien we strive for innovative solutions to transform today's industrial value chains towards resilience, sustainability and human-centeredness with the means of digitization, data science and innovative automation. The scope of our research covers **redesign and optimization of industrial value chains** with their respective systems and processes as well as **human-**

**centered innovation** such as **work system design** and **competence development**.

## Approach

Research at the Fraunhofer Austria Center of Sustainable Production and Logistics and the research area of Industrial Engineering and Human-Machine Systems at TU Wien contributes to the transformation in industry in multiple ways.

- **Context-adaptive and personalized Work Systems**
- **Human Activity Recognition and Natural User Interfaces**
- **Upcycling Economy**
- **Collaborative Logistics**
- **Positive Impact Production**
- **Self-organizing Systems in Manufacturing Planning and Operations**

At Fraunhofer Austria manufacturing innovation is culminating in four ongoing strategic 'lighthouse' topics. Within the topic **Upcycling Circularity**, materials and products are kept within circulations that keep as much of the initial value as possible. Shorter circles such as reuse (of the product or its modules), repair and remanufacture therefore are favoured to a reuse of the material or (in the simplest case) energetic recycling. In order to implement this approach, manufacturing technology innovations (e.g. modular design concepts of semi-finished products, repair and

transformation technologies) as well as process innovations (e.g. improved single-variety sorting systems, multi-criteria decision making) are needed.

**Collaborative Logistics** subsumes concepts to combine logistics streams in order to increase capacity utilisation and to decrease greenhouse gas (GHG) emissions. Therefore, synergies are exploited, in between freight and passenger transport, as well as within individual orders in scalable logistic relations. Furthermore, transport platforms that include sustainability-based decision criteria and standardized but flexible transport equipment as enabler of improved capacity utilization is designed, developed and implemented. Within **Positive Impact Production** combined approaches of factory planning, operations and energy management are researched with the objective to achieve an overall positive impact on the respective sustainability goals, mainly its ecological and human-centered dimensions while keeping industrial competitiveness. In order to achieve this goal, integrated considerations of ultraefficiency, adaptive work systems and synergetic energy consumption and production are considered. **Self-planning Production and Logistics Systems** refers to the inclusion of (semi-)automated cognitive tasks within domain-specific processes. Therefore we apply advanced approaches in design automation, natural language processing as well as in the use of large language models to industrial engineering tasks, mainly towards design and planning of manufacturing and logistics artefacts.

The Fraunhofer Austria Center of Sustainable Production and Logistics works closely together with the research area of Industrial Engineering at TU Wien. At the latter, fundamental topics within the context of **future human-machine interaction** are researched with an emphasis on the manufacturing sector.

**Human-machine systems** play an essential role within this transformation as they at the same time enable and operationalize manufacturing processes. Therefore, the vision of the research area of Industrial Engineering and the research group of Human-Machine Interaction at TU Wien is to shape future work for a competitive industry and a sustainable society. Regarding work system design we follow the objective to create attractive, adaptable and accessible work systems. The work builds on the overarching objective to improve productivity as well as working conditions whilst increasing the perceived level of control of the users in more automated environments.

**Adaptive work systems** are systems that, besides taking requirements of various age groups into account, also focus on the idea of personalization – from age appropriateness to other diversity parameters such as gender, cultural background, or experience. Various sensors, sensor fusion, and wireless data transmission enable the creation of digital twins as digital representations of objects and product-services. However, to this day, there is a lack of underlying standards for the development and deployment of context-aware systems, which is often attributed to a high diversity within domain-specific requirements.

**Attractiveness** within the context of work systems refers to interfaces, usage schemes, interaction and work organization that aligns on human preferences, behaviour and expectations. In order to do so, work system have to provide inherent sensor skills and knowledge about the dynamic status of the human collaboration partner. Furthermore, task assignment is aimed as to consider individual human preferences and interaction schemes as well as natural user interfaces.

**Accessibility** aims at the goal of democratic technology use in the sense as technical systems offer a non-discriminating access to the design, development and use of technology. We consider this concept as somehow indispensable as physical assistance systems such as cobots and exoskeletons are supposed to be used in very close interaction with people. Contrary, today's underlying paradigms still set high access barriers in terms of prior knowledge and experience and limit/restrict potential use cases.



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## **Competencies**

Together with a team of more than 100 researchers at TU Wien and Fraunhofer Austria I strive for the design and development of sustainable and competitive industrial value chains with a focus on human-centered manufacturing systems. Within that context we employ engineering methods as well as data science within interdisciplinary research of socio-technical systems. Recent projects span from European level like various EIT Manufacturing projects over national funding towards regional initiatives. Results have been published in within the manufacturing community (CIRP), IEEE as well as within ergonomics and human factors communities. Various demonstrators of industrial assistance systems, e.g. in the TU Wien Pilot Factory serve as prototypes for our research and evaluations. I am an active member of the industrial engineering and production technology community, for example acting president of the ÖWGP (Austrian Scientific Society of Production Technology), board member of the GfA, member of the IALF (International Association of Learning Factories), the WGMHI (Wissenschaftliche Gesellschaft für Montage, Handhabung und Industrierobotik) and the WGAB (Wissenschaftliche Gesellschaft für Arbeits- und Betriebsorganisation).



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# Sustainable Additive Manufacturing

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## Vision

In terms of resource efficiency and the use of sustainable starting materials, additive manufacturing (**AM**) is already a comparatively environmentally friendly process: (1) the possibility of producing components at short notice in amounts according to current demand prevents excessive stockpiles, (2) using AM reduces material waste, since only the required material is added during the manufacturing process during manufacturing the specific component, and (limited to polymer materials) (3) raw materials from sustainable sources are already being processed under comparatively mild conditions (e.g. low temperature). Examples are epoxides, polyamides and polylactic acid, each of which can be economically obtained from renewable raw materials.

However, light-based processes (stereolithography, DLP) in particular also offer great potential to be used as a sustainable manufacturing method in other areas, such as in the electronics industry and in the production of electrochemical storage devices, and to advance these fields of application in the direction of sustainability. In order to achieve higher performance of electronic components, their components (printed circuit boards, microchips, passive components, ...) have to be manufactured in an

increasingly complex and highly integrated approach. During recycling, this leads to complicated disassembly processes for the separation of the contained materials. Precious metals or rare earths in particular can therefore only be recovered at great expense and often end up in landfills. However, due to the limited availability of these material classes and the increasing global demand for resources, their complete recovery is inevitable in the long term.

- **Additive Manufacturing**
- **3D Printing**
- **Design for Disassembly**
- **Recycling**
- **Sustainability**

## Approach

### *Design for Disassembly (DfD)*

introduces a new concept in which 3D printing is meaningfully integrated into the manufacturing process of electrical components, making them easier to recycle. Components are to be designed in such a way that their individual components can be easily accessed, separated, and further processed. By combining and developing new 3D printing systems and materials, components with the smallest structures in the micrometre range can be produced and provided with targeted predetermined breaking points. The selectively imprinted

breaking points should not affect the mechanical properties of the component during normal service life and should only be activated by certain “triggers”. After the service life, the devices can be disassembled into their individual parts through this activation and the respective components can be separately reused or recycled. 3D printing offers the possibility of high feature resolution, the production of multi-material components as well as the potential for mass production of very small parts. All these advantages combined in one process open up numerous new possibilities in the design and production of electronic components.

## Impact

The concept of **DfD** in **AM** has been developed with the aim of integrating this approach into industrial production processes and moving them towards a circular economy. It represents a transformative approach to recycling and resource recovery from e-waste, but can also be applied to other sectors. By creating products that can be easily disassembled and using additive manufacturing technologies, the potential for recycling, sustainable consumption, and a greater motivation to repair components will be increased. With **AM** and embracing **DfD**, manufacturers can create products that are easy to dismantle and facilitating the extraction of valuable materials. Particularly precious metals and rare earth elements, which can be reused for future manufacturing processes.



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## Competencies

TU Wien is a leading institution in the field of lithography-based 3D printing, starting in 2001 with several completed and ongoing EU projects in this field. Based on this know-how, alumni of our research area (Polymers and Composites) have already founded 6 companies focused on additive manufacturing. A total number of more than 250 employees in these spin-offs indicates the economic relevance of this field. In particular, we have expertise in the field of polymer chemistry, materials science, mechanical engineering and application development. This enables us to tackle challenges along the complete process chain of lithography-based additive manufacturing. Starting with the synthesis of novel initiators and materials, through to printing on our in-house developed AM systems and finally testing the (thermo)mechanical behavior of printed samples. Thanks to a wide range of available analytical and testing equipment, ranging from tensile testing machines, DMA, fracture toughness, to imaging techniques (such as SEM), all relevant methodologies are accessible on site.



# Thermo-Chemical Processes for Decarbonization

Markus Lehner

## Vision

The achievement of climate targets outlined in the Paris Agreement to keep global warming well below 2 °C (preferably to 1.5 °C) is considered as major worldwide challenge of the upcoming decades. Furthermore, the so-called “European Climate Law” sets the goal to reduce emissions to net zero by 2050 and the aim to achieve negative emissions thereafter. In addition, an intermediate Union climate target is anchored which provides that a domestic reduction of net greenhouse gas (GHG) emissions by at least 55% compared to 1990 levels should be reached by 2030. Concurrently, there is increasing scientific evidence that the remaining time to achieve these goals and stabilize the climate is strongly limited and running out rapidly. Achieving these goals will require the interplay of many measures. Academic work analyzing sectoral climate policies in the G20 from 2000 to 2019 found that there are still **significant gaps in the setting of policies** in the various sectors. It was concluded that the climate change mitigation policies currently adopted are not sufficient to reduce emissions to the extent required to achieve the climate targets of the Paris Agreement. **Carbon Capture and Utilization (CCU)** and **Carbon Capture and Storage (CCS)** are seen more and more as inevitable essential components for achieving the climate targets.

Over the past years the research interest in CCU and CCS increased leading to a variety of known CO<sub>2</sub> capture, utilization and storage technologies at different technology readiness levels (TRLs). At the same time, the scenarios developed for the IPCC 6th assessment report found **CCS and CCU as necessary**

**technologies** in order to achieve the 1.5°C or the 2°C goal, respectively. In their special report regarding a limitation of global warming to 1.5 °C, the IPCC analyzed several different pathways, which result in a median of about 15 Gt of CO<sub>2</sub> being captured using CCU and CCS technologies in 2050. According to recent evaluations for the EU this would result in a median requirement for CO<sub>2</sub> capture by CCS of 230–430 Mt/yr in 2030 and 930–1200 Mt/yr in 2050, while the scale for CCU deployment could cover a wide range of 47–800 Mt/yr in 2050. Thus, global efforts must be taken to develop and implement sensible pathways that balance the environmental, geophysical, technical, economic and societal aspects, which have to be

- **Carbon Capture and Utilization**
- **Power-to-X**
- **Low Carbon Hydrogen**
- **Renewable Hydrocarbons**
- **Sector Coupling**

considered when new technologies are rolled out. Consequently, the European Commission reported the **deployment and testing of CCU and CCS** technologies during this decade as critical.

Both the decarbonisation in the energy sector as well as the transition to renewable carbon in the chemical and petrochemical industries have to be accelerated in the upcoming years. Various industries and products rely on **carbon as a feedstock** – up to now based on crude oil, coal (coke) and



natural gas to a great extent. Thus, for a sustainable, renewable circular economy, alternative carbon sources have to be found. Other industries, like cement or refractory production, are **hard-to-abate** since the main part of their CO<sub>2</sub> emissions originates from their mineral feedstock. CCU, either based on renewable sources or holding CO<sub>2</sub> in closed loops, is an option. Furthermore, the **decarbonization** of energy supply, industrial production as well as mobility and transport requires hydrogen with a reduced carbon footprint. A number of different processes can be used for its generation, but these are currently all limited either technologically or with regard to the required energy or raw material supply. Estimates assume that the cross-sectoral **demand for hydrogen** in the EU in 2050 will be around 2250 TWh. This corresponds to about a quarter of the projected total energy requirement of the EU in 2050. By using hydrogen, the EU's CO<sub>2</sub> emissions can be reduced by around 560 Mt per year. Today, hydrogen is mainly used in chemical and petrochemical processes as an important reaction partner. Currently, in the European Union the annual hydrogen consumption summarizes to 339 TWh, which corresponds to about 10 million tons per year. The largest amount of hydrogen is used by refineries during refinement of crude oil or the refinery intermediate products, including desulfurization ("hydrotreating") and in the conversion of higher molecular weight compounds into middle distillates ("hydrocracking"). In chemical processes hydrogen is mainly used in the Haber-Bosch process for ammonia production. Around 27 TWh or 0.8 million t of hydrogen is expended for the synthesis of methanol. All other areas of application, as in metallurgy, glass manufacture, semiconductor production or in the field of mobility, are currently still of secondary importance in terms of hydrogen consumption.

Additionally, hydrogen will be needed for the **chemical storage of surpluses from renewable electricity** production. Sector coupling, i.e. the interconnection between energy generation, industrial production, mobility, heat supply as well as the gas grid will play a vital role in the transformation to a sustainable circular economy and an industrial production which relies to a great extent on renewable energy sources. Both coupling technologies and chemical storage options, i.e. the **transformation of electrons in molecules**, are required which utilize existing infrastructure and thus enable a fast transformation. Beside electrification, **Power-to-X technologies** are a backbone of

future renewable energy supply and industrial production. Their further technological development as well as their systemic integration in existing industrial production, transport and heat supply are key for the necessary decarbonization and for achieving the climate goals set out by the European Union. **Thermo-chemical conversions** play an important role, in Power-to-X process chains, CCU technologies as well as in the production of hydrogen with a reduced carbon footprint.

## Approach

The methodical approach comprises a combination of experimental investigations, both in laboratory and bench to pilot scale facilities, simulations, both on process as well as reactor level, combined with techno-economic, and partially also socio-economic as well as legal analyses. A series of projects investigated the **in situ microbial methanation** of carbon dioxide and hydrogen in depleted natural gas reservoirs, known as Underground Sun Conversion (USC), and aimed to develop a process chain for its industrial utilization. The overall objective was a comprehensive assessment on technical, economic and legal aspects as well as greenhouse gas impacts to be concerned for establishing the USC technology concept. This is achieved by applying **multidisciplinary research approach** combining process simulation, techno-economic and greenhouse gas assessment as well as legal analysis which allow answering questions about technical, economic feasibility and greenhouse gas performance as well as on legal constraints related to large scale CCU using geo-methanation in depleted hydrocarbon reservoirs. CO<sub>2</sub> from industrial sources and renewable H<sub>2</sub> from a electrolyser are converted to geomethane in an underground gas storage and used in industry again to close the carbon cycle. Process simulations reveal that the conversion rates vary due to operation mode, and gas cleaning is necessary in any case to achieve natural gas grid compliant feed in quality. The **geomethane production costs** are found to be similar or even lower than the costs for synthetic methane from Above Ground Methanation (AGM). The GHG-assessment shows a significant saving compared to fossil natural gas and conventional power-to-gas applications. From a legal perspective the major challenge arises from a **regulative gap** of CCU in the ETS regime. Accordingly, a far-reaching exemption from the obligation to surrender certificates would be fraught with many legal and technical

problems and uncertainties. [1]

In industrial production still high amounts of non-renewable CO<sub>2</sub> is emitted. These emissions cannot easily be fully omitted in the short- and mid-term by electrification or switching to renewable energy carriers, as they either are of inevitable origin [2] (e.g., mineral carbon in cement production) or require a long-term transition of well-established process chains (e.g., metal ore reduction). CCU is an option to **reduce net CO<sub>2</sub> emissions**, and, in this context, the production of **synthetic natural gas** (SNG) through power-to-methane (PtM) process is expected to possess considerable value in future energy systems. Considering current low-temperature electrolysis technologies that exhibit electric efficiencies of 60–70%el,LHV, and methanation with a caloric efficiency of 82.5%LHV, the conventional PtM route is inefficient. However, overall efficiencies of >80%el, LHV could be achieved using co-electrolysis of steam and CO<sub>2</sub> in combination with thermal integration of waste heat from methanation. Such a **thermally integrated system** in the context of different application scenarios allows for the establishment of a closed carbon cycle. [3] Considering potential technological learning and scaling effects, a techno-economic assessment reveals that compared to decoupled low-temperature systems, synthetic natural gas generation cost of < 10 cents/kWh could be achieved. [4] Additional benefits arise from the direct utilization of the by-product oxygen. With the ability to integrate renewable electricity sources such as wind or solar power in addition to grid supply, the system can also provide **grid balancing services** while minimizing operational costs. Therefore, the implementation of highly-efficient power-to-gas systems for CCU applications is identified as a valuable option to reduce net carbon emissions for hard-to-abate sectors. However, for mid-term economic viability over fossils intensifying of regulatory measures (e.g., CO<sub>2</sub> prices) and the intense use of synergies is considered mandatory.

Flow sheet simulations of carbon capture and utilization (CCU) processes give insights in the effects of technological as well as process structure options. For a CCU process in which process-related carbon dioxide is converted with green hydrogen in a **Fischer Tropsch synthesis** to liquid hydrocarbons, the influence of hydrogen production technology, such as PEM and SOEC, thermo-chemical conversion technologies on plant specific efficiencies, product volumes, as well as investment, operating and net production costs have been investigated. [2] The **techno-economic assessment**

reveals that in this case the use of a SOEC and electrified reactors offers the technologically best and economically most optimized process chain.

The steel industry is one of the most important industry sectors, but also one of the largest greenhouse gas emitters. The process gases produced in an integrated steel plant (blast furnace and basic oxygen furnace gas, BFG and BOFG) are due to high shares of nitrogen in large part energy poor but also providing a potential carbon source for the **catalytic hydrogenation to methane** by integration of a power-to-methane (PtM) plant. Furthermore, by interconnecting a biomass gasification, an additional biogenic hydrogen source can be provided. A direct conversion of process gases results in high shares of nitrogen in the feed gas of the methanation. Laboratory experimental tests have shown that the methanation of BFG and BOFG is technically possible without prior separation of CO<sub>2</sub>. The methane-rich product gas can be utilized in the steel plant and **substitutes for natural gas**. For a mid-sized steel plant, the implementation of renewable energy sources results in a significant reduction of CO<sub>2</sub> emissions between 0.8 Mt CO<sub>2</sub>eq and 4.6 Mt CO<sub>2</sub>eq per year. [5] However, a significant limitation in terms of available electrolysis plant size, renewable electricity and biomass exist. In a techno-economic analysis of the system, three extreme value scenarios and three constrained scenarios were defined and evaluated. The biomass gasification plant, set to a maximum nominal power of 105 MWth, was the main limiting factor for the constrained scenarios. It was found that the main cost influencing factor throughout all six scenarios was the energy supply cost (electricity and biomass). [6] Several parameters are subject to **dynamic changes** during the standard production of steel, such as the available amount and composition of the accumulating process gases, the temperature and operating pressure as well as their periodicity. In addition, the available amount of hydrogen can vary depending on the available **fluctuating renewable energy** for the installed electrolyzer. Analysis of operating parameters and process routes in steel-making revealed that only one realistic application-based scenario exists which is based on high variations in the availability of hydrogen. In experiments performed with a three-stage methanation setup in lab-scale it was possible to achieve very stable product gas compositions, even with significant load changes in gas input power. [7] These investigations showed the opportunities, but also the remaining **challenges of decarbonizing** steel production with the implementation of

thermo-chemical processes into existing industrial infrastructure and driven by renewable energy.

Hydrogen is a key driver for reducing greenhouse gas emissions in a whole range of sectors (mobility, heat, industry). However, the basic prerequisite is that the hydrogen was produced with no or only a small CO<sub>2</sub> footprint. Beside other options, low carbon footprint hydrogen can be produced from fossil fuels by means of reforming or partial oxidation. A reduction in greenhouse gas emissions can be achieved by subsequent storage of the resulting CO<sub>2</sub> (CCS). The advantage here is clearly the potentially **fast scalability** of these processes for generating large amounts of hydrogen, since both the necessary fossil feedstock and the necessary technologies are available. However, the difficulty lies in the subsequent storage of the CO<sub>2</sub>, for which there are currently no real options, especially in Central Europe. **Methane pyrolysis** is an alternative process for generating hydrogen with a reduced CO<sub>2</sub> footprint in which methane or natural gas is cracked into hydrogen and solid carbon at temperatures between 800°C and 1200°C. The methane cracking can take place purely thermally or catalytically. Processes in moving bed

reactors, in fluidized beds, in **liquid metal baths** or molten salts and in various types of plasma reactors have been investigated on a laboratory scale. A significant advantage of this process is that the energy requirement for methane pyrolysis is around 80% lower than for water electrolysis. If this energy requirement is met in a renewable way, for example with renewable electricity, then the CO<sub>2</sub> footprint of methane pyrolysis is very small. In addition, the **solid carbon** can potentially be converted into various usage options, which can generate additional value. The main disadvantage is the low level of technical maturity achieved so far. In many methane pyrolysis processes, the scalability to larger scales and the long-term stability of the processes are not yet given. [8] At Montanuniversität Leoben, an interdisciplinary team is currently working intensively on the development of a methane pyrolysis process and the use of the solid carbon produced as a “by-product”.

## Impact

This research is expected to create scientific impact in understanding how Power-to-X and CCU process chains can be optimized in terms of their efficiency and of their key performance indicators. Furthermore, their beneficial implementation in and coupling with existing industrial production infrastructure is described and understood. Thus, this research enables the **integration of renewable energy into industrial production**, and consequently the reduction of GHG emissions in hard-to-abate or energy intensive industries, respectively. Furthermore, the fluctuating nature of renewable energy supply can be handled by **dynamic operation of thermo-chemical conversions**. The simulation of process chains as well as of reactor behavior enables the up-scaling of the systems to pilot and finally industrial scale while **minimizing the risks** of these new technologies. A series of projects are already transforming the laboratory systems to pilot and demonstration scale in real environments.

Thermo-chemical processes are a cornerstone of the development of a **sustainable green** society with significant positive impacts on economy, human health and nature. It contributes to European Union's goals of sustainability. The implementation of low carbon hydrogen fits perfectly to the **long-term transition strategy** of a low-carbon industrial production.

To reach **climate neutrality**, thermo-chemical processes and alternative production routes for low carbon hydrogen, like methane pyrolysis, in combination with CCU applications are required.



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## Competencies

The main targets of the research group Energy Process Engineering at the Chair of Process Technology and Industrial Environmental Protection are the integration of **renewable energy in industrial production**, the **utilization of CO<sub>2</sub>** as feedstock as well as the development of processes for **closing the materials cycle**. The working group deals with chemical-catalytic processes for the utilization of CO<sub>2</sub> as feedstock. The main focus is process development by experimental works and process simulation. A long-term emphasis is given to catalytic methanation, where both process concepts for load management as well as dynamic operation are developed. Furthermore, application scenarios for the implementation in industrial production and coupling with technologies for the production of renewable hydrogen are addressed. These works are complemented by catalytic reforming of CO<sub>2</sub> rich process gases from industrial processes. Additionally, the development of a process for **thermal cracking** of polyolefins embedded in a crude oil refinery is supported by kinetic modeling. Also, the mechanical treatment of post-consumer plastic containing waste streams for the derivation of a polyolefin rich feedstock for the thermal cracking process is investigated. The working group co-operates in all projects with industrial partners working in the fields of plant engineering, oil and gas processing, waste treatment as well as automotive industry. Many projects are based on the collaboration with national and international scientific working groups.

The Chair of Process Technology and Industrial Environmental Protection runs outstanding, state of the art laboratory equipment, experimental infrastructures as well as simulation tools. Laboratory plants in different scales are available, like a methanation plant consisting of three serial pressure reactors w/wo cooling, a reforming plant, analytics (infrared sensor, GC, REM-EDX, etc.) and various commercial as well as proprietary simulation tools (Aspen Plus®, Comsol Multphysics®, proprietary codes based on Matlab®).

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# Biotechnological Tools for Sustainable Production

Matthias Slatner, Martin Walpot

## Vision

Modern Biotechnology has very high potential to accelerate the transition to a circular economy. The Austrian Centre of Industrial Biotechnology (acib) has been working for more than 25 years in the development of sustainable production processes using the power of microbes and enzymes.

Since its foundation in 2010, acib, an NGO, has specialized in the development of innovative, eco-friendly and economic processes in the biotech-, chemical- and pharmaceutical industries. acib carries out research in all fields of industrial biotechnology. Its expertise covers 12 research areas from biocatalysis and recombinant protein production to modelling and engineering and bioprocessing. The non-profit organization with its headquarters in Graz has additional sites in Innsbruck, Tulln, Vienna (AUT) and abroad. The Centre is jointly owned by the University of Natural Resources and Life Sciences (Vienna), University of Technology (Graz), Universities of Innsbruck and Graz and Joanneum Research. Today, the combination of digitalization and life sciences leads to novel methods with increasing potential to enhance sustainable production. acib's vision is to close the gap between academia and industry by transforming recent results of biotech research into practical tools for the industrial production. Therefore, acib aligns its goals along the following key topics, such as the (i) Replacement of harsh chemicals by green chemistry, (ii) development of new sustainable materials and recycling routes, (iii) optimization of recombinant proteins and new production paths for next-generation biopharmaceuticals,

(introduction of biobased feedstock and novel food and feed products and (v) inter- and transdisciplinary approach to science communication and linking biotechnology with other science fields, e.g. art, architecture, culture etc.

By providing and using state of the art biotechnological tools, acib and its international network of universities and industrial partners paves the way to a circular economy and sustainable innovations that benefit us all.

- **Green Chemistry**
- **Fermentation**
- **Biopolymers**
- **Protein Engineering**
- **CO<sub>2</sub> Reduction**
- **Sustainability**

## Approach

Biotechnology is one of the oldest existing industrial techniques: The production process of beer has already been described 1.700BC in the "Codex Hammurabi" and by early medieval monastery monks in Europe. Since the introduction of steam by James Watt in 1765, industrialization of beer production, as well as from other foods and beverages started, leading to application of biotechnology in countless industrial processes today. Beside food production, biopharmaceutical processes, energy systems like bioethanol, aquatic systems using algae and many more examples are essential processes in modern life. acib also elaborates biotechnology applications for



sustainable production. The framework is to use microorganism and enzymes to replace harsh chemical processes by low-risk and greener, more sustainable biological steps.

The following examples and success stories give a short overview of acib's research activities.

## Impact

### (i) Replacement of harsh chemicals by green chemistry

For many chemical processes you need chemicals, which are harmful to both health of animals and humans and the environment. Their disposal and neutralization are complex and expensive. Therefore, the Austrian Centre of Industrial Biotechnology (acib) is working hard to make a variety of these processes more ecofriendly – by using enzymes. These catalyst from nature enable different reactions and can be used instead of chemical reactions. One of the most popular chemical transformation methods is the so-called Friedel-Crafts Acylation. This reaction method is applied to produce ketones, important intermediates for the production of pharmaceuticals such as Ibuprofen or Paracetamol, cosmetics, perfumes or acetophenone resins. The FCA performs a regioselective, which means targeted, coupling of acyl residues to aromatic compounds to produce a desired carbon bond (C-C). To achieve this, this reaction required a chemical catalyst such as toxic aluminum trichloride (AlCl<sub>3</sub>). Another drawback are the process parameters, because these chemicals only work in highly reactive environments, with high temperatures and with the aid of organic solvents – resulting in unwanted by-products which require complex and expensive neutralization and disposal.

The scientists of acib came across an enzyme extracted from strains of forest and meadow organisms that would trigger this reaction, adding an important piece to the enzyme toolbox of acib. This means, that C-C bonds can be achieved with natural means, without the use of toxic substances, enabling innovative possibilities for the construction of molecule structures. Once in industrial scale, the new method can help sun screens, cosmetics or flu drugs to soon be “organic”. The future will see both a diversification of available enzymes and the development of novel hybrid catalysts with new to-nature activities.

### (ii) Introduction of new, sustainable materials and recycling routes

Various research activities worldwide are dedicated to discovering solutions to fight global plastic pollution. acib is among the leading research institutes worldwide in the field of PET recycling using natural enzymes and introducing new biobased polymers. First, acib discovered the ability of bacteria and fungi, including *Fusarium solani*, to produce natural enzymes that can decompose PET. In a second step, the researchers asked themselves how this natural process could be translated into industrial applications in order to manage eventually to recycle polymers by natural means. But first, they had to find an answer the question, how a natural substance can decompose a synthetic material into its individual elements?

Soon after, a method was developed for the targeted adjustment of enzymes to the synthetic polymers that are to be decomposed. These polyesterases were able to work in a more stable and significantly more efficient manner. This means, that today the scientists are able to break down huge plastic molecules into their individual components within less than 24 hours. The process is gentle on the environment, takes place at 37° Celsius under

natural atmospheric pressure, in a neutral pH environment and water suspension, and without the need for toxic chemicals such as heavy metals. As well, the synthetic components in their pure form that result from enzyme recycling can be used to produce high-quality, new products such as functional clothing, PET bottles and even active substances for medication. Nearly 90 percent of the input material can be reused. Recent approaches in that area were done by using rumen based enzymes.

Other research activities undertaken by acib in this field focus on the enzymatic recycling of textile waste and waste of different source materials, the anaerobic decomposition of plastics in biogas plants or the production of biopolymers from regrowing sources, to name but a few. All of these are geared towards offering alternative options for petrol-based production of polymers.

### **(iii) Recombinant Proteins and new production paths for next-generation biopharmaceuticals**

#### **Virus-like Particles**

There are a multitude of challenges associated with the production of next-generation biopharmaceuticals and vaccines. acib together with international partners developed a production platform that promises faster, more economic and safer production of modern pharmaceuticals. Today, modern biopharmaceuticals are often based on the mass production of designer proteins, such as virus-like particles (VLP) for gene therapy or for the development of vaccines, to support the organism in producing antibodies against various pathogens. Imagine the immune system as a memory match player busily identifying the surfaces of any virus that appears and developing resistances as soon as it gets into contact with the virus. VLP make use of this principle: they imitate the surface of the virus and feign an infection without damaging the body, because the dangerous genetic material inside the virus envelope that is responsible for infection, has been removed. Since the surface proteins of VLP can be tailored to various applications, this technology is becoming ever more interesting for industry. However, the production of this specialized biomolecules calls for improved and above all, more robust production procedures. Vaccines have been mostly produced by means of seed viruses. These are living pathogens that multiply in cells from chicken eggs. Seed viruses are used, for example, to produce approved influenza vaccines. But these production vehicles as well as alternative platforms e.g. in production in cultured cell lines of eukaryotic organisms such as yeasts and insects, have the disadvantages of instability and limitation.

Therefore, acib and partners investigated a platform technology for the optimised production of diverse proteins. Using a sophisticated fermentation process, the genetically optimised insect cell line is stimulated to grow and produce protein in a bioreactor, before the scientists introduce the genetic information for the generation of designer proteins, which are purified from the insect cells after several days of production. As a new platform technology, the process entails great potential for the pharmaceutical industry and could in a few years enable new next-generation biopharmaceuticals – from gene therapies for neurodegenerative disorders such as Parkinson's or Alzheimer's, to cancer therapy and modern preventive vaccines against influenza, HIV, dengue or zika virus.

### **(iv) Biobased feedstock and novel food and feed products**

#### **Econutri**

Global CO<sub>2</sub>-emissions are rising continuously. At the same time, the world population is growing and with it the production of food. In particular, the demand for high-quality proteins will almost double by 2050. Alternative, sustainable sources for protein production

are therefore in high demand. The Austrian Centre of Industrial Biotechnology (acib) and the start-up Econutri are using a special microorganism called *Cupriavidus necator* to convert the harmful greenhouse gas CO<sub>2</sub> into high-quality protein. The process does not pollute the oceans or land areas and, as an alternative source of food and feed, thus prevents overfishing of the oceans and is a sustainable answer to factory farming, which is widely regarded as climate killer. A pilot plant is currently under construction. Planned large-scale plants, coupled to industrial facilities such as cement plants, have the potential to use CO<sub>2</sub> from exhaust gases to produce proteins for the animal feed industry but also human nutrition. Another application could be the production of environmentally friendly bioplastics.

### **Alternative Meat**

Another field, where acib is paving the way, is the development of Alternative meat. Products from alternative sources are getting more and more relevant, especially Alternative meat, since current crises and a growing population are causing a demand for meat to rise sharply worldwide.

Traditional meat production, especially factory farming, consumes too many of the increasingly scarce resources available, requires too much land and produces the same amount of greenhouse gases as the entire transport sector. Graz-based researchers from the Austrian Centre of Industrial Biotechnology (acib) and the Institute of Molecular Biotechnology at Graz University of Technology (TU Graz) are researching a new, more environmentally friendly meat alternative. Produced using biotechnological methods, this could be on supermarket shelves in the next few years. With a 95% reduction in space requirements, a tenfold reduction in CO<sub>2</sub> emissions and the avoidance of animal suffering, this new, alternative type of meat has above all climate-relevant and ethical advantages compared to traditional animal husbandry - and, last but not least, market potential worth billions: according to surveys, in 15 years 20 percent of the meat consumed worldwide will already come from environmentally friendly alternative production processes.

### **(v) Biotechnology meets art and history**

#### **Fermenting Futures**

Yeast plays a major role in our human evolution, shapes our historical understanding of the past as a bioarchaeological trace on cultural artefacts, and is one of the most important tools of modern biotechnology. Therefore, BOKU Vienna, acib and the renowned artists Anna Dumitriu and Alex May dedicated their own exhibition to yeast named „Fermenting Futures“. It combines bioart, digital technologies, sculpture and installations with the research field of biotechnology. To understand how yeast fermentation has evolved over millennia, the researchers reconstructed different species of yeast and recreated the evolution of yeast in the laboratory. The goal is to make yeast fit for industrial applications. This project tells the story of yeast from its beginnings to the present day from a cultural, aesthetic and historical perspective, but also highlighting its future potential - including the ability of a new biotech yeast to capture CO<sub>2</sub> from the atmosphere to produce bioplastics. The central artwork of „Fermenting Futures“ was 3D-printed from this plastic filament produced from CO<sub>2</sub>. The artwork thus simultaneously captures carbon and produces plastic from it. At first glance, then, it solves one problem while creating another. This paradox can inspire reflection on global warming caused by too much CO<sub>2</sub> in the atmosphere or large amounts of microplastics in our oceans. Since the plastic produced is biodegradable, the process in fact solves two problems at once.

Another part of the exhibition, the work, „The Bioarchaeology of Yeast,“

examines the traces left by yeast on artifacts of human culture. As the habitat of extremophilic fungi, also known as black yeasts, they are not something to be removed, but objects of aesthetic appreciation in their own right. To depict this interaction, the artists allowed black yeast colonies to form complex morphological structures in the laboratory for months. From their image, they created three-dimensional sculptures on which organisms left their colourful traces.

A significant part of the exhibition explores the relationship between fermentation for the production of bread and beer and human settlement. In an artificially created city of metaphorical architecture, a series of bread-crumbs encrusted architectural houses emerge, their rooms furnished and lit by tiny screens. The artists aim to inspire a sense of awe and curiosity about yeast biotechnology, and invite the public to interact with the works and reflect on our millennia-long, historical connection with yeast.



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## **Competencies**

### **Biocatalysis & chemical analytics**

This research field describes the use of biocatalysts for the conversion and synthesis of molecules and to replace common chemical processes by efficient and environmental-friendly approaches.

### **Enzyme technologies & protein engineering**

In this research field acib is dealing with new enzymatic conversions within synthetic approaches in order to close current gaps in enzymatic process applications.

### **Microbial biotechnology**

The research field includes the biotechnological utilization of microorganisms (bacteria, yeasts, fungi) and their compartments.

### **Cell line development & epigenetics**

The projects carried out in this area deal with a detailed, molecular understanding of the properties of production cells that are used for manufacturing biopharmaceutical products.

### **Bioinformatics & simulations**

Genes, RNA, proteins, and metabolites are the key players in biological systems. The sum of these parts is less than the whole because these actors never act alone, but are integrated into complex and multi-layered networks. The decoding of these networks and their structures as well as the interactions between them is therefore essential for an understanding of biological processes.

### **Bioprocess technologies**

The research area Bioprocess Technologies deals with the development of improved or new biotechnological processes, control, and regulation algorithms.

### **Bioeconomy & environmental biotechnology**

Optimizing recycling and recycling processes has been one of acib's key issues for a long time. Only a small part of all plastic waste is recycled; Huge amounts end up in the environment, where they are degraded very slowly. The aim is to optimize these processes to create a natural recycling process in the long term.

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# Electrochemical Component Production

Viktor Hacker, Merit Bodner

## Vision

The implementation of **sustainable production for new technologies** is the logical next step in the context of the upcoming transformation process towards CO<sub>2</sub>-neutral manufacturing. In particular, this involves the use of innovative processes for the continuous mass production of innovative energy technologies. The **Institute of Chemical Engineering and Environmental Technology (CEET)** is working on manufacturing processes for fuel cells and electrolyzers. These technologies serve as source of energy or energy carrier, respectively to fuel the transport sector, such as cars, trucks, buses, ships and aircraft, but also in stationary applications, e.g. for seasonal energy balancing. The sustainable production of **electrochemical components** requires research into very thin layers applied with innovative coating processes to produce large quantities of the thin-film components. Currently, reducing system costs and increasing lifetime and efficiency are crucial for economic competitiveness compared to conventional thermal engines. **The membrane electrode assemblies (MEAs)** of the electrochemical energy converters are the most expensive component of the repeating unit in the cell stack and account for 50-70% of the costs [1].

The reproducibility of the production and the guaranteed lifetime and performance are important parameters for commercialisation and possible applications. The currently achievable operating times are already quoted as tens of thousands of hours [2]. In order to **reduce investment costs** per service hour and reach the cost level of conventional energy converters (e.g. combustion engines), the service life must be further increased [2].

The power requirements in the stationary range are at least 1 W/cm<sup>2</sup> at operating cell voltages of  $\geq 0.65$  V [3]. In ongoing research projects at the CEET, commercial MEAs are purchased from established manufacturers and characterised. The costs for small purchase quantities are around 6,000 EUR/kW. This price is set as an initial threshold for small-scale production and must then be significantly undercut for larger volumes. Figure 1 shows a target price for MEAs of 87 EUR/kW for a purchase volume of 1,000 pieces, i.e. about 5,000 m<sup>2</sup> (1 piece = 5 m<sup>2</sup>). The extrapolated course

- **Fuel Cells**
- **Electrolyzers**
- **Membrane Electrode assembly (MEA)**
- **Catalyst**
- **Coating**

of the curve shows on the one hand the prices for the production of small quantities (more than seventy times as expensive) and on the other hand the potential cost reduction through mass production rates above 500,000 units to approx. 12 EUR/kW, through optimized production steps and fully automation [1]. At the same time, production processes for these technologies must adhere to the same requirements for green and sustainable production as any other manufacturing process.

This vision of **sustainable production of future technologies** includes research into fuel cell components that (i) meet the requirements of low prices at high volumes, while (ii) achieving high power densities and long lifetimes and (iii)



minimising resource consumption, waste production, emissions and energy waste in the spirit of the circular economy by slowing down, reducing and closing energy and material cycles.

## Approach

The challenge in electrode production is the manufacture of catalyst layers with **precisely defined porosity** for the necessary mass transport for cells with high current densities. The methods of catalyst ink composition (catalyst powder, ionomer and solvent) and electrode deposition must be optimised to such an extent that the agglomeration of platinum particles in the solution is prevented and a sufficiently high catalytically active surface is achieved. In **electrode fabrication**, it is also important that the ionomer is evenly distributed so that some catalyst particles are not completely covered with ionomer,

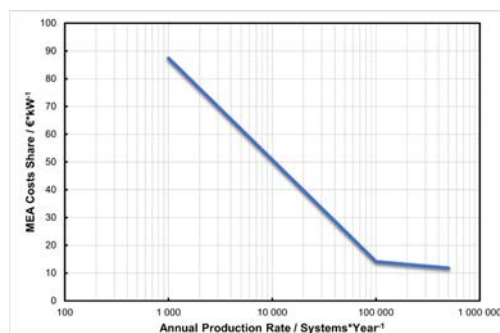


Fig. 1. MEA cost development with increasing production rate [1]

blocking the mass transport of reactants to the catalyst particle, while other particles are not in contact with the ionomer at all and supply the catalyst with protons during operation [1]. These challenges can be addressed by an optimal electrode fabrication method.

Of the numerous electrode fabrication methods [1], most use **catalyst ink-based methods** such as spraying or printing [1,4,5]. In these methods, the ink is applied either to the gas diffusion layer to form gas diffusion electrodes (GDEs), or to the membrane to make catalyst coated membranes (CCMs). Other methods include sputtering, atomic layer deposition, electrochemical deposition, dual ion beam assisted deposition or electrospinning. Each method is, however, distinctly different and has individual advantages and disadvantages [1].

**Ultrasonic spray coating** is an improved form of the conventional hand-spray technique, where an ultrasonic nozzle is built into the spray gun that is mounted on a three-axle motor (see Figure 2) [1,4,5]. This achieves a higher dispersion of the catalyst particles in the ink and both CCMs and GDEs can be produced reliably and reproducibly using this method. Since only small amounts of solvent reach the substrate during coating, it is possible to coat directly onto thin membranes.

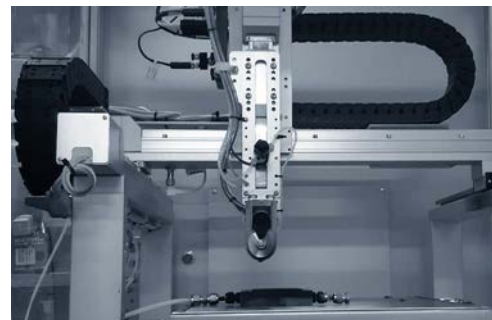


Fig. 2. Ultrasonic spray coating machine at the CEET institute of TU Graz

## Slot die coating

Slot die coating is a thin film process used to produce catalyst layers and electrolyte membranes. In this process, a substrate is moved under a slot die through which a liquid such as catalyst ink or ionomer is pumped. In this way, a thin film is applied to the substrate, the properties of which can be controlled by the flow rate, lateral movement and distance between the substrate and the slot nozzle. The viscosity of the ink can be adjusted and is crucial for the quality of the layers produced [1,6]. Slot die coating can be integrated into the roll-to-roll coating process once the lab-scale manufacturing process has been developed and optimised [1]. It is considered the most promising method for large-scale MEA fabrication. A picture of the slot-die coating line is shown in Figure 3.

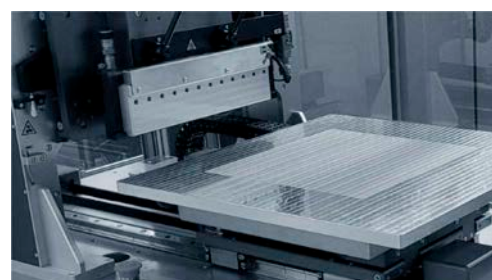


Fig. 3. Slot die coating machine at the CEET institute of TU Graz

## Electrospinning

Electrospinning proven to be a fuel cell fabrication technique that can produce electrodes with large surface area and porosity and membranes with high ion conductivity, resulting in excellent performance (Figure 4). In this process, a high voltage is applied to a polymer solution (or melt), creating a charged liquid jet that is rapidly stretched and solidified into a fibrous structure. During this process, the solvent evaporates leaving behind a fine, continuous fibre. These fibres are typically nanoscale in diameter and can be tailored to specific compositions and morphologies [1,7]. Various materials such as conductive carbon, electrocatalysts and ion-conducting polymers (e.g. Nafion™) can be spun into individual fibres, which are then joined together to form a fibre mesh. This method can be used to produce single and multilayer electrode configurations. The morphology of the fibres can be controlled by adjusting solution properties such as viscosity and surface tension, and by varying processing parameters such as electric field strength, solution flow rate and collector spacing [1,7].

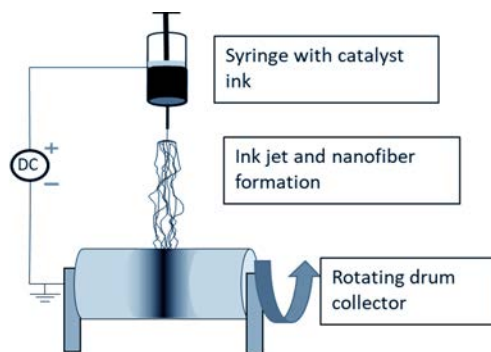


Fig. 4. Schematic depiction of the electrospinning setup.

The biggest advantage of electrospinning is the large surface area of the electrodes, which leads to effective use of the expensive electrocatalyst and thus reduces manufacturing costs. Another important advantage of electrospinning for the production of fuel cell electrodes is that the morphology and composition of the fibres can be precisely controlled. This means that the properties of the resulting electrode material can be tailored to specific performance requirements. For example, the surface area, pore size and porosity of the fibres can be adjusted to optimise fuel cell performance. Finally, electrospinning can be combined with other manufacturing processes such as roll-to-roll processing to produce continuous electrodes [1]. Overall, the use of electrospinning for the

production of fuel cell electrodes is a promising area of research that has the potential to significantly improve the performance and durability of fuel cell systems in the future and, with continued innovation and development, pave the way for a more sustainable and energy-efficient future [1].

## Impact

Driver of the **Green Transition** is urgent need to move towards carbon neutral energy technologies and facilitated by the European Commission's Hydrogen Strategy and the REPowerEU Plan. These have established a framework to promote renewable energy and **green hydrogen** in order to decarbonise the EU and reduce its dependence on imported fossil fuels. The expected cumulative investment in green hydrogen in Europe alone is estimated to be up to EUR 470 billion by 2050, encompassing the future technologies for prosperity including **smart materials manufacturing** and hydrogen production and conversion. Strong and subsidised competition from Asia and North America, combined with high energy prices lead to the risk of deindustrialisation in Europe. Disruptive research into new manufacturing processes for green technologies, securing know-how and regional production of electrochemical components are crucial for maintaining industry and prosperity.

The special features of **electrochemical energy conversion** include low operating temperatures, high power density and easy scalability, making it ideal as a replacement for internal combustion engines in motor vehicles and for stationary applications. Hydrogen-powered vehicles combine the advantages of fossil fuel vehicles and vehicles powered by batteries. They emit only pure water vapour. They achieve long ranges and can be refuelled quickly. The efficiency of fuel cell vehicles (FCEVs) is twice that of diesel combustion engines. The production of electrochemical components has implications for the **transport sector and for stationary systems**. Fuel cell electric vehicle fleets are already in use in the transport sector and new applications such as for the heavy duty and the maritime sector are explored. Decentralised low-temperature fuel cell systems are primarily targeted at small power demand (50-250 kW for decentralised use and <10 kW for households). Emergency power solutions for data centres, banks, hospitals and telecommunication companies have recently gained importance. For portable devices, fuel cells can provide power for laptops, chargers, portable electrical devices and military radio/communication equipment.

**SDG 7**, access to affordable, reliable and sustainable energy aims to significantly increase the share of renewable energy in the global energy mix. Fuel cells can be usefully applied in trucks, buses, trains, ships and aircraft. Establishing new processes in Austria is a step towards **SDG 9**, which aims to build a high-quality and sustainable infrastructure and enable the implementation of parts of the value chain in the hydrogen industry. MEAs still require platinum as a catalyst for their production. The increase of the utilisation of this metal in fuel cells is in line with **SDG 12**, which focuses on sustainable consumption and production.



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## Competencies

**Prof. Viktor Hacker** is head of the Institute of Chemical Engineering and Environmental Technology (CEET) and of the Working Group for Fuel Cells and Hydrogen Technology. Together with **Ass.Prof. Merit Bodner**, he is supervising 15 PhD students working in the research fields of fuel cells and electrolysis and hydrogen production. He was appointed professor for hydrogen technologies, has habilitated on electrochemical energy technologies, has more than 20 years of experience in coordinating international research projects and is heading the Center of Hydrogen Research of TU Graz. He received the 2017 State Prize (bmvit) for the H2 Mobility project as well as the Houska Audience Award and Recognition Award for successfully implemented industry-related research projects, is co-author of more than 100 peer-reviewed articles [8] in journals and books in the field of hydrogen and fuel cell research (2021-2023 published [1,4,16,5,9-15]) and regularly organizes international events, summer schools and workshops.

At CEET, a vastly equipped **laboratory infrastructure** for physical, chemical and electrochemical analysis is available for catalyst research and the characterization of gas diffusion electrodes. An ultrasonic spray coating system, a slot-die coating system and an electrospinner are accessible for the production of active layers for fuel cells and electrolyzers. A laboratory for the installation of a coat&roll multipurpose unit is being planned. **Catalytic layers** can be characterized ex situ by Hg porosometry, light and scanning electron microscopy including EDX, IR-thermography and FT-IR as well as UV-Vis spectroscopy. **Fuel cell measurements** in single cells up to short stacks can be performed in fully automated test rigs. The Fuel Cells and Hydrogen Technology working group has been researching the production and characterisation of low temperature fuel cells, redox flow batteries, electrolyzers and hydrogen production by chemical looping for over twenty years. The institute has vast experience with the transition from **basic chemical research to industrial processes**. International cooperations such as the recent joint PhD project with TU Darmstadt as part of the university network for innovation, technology and engineering "Unite!" further promote this expertise.

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# Bioresources, Buildings and Products for the Circular Economy

Alexander Petutschnigg

## Vision

The Campus Kuchl of the University of Applied Sciences Salzburg is dedicated to the ideas of Green Engineering and Circular Design. The development of Green Technologies and Processes as well as the ideas of circular usage of resources are seen as main factors to overcome the issues of uncontrolled climatic gas emissions and exhaustion of limited planetary resources. Therefore mainly the following Sustainable Development Goals of the Department of Economic and Social Affairs of the United Nations are addressed:

9. Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation

11. Make cities and human settlements inclusive, safe, resilient and sustainable

12. Ensure sustainable consumption and production patterns

The change of existing production-, building- and product design will only change if the people dealing with these tasks will be able to do these changes. For these reasons another main issue to be addressed is the concept for the academic and professional education of recent and future employees and entrepreneurs. The vision is to establish

an educational concept for experts in the field of Green Engineering and Circular Design in the different levels of qualifications and expertise on our campus.

## Approach

We aim at the development, engineering and the design of products, processes and buildings. The research is based on contents of the study programs, and the structure is shown in table 1.

The educational concept is shown in Figure 1 based on the strategic collaboration of the so called "Wissenscampus Kuchl". The campus offers professional education ("Lehre" and "Meisterausbildung") as well as secondary teaching institutions ("Fachschule" and "Höhere Technische Lehranstalt") as well as academic education ("Fachhochschule").

- Green Engineering
- Circular Design
- Circular Economy
- Smart Building
- Smart City

Study programs	Development, Engineering and Design of:		
	Product	Processes	Buildings
Design- and Product Management			
Forest Products Technology and Timber Construction			Y
Smart Building/ Smart Cities			

Table 1: Sketch of Research Topics per Study Program



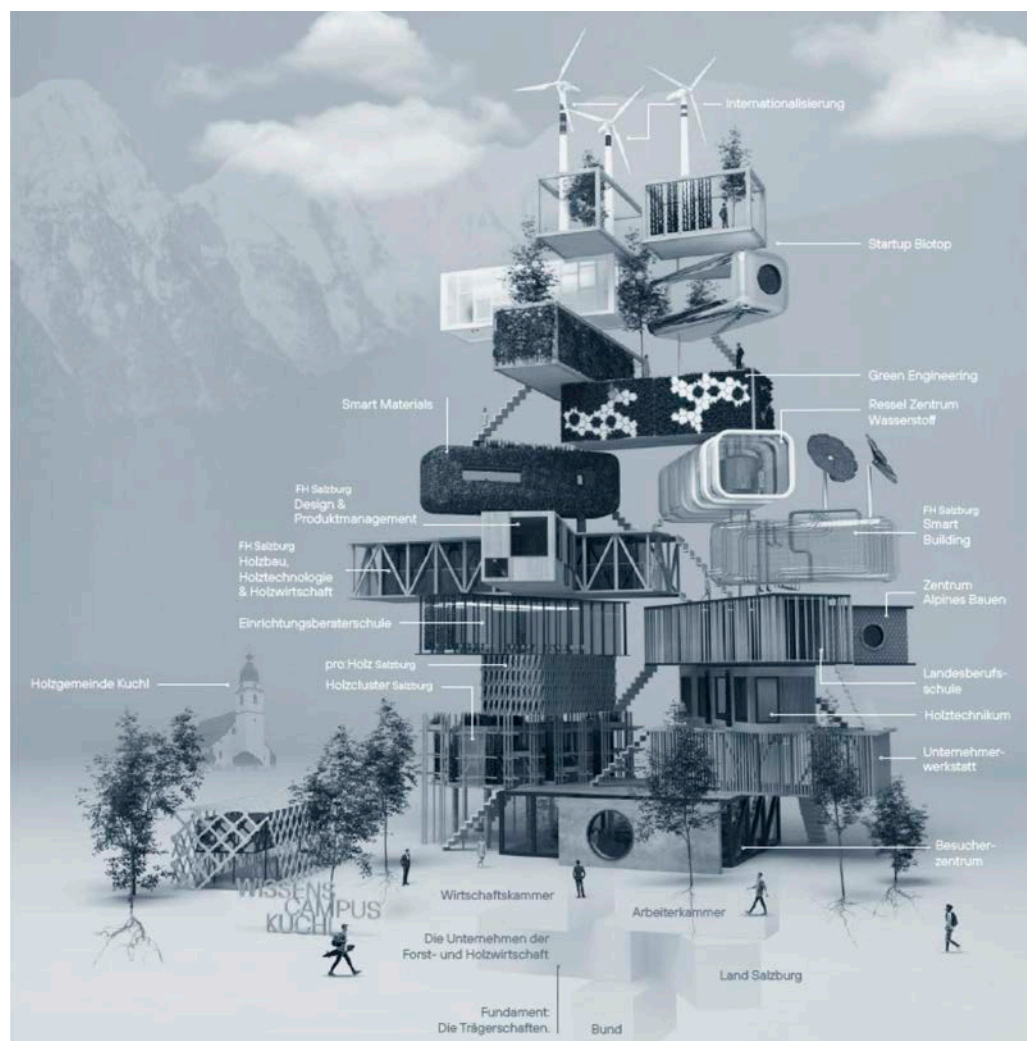


Fig. 1. Sketch of the "Wissenscampus Kuchl" concept

In figure 1 it can be seen that the students and scholars which are affiliated to one educational institution of the campus, should be able to

develop within the educational system and can decide if, when and where they would choose to develop into a higher level in education.

## Impact

The impact can be seen in following directions:

### 1. Employees and Decision makers

The campus delivers experts in the different levels of education and with different specializations. This satisfies the need of a competitive and future oriented economy to ensure the transition of the existing structures into a more sustainable direction.

### 2. Transfer of research into companies

The campus enables companies to participate in the recent developments of production processes, material science and building technologies to improve their daily tasks as well as their competitiveness and their future potentials.

### 3. Research

The campus is taking part in international research collaborations and is performing different research projects especially in the field of renewable resources and their processing, the development of building structures and the integration of technological equipment and technological sub-structures in buildings.



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# Sustainable Biocatalytic Production

Robert Kourist, Hanna C. Grimm

## Vision

In 2022, up to 80 % of the energy and material consumption in the world is provided by fossil resources.[1] At the same time the earth overshoot day moves forward every year and the development of sustainable alternatives becomes increasingly urgent. **Biocatalysis** uses natural catalysts such as **enzymes** to produce bulk and fine chemicals with clear environmental benefits. Currently, in light of the ongoing climate crisis, biocatalysis is expected to develop more environmentally friendly, “green” processes; indeed in 2009, Anastas and Eghbali postulated twelve principles to reach this aim.[2] These include goals such as reducing waste, using safer chemicals and synthesis routes as well as achieving high atom efficiencies. Here, enzymes meet the modern requirement for sustainable catalysts: They are biodegradable, operate under mild reaction conditions and their application is generally associated with low waste formation and the use of less toxic reactants. Finally, enzymes exhibit superb regio-, stereo- and chemoselectivity [3,4] which increases yields and simplifies the production of chiral compounds as well as downstreaming processes. Due to these reasons, enzymes are expected to make a major contribution to achieving the EU’s objectives for reducing CO<sub>2</sub> emissions and creating a circular economy. In 2020, the total global enzyme market size reached a volume of about 117 kilotons and is expected to grow approximately to 6.4% between 2021 and 2026.[5]

Obstacles on the way to the industrial implementation of biocatalytic reactions start with identifying an optimal enzyme.[6] Furthermore, enzymes are rarely ready-to-use but

need to be adapted to meet process requirements. Typical factors such as (i) a low stability of the enzyme, (ii) cofactor dependencies, (iii) a lack of promiscuity for unnatural, industrially relevant substrates and (iv) divergent reaction conditions in multistep synthetic pathways hinder their use for the desired process. We envision (i) to **establish novel biocatalytic reactions** with industrial relevance and (ii) to overcome bottlenecks by **enzyme engineering - the systematic optimization of enzymes**.

Existing chemical routes are complex and require numerous chemical transformations under very different reaction conditions. The isolation and purification of reaction intermediates is cost and energy intensive and results in the accumulation of toxic waste.[7] In contrast, most enzymes

- **Biocatalysis**
- **Renewable Resources**
- **Directed Evolution**
- **Machine Learning based Enzyme Engineering**

can operate in water, which allows their assembly to environmentally friendly one pot multistep syntheses. From an environmental point of view, **multi-enzyme and chemoenzymatic cascade reactions** represent a very promising approach, mainly due to the avoidance of intermediate extraction and purification steps, resulting in a significant reduction of both waste and production costs on industrial scale. There are, however, some technological and scientific challenges to be overcome en route to industrial

scale implementation of cascades. Here, enzyme engineering allows the creation of **tailor-made enzyme variants** with optimal catalytic properties for cascade reactions. In addition, future biotechnological production must be truly renewable. A highly promising approach is the use of CO<sub>2</sub>-fixing production systems such as cyanobacteria and hydrogen-oxidizing bacteria as catalysts. Cofactor dependence, especially for NAD(P)H, is an intrinsic limitation for the industrial application of many oxidoreductases since stoichiometric addition is economically not feasible. The solution is a cofactor regeneration system which recycles the required cofactor. Conventionally, applied cofactor recycling systems often rely on sacrificial cosubstrates as electron donors such as isopropanol or glucose which is accompanied with the formation of by-products and a low atom efficiency. While cyanobacteria are **photoautotrophic** and require light, carbon dioxide and water for growth, **chemolithoautotrophic** *C. necator* can utilize waste streams containing oxygen, hydrogen and carbon dioxide. Both organisms can regenerate cofactors such as NAD(P)H which can be redirected towards a recombinant reaction. Thus, the autotrophic metabolism can be used as an **atom-efficient cofactor recycling system**. Since the low liquid-gas transfer hinders the use of molecular oxygen as oxidant, the in vivo production of oxygen in cyanobacteria poses another benefit. We were able to show these biotechnological potentials of both organisms.[8–10] Our main goals are (i) the characterization and the establishment of gene regulatory elements to improve the production of recombinant enzymes, (ii) the improvement of electron shuttling towards our recombinant reactions and (iii) the design of suitable reactors for the upscaling of existing reactions.

In summary, enzymes constitute sustainable catalysts with manifold areas of applications. With their selectivity and their environmentally friendly, inexpensive production and operation conditions they might outcompete chemical catalysts. On the other hand, limitations such as stability, the required optimization time, the lacking promiscuity for unnatural, industrially relevant substrates and divergent reaction conditions in multistep synthetic pathways are challenges on the way to industrial applications. These problems are constantly being addressed and solved by rapidly advancing research in biocatalysis.

## Approach

**Enzyme engineering** and **directed enzyme evolution** have provided highly improved biocatalysts for sustainable production. Achievements in biocatalysis and new methods were immensely influenced by developments in computer modelling and bioinformatics.[11] Specifically, next generation DNA sequencing (NGS) drastically reduced the price for genome and metagenome sequencing and fueled DNA sequence data bases. Homology search and multiple sequence alignments enabled (i) the identification of new biocatalysts [6], (ii) sequenced-based prediction of enzymatic activity, (iii) the identification of enzymes with similar activities and of consensus sequences, (iv) the determination of the degree of relationship between enzymes and enzyme families and (v) the reconstruction of ancestral biocatalysts in order to increase the operational stability.[12] Furthermore, the ability to synthesize DNA inexpensively revolutionized cloning: tedious gene isolations were replaced and genes could be codon-optimized for more efficient transcription in host organisms. Regulatory elements for gene expression could be introduced more conveniently and synthesis of segments of chromosomal DNA facilitated the engineering of metabolic pathways.

Today, the creation of high-quality DNA libraries is standard practice. At the protein-level, the RCSB protein data base (rcsb.org) provides information on protein structures with over 200,000 entries and structural alignments of related proteins deepened the understanding of sequence-function relationships and facilitated rational protein design. To the same time, experimental routes can be shortened due to the enormous technical progress. For example, programs like AlphaFold developed by DeepMind can predict three dimensional structures from amino acid sequences with steadily increasing preciseness.[13] Via computer modelling, interactions between enzymes and molecules can be calculated to reveal potential amino acid residues involved in catalysis, selectivity or with structural function.[4] These can be selected for mutagenesis, and the derived enzyme variants are screened for altered properties. A striking example is the rational design of biocatalysts for the synthesis of enantiomerically pure pharmaceutical molecules. [3] We believe that computer-aided enzyme engineering has just begun

to revolutionize biocatalysis and will in future immensely accelerate the time required to optimize an enzyme to meet the process requirements.

The application of biocatalysts encompasses highly selective transformations [4], cascade reactions and new reactions concepts such as photobiocatalysis. We demonstrated the coupling of oleate hydratases and fatty acid decarboxylases to a **multi-enzyme cascade reaction** for the synthesis of optically pure long-chain secondary alcohols that would be very difficult to obtain with other methods.

[14] **Chemoenzymatic cascades**

combine the unique selectivity of enzymes with the versatility of chemical catalysts. Here, required reaction conditions for both types of catalysts need to be considered.

By compartmentalization, we could combine two mutually incompatible catalysts and develop a new method to produce highly valuable biobased antioxidants.[7]

The field of **photobiocatalysis** uses light as energy source for biochemical transformations. The Kourist group has pioneered the use of genetically modified cyanobacteria as selective catalysts.[15] Cyanobacteria produce themselves with light as energy source and atmospheric carbon dioxide as sole carbon source. By oxygenic photosynthesis, the cyanobacterial hosts can regenerate the redox cofactor NADPH in an atom efficient way for a biochemical redox transformation. Recently, we were able to boost the electron supply for our model reactions by deactivating a competing electron sink.[9,10] Due to the novelty of the field, suitable photobioreactors need to be developed to reach industrial relevant product titers. Examples such as a bubble column reactor with internal illumination fueled by induction [16] and continuous flow photobioreactors [17] demonstrate how the volumetric productivity of photobiocatalytic reactions can be greatly increased.



## Impact

Fossil fuel depletion, climate change and the energy crisis are increasing the demand for sustainable production concepts from renewable resources. According to the European Chemical Industry Council, the production of chemicals from bio-based feedstocks will double by 2050 compared to 2018 [18] and with this research, we contribute significantly to the development of **new enzymatic synthesis routes**. Our work holds **great economic and environmental potential**.

In contrast to the scarcity and the fluctuating prizes associated with metal catalysts, the costs to produce enzymes are predictable and stable. In addition, labor and costs can be saved when carrying out enzymatic reactions. First, harsh reaction conditions such as high pressure, high temperatures or the use of organic solvents are reduced, which saves costs for energy and waste disposal. In addition, harsh reaction conditions are associated with increased occupational safety and health risks that can now be circumvented. Second, chemical pathways can be shortened by using enzymes, saving time and money.[3] By combining enzymatic reactions in multi-enzymatic or chemoenzymatic cascade reactions, intermediate purification steps are even further reduced. The environment benefits from the reduced amount of toxic reaction components such as organic solvents, the reduced waste, and the biodegradable nature of enzymes. Our approach of using **CO<sub>2</sub>-based catalysts** further reduces the environmental impact. Producing chemicals from a greenhouse gas and a renewable energy source such as light or hydrogen holds great potential as a **key technology** in the chemical and pharmaceutical industries. Currently, implementation of these reactions is hampered by a lack of scalability. We are convinced that our research will have a significant impact on the development of suitable production strains and bioreactors.

The optimization of biocatalytic reaction to meet our goals occurs by combining strain-, enzyme- and process engineering. For this, the fast-developing research field of biotechnology constantly provides novel tools to increase speed, precision, and success of the optimization strategy. Our work is part of this process and paves a way for sustainable reactions in future.



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## Competencies

Research at the Institute of Molecular Biotechnology (IMBT) on biocatalysis and enzyme engineering is well integrated in international EU funded research projects in Horizon 2020 and Horizon Europe. Recent research has been done in **Biocatalysis** (coordination of Horizon 2020 MSCA-EID BIOCASCADES, Horizon 2020 MSCA-EID INTERFACES), **Enzyme Engineering** (Horizon Europe MSCA-DN projects BiocatCodeExpander, DECADES, FWF doc.funds CATALOX, FWF project Active Site Design, FFG Project XR Scanning, FFG COMET at the Austrian Centre of Industrial Biotechnology) and **Photobiocatalysis** (Horizon 2020 FET Open FUTUROLEAF, coordination of Horizon 2020 MSCA-EJD project PhotoBioCat, FWF projects Cyanobacterial Oxyfunctionalization, Cyanobiotrans) and **Biotechnological Hydrogen Utilization** (Horizon 2020 MSCA-EJD CONCO2RDE, FWF project A cellular biosensor for hydrogen). Translational research cooperation with industrial partners focuses on sustainable biocatalysis (Bayer AG, Henkel AG, various European SMEs), with strong focus on the optimization of enzymes and whole-cell biocatalysts for sustainable and cost-efficient production of biobased chemicals, including biologically active molecules and high-performance adhesives.

The IMBT and the Austrian Centre of Industrial Biotechnology (acib) offer outstanding laboratory facilities for molecular biology (cultivation from 50  $\mu$ L - 20 L), genetical engineering, protein chemistry (protein purification, MST), analytics (GC, GC/MS, HPLC, LC-MS), directed enzyme evolution (semi-automated screening pipeline) and photobiocatalysis (algae engineering and cultivation, photobioreactors from 1 mL - 1 L).

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# Value Contribution through Human-centric, Circular and Resilient Production

Gerald Reiner

## Vision

From a socio-economic and technical perspective, it is expected that the digital transformation will disrupt the production of the future as well as the entire “**value chain**”. Of particular interest are new industrial technologies of digitalization, such as the Internet of Things, Big Data such as Internet of Things, Big Data, Cyber Physical Systems, Blockchain Technologies and the associated related new production technologies, such as additive manufacturing (3D printing, etc.). The digitization and integration of the entire value chain related to Industry 4.0 follows a merging of the virtual and physical worlds to ensure sustainability, energy and resource efficiency, as well as increased productivity and innovation (www.semi40.eu). In this context, the OECD has introduced the term “**Next Production Revolution**” to describe the potential of these new developments on production and service systems (doi: 10.1787/9789264271036-en). However, the exploitation potential requires comprehensive knowledge of the underlying business processes and workflows. This assessment is supported by an OECD study from 2017. According to this study, **relative productivity gains** (labor productivity) have been reduced since the early 1990s (doi: 10.1787/888933367500). It is therefore necessary to develop new business models (value proposition, value creation and value capture) that are also capable of **exploiting the benefits of digital transformation** both internally as well as along the value chain.

Digital transformation requires a rethink and a **change in the mindset** that determines **how products and services are produced**, distributed and delivered, sold and used [2]. This will

lead to a significant structural evolution and revolution in production and supply chain management. This development poses new challenges for companies in terms of **sustainable competitiveness**, such as rising costs, changing quality requirements, resource efficiency, emissions reduction, due diligence requirements, dynamic customer requirements, as well as the necessary improvements in customer satisfaction, productivity & flexibility, and it enables companies to expand their dynamic capabilities and strategic management objectives [2].

- **Industry 5.0**
- **Business Models**
- **Circular Supply Chains**
- **Resilience**
- **Operations Strategy**

The contribution of digital transformation adoption for production can be considered at a strategic level. The following stages are of interest for **operations strategy**, i.e., internal operations, supply chains, markets and societal impact [3].

- (i) Adoptions that improves **internal operations** with limited overall contributions in terms of, e.g., lower costs, faster new product development, reduced material waste,
- (ii) adoptions leading to changes beyond a single organization, and affecting **suppliers and supply networks**,
- (iii) adoptions impacting on competition in the **market** by offering new value propositions to customers, and
- (iv) adoptions impacting on **society**,

i.e., the humanitarian, social and environmental credentials. The **operations strategy** and the related **supply chain strategy** does express the **customer value proposition**, which reflect the competitive strategy that is based on macroeconomic, political, and technological factors as well as global competition [4]. The comparison of the market view and the resource view identifies gaps and may eventually require an adaption of the competitive strategy or the operations strategy as well as supply chain strategy.

The adoption of emerging technologies like additive manufacturing will change product **designs as well as the structure of supply chains** [3]. The supply chain design in this environment is no longer characterized by centralization and globalization but by decentralization and localization [4]. **Localization** may enable supply chains to operate in a **VUCA** (volatility, uncertainty, complexity, ambiguity) environment (doi: 10.1007/978-3-319-16889-0\_9).

The synchronization of production with customer demand might reduce the volatility, uncertainty, complexity, ambiguity elements, i.e., this type of make-to-order production is called **customer-responsive concurrent production** (doi: 10.1016/j.jom.2016.12.006). Digital transmitted knowledge and materializing products as locally as possible with the objective to minimize physical moves and storages can be enabled by the combination between the physical internet and open distributed production centers via disruptive manufacturing technologies, e.g., additive manufacturing [5].

The World Economic Forum Report [6] suggests that supply chains are the key unit of action with regard to **Circular Economy** implementation and success. Combining Circular Economy, Operations Strategy and Supply Chain Strategy will be the foundation for driving needed changes that will be facilitated by the adoption of emerging technologies. Circular supply chains request to engage the customers/consumers to rethink the value chain (demand and supply). All supply chain partners need incentives to participate in the circular supply chains (ctl.mit.edu/sites/ctl.mit.edu/files/SCMR1409\_InnovationStrategies.pdf). These requirements demonstrate the importance of innovations (technical & operations) as well as new types of **Supply Chain contracts for cooperation and collaboration** and the training of experts for circularity [4].

**Business models** have been identified as an important means of enabling and promoting the circular economy and reaping the benefits of digital transformation, as they provide a holistic perspective and link internal and external activities. Thus, they are considered enablers to transition from a linear take-make-dispose system to a circular one, including new innovative ways of doing business and creating value as is the case with **integrated product-production service-systems**. Despite the general interest, there remains concerns and doubt regarding the applicability and quantification of integrated product-production service-systems in real-life (doi: 10.1007/s00170-019-03740-z). Recent research studies provide interesting insights of production companies, that shifted to integrated product-production service-systems and often failed to achieve sound financial performance compared to “classical” manufacturing companies, i.e., the findings indicate that integrated product-production service-systems lead to greater bankruptcy risks for the provider based on higher internal and environmental risks. The empirical results provide evidence about the dependency of the type of service offering on these risks (doi: 10.1108/IJOPM-02-2014-0052). Furthermore, factors that may impact the shift of manufacturing to integrated product-production service-systems such as leadership, technology related to the digital transformation, service modularization and degree of competition require analysis and innovative solutions (doi: 10.1016/j.techfore.2019.01.014).

**Industry 5.0** is an extension of the industry 4.0 paradigm that will be of interest to search for related technical and process innovations to create impact, “Industry 5.0 complements the existing Industry 4.0 paradigm by highlighting research and innovation as drivers for a transition to a sustainable, human-centric and resilient European industry. It moves focus from shareholder to stakeholder value, with benefits for all concerned. Industry 5.0 attempts to capture the value of new technologies, providing prosperity beyond jobs and growth, while respecting planetary boundaries, and placing the wellbeing of the industry worker at the centre of the production process.” (doi: 10.2777/308407)

Multiple crises related to climate change, shortage of raw materials, structural change in the world of work, and geopolitical shifts requires **resilient operations and supply chains**. Surveys show that the implementation of resilience strategies

in companies is lacking behind (doi: 10.1108/IJOPM-03-2020-0165). A reason might be the lack of transparency and information sharing between different supply chain partners. While **information sharing** could help reduce uncertainty and improve **supply chain visibility**, the risk of revealing too much information and the potential loss of data to competitors make companies reluctant to share information [7],

(i) Innovative technologies (i.e., Blockchain Technology) enables to define and negotiate procedures for different states of the systems in advance and follow them automatically if such a state is detected, which saves time, increases transparency, and contributes to better monitoring of the system (doi: 10.1109/ICCCNT.2018.8494045).

(ii) SC partners can use the zero-knowledge proof to solve the problem of sharing too much data. This cryptographic method enables the user to prove to another user that he/she possesses certain information or that certain information is true without revealing the information itself (altoros.com/blog/zero-knowledge-proof-improving-privacy-for-a-blockchain/).

(iii) Secure multiparty computation is a method that enables to combine data from multiple users and perform computational operations on them without sharing the data of individual users between each other or with some central authority computing the results [7].

## Approach

Typically, each industry 5.0 related research project is based on a thorough systematic literature review which forms the base of the initial research. Once the existing research has been reviewed, and the current state-of-art strategies and practices have been identified and understood, quantitative models will be build based on empirical data that are derived from exploratory case study research with company partners. Applying different simulation methods, i.e., agent-based simulation, discrete-event simulation and system dynamics simulation allows greater insights. The application of agent-based simulation allows to cover the behavior of crucial stakeholders within the supply chain like the provider and customer [8]. Discrete-event simulation enables the analysis of manufacturing processes to explore the “real” situation, to conduct experiments regarding process alternatives and to measure relevant performance measures [9]. System dynamics simulation allows to capture related long-term systemic impact [10]. In addition, game theoretic models are suitable to analyze different types of supply chain coordination mechanisms and evaluate them through the agent-based simulation models. It is necessary to consider these different viewpoints, to develop and achieve process innovation. Hence, this mixed method research will enable the assessment and development of feasible solutions.



## Impact

Industry 5.0 and its extension of autonomous production systems and their behaviour in terms of interactions from human-to-machine will affect production performance. To analyse these impacts, a set of performance indicators in the economic, environmental and social sphere are required to capture the respective changes [2]. Any performance win of a new technology should therefore not only be measured in financial and/or productivity terms. Equally important is to better understand non-financial consequences, perceived quality of products/services, impacts on image/reputation of the company, their value added to the effectiveness of organisational processes, or the link to the workforce for successful adoption [2]. In this context standards are of special interest, e.g., EMAS, ISO 22400, SA8000 and the GRI, to facilitate a proper impact assessment covering all three relevant domains (economic, environmental and social) [2].

Manufacturing firms tends to focus on easily-measurable cost (<https://doi.org/10.1002/joom.1113>). This is represented by well established financial measures, like return on Investment (ROI), return of equity (ROE) and by related financial statements, i.e., balance sheet & profit and loss account. Anyhow, important measure are not part of the financial statements that may cause misleading decision support for investment decision related to industry 5.0 technologies, i.e., opportunity costs, like markdowns (discounts to convince customers to buy excess inventory) and lost sales (customer sales that did not materialize because of stock-outs).

A shift from Total Cost of Ownership (TCO) to Total Value Contribution (TVC) aligns decision makers with value rather than cost, in addition, TVC replaces the term “ownership” with the more appropriate term “contribution,” thus avoiding narrowing the view ([doi: 10.1002/joom.1113](https://doi.org/10.1002/joom.1113)).



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## Competencies

The Institute for Production Management has comprehensive competencies in the planning, analysis and evaluation of manufacturing and supply chain processes. The measurement, analysis and evaluation of operational performance taking into account economic, ecological and social aspects in connection with integrated supply and demand management form a research focus that is also highly relevant for industry 5.0 projects. The mismatch of supply and demand is a main driver for technological and process innovations. The institute for Production Management has a proven expertise in modeling, simulation and optimization of manufacturing processes as well as supply chains based on research in cooperation with other research institutions as well as with companies. My research team investigated, e.g., how revolutionary queuing based modelling software helps **keep jobs in Europe**, via the development and application of a lead time reduction software that increases industry competitiveness and supports academic research (FP7 Marie Curie Actions-Industry-Academia Partnerships and Pathways). Recent research work is allocated to development of a comprehensive **assessment** method, taking into account **economic, environmental and social factors** (Horizon 2020 / FFG: Power Semiconductor and Electronics Manufacturing 4.0, [www.semi40.eu](http://www.semi40.eu)), development of a methodological assessment framework based on **rapid modeling tools** for the **analysis of technical innovations in production processes** (Horizon 2020 / FFG: Integrated Development 4.0, [www.idev40.eu](http://www.idev40.eu)), and **human-centred AI** for the optimization of **robust and competitive manufacturing network** (Horizon Europe / FFG: Artificial Intelligence in Manufacturing leading to Sustainability and Industry5.0).

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# Research & Development on Reclaimed Cross-laminated Timber

Anton Kraler, Stephan Kaiser

## Vision

In timber construction, cross-laminated timber (CLT) has been a very modern and widely used building product for more than 20 years. However, due to the increase in the number of CLT producers, there is an increasing price neutrality, therefore the topic of unique selling proposition in terms of quality and sustainability is of immense importance in order to keep up with competitors on the sales markets. CLT is a building product that actively contributes to **reducing the CO<sub>2</sub> footprint in the construction industry**. The share of grey energy, i.e. primary energy consumption for the production (kWh = kilowatt hour) of sawn goods added to the stored energy (calorific value) results in a positive energy balance, which has a ratio of 1:6 between grey (consumed) energy and stored (embodied) energy [1]. The use of CLT in timber construction as wall or ceiling elements works well, especially in the field of prefabrication. By 2022, production capacities of 1.28 million m<sup>3</sup> of CLT per year have been installed in the D-A-CH region (with Germany, Austria and Switzerland), as well as Italy and the Czech Republic. After further companies went into operation in 2023, a CLT capacity of more than 2.3 million m<sup>3</sup> per year has been reached in Central Europe [2].

With the currently used CLT production layouts, between 10 and 15 % cutting waste is produced in large-format wall or ceiling cutouts [4], which is of high material quality. A downcycling system is currently rigorously applied to re-use this waste. For this purpose, the large-format cut-outs (e.g. 1 to 3 m<sup>2</sup>) are chopped up and used only linearly, for example to heat drying chambers. As a result, the waste product from the quality product CLT loses its **high**

## ecological and economic value.

There are various approaches to **avoiding the high-grade CLT residues**, but these are rarely used on a wide scale. One method is sawing the remnants in layers and processing them (e.g. planing) to be re-used as recycled middle layers in CLT. Another method to avoid CLT cut-outs is a production technique in which the large-format openings are not cut out. A third method is striving for material-saving design, i.e. lengths and widths are selected in such a way that fewer cutouts are produced. Since these

- **Renewable Resources**
- **Circular Economy**
- **Recycling**
- **Circular Production Processes**
- **Cross-laminated Timber**
- **Resource Conservation**

three methods described are hardly ever used, mainly for economic reasons, further viable solutions are being researched.

A new solution that is already being researched involves a **recycling process**. The idea here is to produce a new CLT panel from the cuttings. This makes it possible to **reuse CLT** along a circular economy scheme. The same recycling process can also be applied in the **dismantling process** of timber structures made of CLT. This research approach thus takes on even greater significance, because it means that the quantities of wood repeatedly remain at their intended **level of use**. In other words, they are used as CLT and not

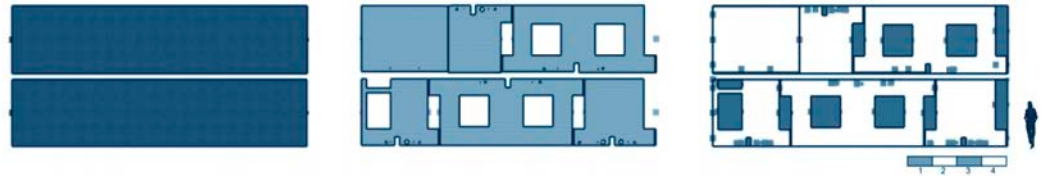


Fig. 1. CLT raw panel (12 m \* 2.7 m), CLT wall element during joinery, resulting CLT cutouts [6].

in a different wood material form. This generates a **longer service life** and keeps down the primary energy input for possible recycling.

In a master's thesis (MA) at the Salzburg University of Applied Sciences in Kuchl from 2022, 60 CLT timber construction projects were investigated for the extent of their waste and recycled material. The mean value of the **share of waste** was determined at 13.4 %. Furthermore, it was possible to establish in the MA that a **recycled share** (for the production of recycled cross laminated timber) of 78.4 % is achieved from the offcuts [6]. Building on this MA, further research will follow at the University of Innsbruck (UIBK) in a dissertation, dealing for example with a digital analysis of all material and energy flows that are necessary for the individual production steps of CLT.

One objective is to obtain "the best possible use of energy and materials (through transparency of information in production process)". In addition, differences in the individual production methods also play a part in this investigation, in order to include or further develop already existing solutions in research and development. At the same time, **constructive cooperation** with several industrial partners is essential to obtain **real data** from the production sector.

## Approach

The research approach consists of several facets, which are comprised in the fields of activity in engineering for forest production technology and timber construction. **Circular business models** have been proven to be an essential success factor and do not only lead hidden champions to very good business results! A **higher material utilisation** in an adapted production process leads to a reduction in material requirements and waste. If, as in the example of CLT, the large-format production waste is used for the production of new panels (reCLT), only the material and energy costs of, for example, 50 to 60 % are to be subtracted from the unit cost calculation and can be considered as value added [5]. In the future, the re-

processing and reuse of already built-in CLT will also be demonstrated by a functioning recycling scheme for the (reprocessing) production processes. The development of a production layout for the recycling of CLT cutouts can be researched through digital material and production process simulations at the University of Innsbruck. In doing so, research activities on **innovative recycling processes** will continuously advance the transformation from a linear economy (production, single use and waste) to a **circular economy** (reuse of resources)!

As a solution approach for recycling, the CLT residues could be transferred to an automatic high-bay warehouse after trimming, sorted and temporarily stored in order to have a critical quantity available and to carry out the production of reCLT in a resource-saving manner at the appropriate time interval when sufficient surplus renewable energy is available. An essential point in the introduction of recycled CLT is that the circular economy is anchored in standardisation for implementation and application. For this purpose, it is necessary that the corresponding research and development work is carried out. The inclusion of recycled materials in the standards increases motivation and supports the strategic considerations of the manufacturing companies. **Sustainable products** are considered particularly worthy of support by the European Union (EU) and the individual countries in terms of resource efficiency and the circular economy, and they provide respective research funds. In order for such developments to succeed and to deliver usable results, the cooperation between the CLT industry and research institutions such as the University of Innsbruck's Department of Timber Construction must be seen as a necessary requirement.

## Impact

In times of increasing resource scarcity, the extraction, application and circular use of raw materials in terms of efficacy and efficiency is a significant research topic. The storage period of the stored carbon in the amount of wood should bring the duration of natural reproduction (in the forest) in line with the respective harvesting cycles (wood species, growth area, forest management) without exploiting **the natural resource**. From an economic perspective, the use of wood as a building material and thus also as a **CO<sub>2</sub> store** is more valuable than its use as an energy source. The processing of wood for energy use requires additional grey energy, which in turn releases CO<sub>2</sub> and consumes additional resources. Currently, the purchase of **CO<sub>2</sub> certificates** can be used to offset greenhouse gas emissions. The consequences of this scheme are that on the one hand this leads to additional costs for producers and consumers and on the other hand it does not reduce **CO<sub>2</sub> emissions** in the respective production sector, unless the resulting income from the sale of CO<sub>2</sub> certificates is used effectively and efficiently for the general **reduction of greenhouse gases**.

In summary, the linear type of production is not conducive to a sustainable economy and the counter-strategies to combat climate change. The material and energy balance of the currently installed production systems provides the impetus for new solutions leading to a circular economy. The building product CLT is in a worse position than competing products in the market economy. This is because the building owner pays for the waste of large-format openings (windows, doors) at the time of purchase, for example. For an average residential building, the additional costs can amount to an average of up to 13.4 % of the CLT. The above facts lead to the research approach of developing a **recycling product** including a **recycling layout** that can be integrated into existing production facilities. Making adjustments to planned new production plants can prove viable.

In connection with the topic of energy saving, there are already successfully modified production processes. These were divided into individual production steps after a thorough analysis of production-related material and energy flows, and further developed and implemented by modifying production processes with circular resources. In this way, the costs of energy-intensive production processes could be greatly reduced by switching to flexible production scheduling, taking into account the available natural resources, such as wind or solar energy. The savings are achieved by linking the consumption of solar and / or wind energy to their availability.

An important indicator for the circular economy is the **Circular Material Use Rate** (CMU), which indicates the proportion of materials that are recycled in relation to the overall use of raw materials in the economy [3]. In Austria, the CMU is 12 %. By comparison, the leading nations in CMU in Europe are the Netherlands with 30.9 %, followed by Belgium and France with 23 and 22 % CMU each (eea.europa.eu 2023). However, the CMU (including all materials used) is much lower than other indicators (e.g. recycling rate with 56 % within the EU).

Through multi-faceted transformations in material consumption in production and extended use, the circular economy rate can have a very extensive leverage on material consumption. In the process, society will undergo a comprehensive rethinking process and major efforts and adjustments to **resource consumption** in relation to **resource deposits** will follow. In the case of renewable biomass, for example, a large contribution can be made to material consumption



by avoiding combustion as much as possible in the future. From the industry's point of view, this requires more sufficiency-oriented production technologies, and from the consumer's point of view, a longer use of products. Another indicator will be the **product carbon footprint**. From 2024, this will provide a further indicator throughout the EU, due to the obligation to report on sustainability issues (Corporate Sustainability Reporting = CSR), depending on the size of the company, in order to be able to use additional monitoring methods [3].

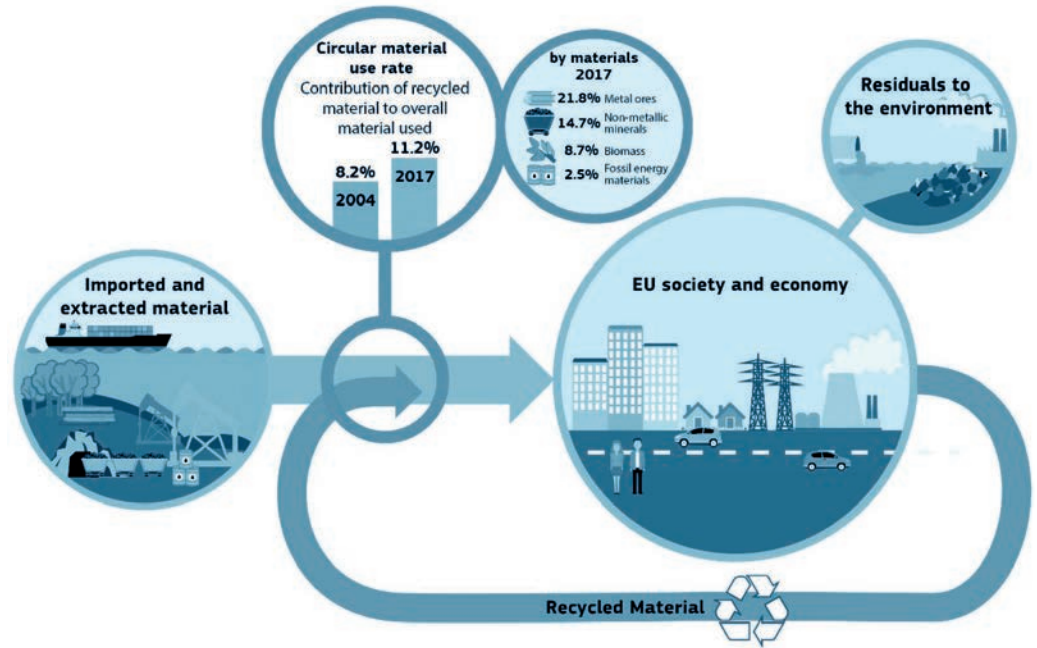


Fig. 2. Circular material use rate in the EU



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## Competencies

The Department of Timber Construction at the Institute of Construction and Materials Science of Innsbruck University, has **modern research facilities** and sought-after experts who carry out **interdisciplinary research** and development. Modern laboratory facilities and digital infrastructure are available for this purpose. The Technical Research Institute (TVFA) of UIBK and TiroLignum, a competence centre for **cooperation** between the timber construction guild, the vocational school for wood technology and the UIBK Department of Timber Construction, can be named as particularly important research institutions.

The core competence of the timber construction department lies in practice-oriented research and quality assurance, in the area of structural timber engineering, building physics with special requirements in sound insulation and fire protection, besides participating in international research projects. In cooperation with the accredited testing laboratory TVFA, investigations are carried out and test reports, expert opinions and scientific evidence are provided. The TVFA operates in various specialist areas: Timber construction, materials technology, strength of materials and structural analysis, steel construction and mixing technology, applied mechanics, and energy-efficient construction.

Particularly noteworthy are successfully completed research projects with cross laminated timber. These include the “Spider Connector”, which won the “Product Innovation Award 2019”, the “CNC-manufactured wood-wood connections” and the “curved CLT radius timber”. In the field of building physics, the research project “Prefabricated facade elements for serial renovation and new construction in multi-storey buildings” with special requirements in sound and fire protection needs to be mentioned. The CLT is a component of the research services for the projects listed.

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# Innovative Solutions for a Circular Bioeconomy

Boris Hultsch

## Kompetenzzentrum Holz GmbH, Wood K plus:

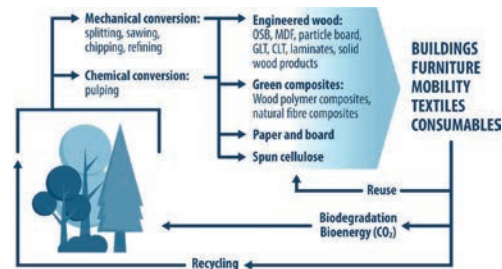
We are a **leading research organisation** in the area wood and wood-related renewable resources in Europe. Our core competences are **materials research and process technology** along the complete value chain – from raw materials to finished products. We develop methods and basics and perform applied research on the **economy-science interface** in order to enable resource-efficient management in the **circular bioeconomy**.

As COMET K1-Center of the COMET Programme – Competence Centers for Excellent Technologies - we are funded by the Austrian ministries BMK, BMAW and the federal states UpperAustria, LowerAustria & Carinthia. The programme COMET is operated by the Austrian Research Promotion Agency (FFG). In the K1-Center research is carried out together with more than 30 company partners and 15 scientific partners - among them many well-known Austrian and international partners - at three locations in Linz (headquarters), Tulln and St. Veit an der Glan. Wood K plus also performs **contract research** for companies and participates very successfully in numerous **international and national project programmes**. In 2022 alone, 5 EU projects were granted in the *HorizonEurope* programme. Thus, the centre is also a beacon internationally and is very well networked.

At Wood K plus, around **120 researchers** develop bio-based functionalised materials - such as new wood-based materials for furniture and construction, high-performance carbon materials, sustainable packaging, high-quality fibres, thermal insulation and

natural composite materials for many applications, e.g. vehicles and wind power plants. There is also a focus on **improving the carbon footprint** of the construction sector. One hundred percent bio-based composites and wood-based materials with bio-based binders are to massively increase durability and functionality in timber constructions. Using raw materials efficiently, protecting the environment and increasing productivity - **closing material cycles** is becoming increasingly important.

- **Circular Bioeconomy**
- **Biorefinery**
- **Chemical Process Engineering**
- **Wood Materials Technologies**
- **Composite Materials**
- **Paper & Surface Technologies**



## Biorefinery Processes & Composite Materials

The research focus of the Linz area Biorefinery Processes & Composite Materials is on optimising the use of biomass - primarily wood - but also other renewable raw materials. We are a leading research partner for industrial and strategic questions in the fields of wood and wood component chemistry, pulp quality and **chemical or biotechnological utilisation of lignocellulosic raw materials**.

Our expertise ranges from the pre-treatment of biomass to the digestion in pressurised reactors, the separation of waste and value streams and the development of methods for the required instrumental analysis.

Another focus of our research activities is on **composite materials** made from renewables (NFC - Natural Fiber Composite) as well as **bio-based carbon materials**. By means of extrusion, injection moulding, pressing, melt spinning or 3D-FLM printing, these materials can be processed into innovative products with specifically adjustable property profiles. Our unique know-how also enables us to produce **hybrid materials, carbide ceramics and porous carbons** from biogenic raw materials and to process them into complex parts. In addition, research is being conducted on the development of bio-based carbon fibers, carbon fiber precursors and in the area of bio-based electrochemistry.

### The research topics of this area comprise:

- Understanding of chemical reactions in digestion processes and translation into new or improved processes
- Pretreatment of biomass to optimise digestion processes
- Efficient cellulose-based specialty products
- Intelligent processes for selective recovery of components in biomass and their further use – as material and/or energetically
- Chemical and/or biotechnological conversion of degradation products of lignocelluloses to platform chemicals
- Downstream chemistry of cellulose, hemicellulose and lignin-derivatisation and functionalisation

- Development of analytical methods - from laboratory to industrial process applications
- Optimisation of thermoplastic processing: Compounding, Profile extrusion (also foaming and coextrusion), Injection molding (also foaming), Melt spinning, Production of filaments (also short and continuous fiber reinforced) for 3D-FLM printing
- Material development and optimisation of thermoplastic formulations (focus on biopolymers)
- Development of biobased carbide ceramics
- Development of carbon fibers and carbon fiber precursors from biobased raw materials
- Research and development in the field of bio-based components for electrochemical applications (batteries, fuel cells, supercapacitors)



## Wood Materials Technologies

The Tulln area Wood Materials Technologies focuses on different wood technological processes as well as on the **destructive and non-destructive testing** of wood and wood products. Research activities focus on the characterisation of wood and its primarily (thermo-) **mechanical transformation into materials for construction and furniture**. Their recalcitrance against negative effects of moisture and humidity, their fire resistance, and the significance of emissions from wood-based materials are being closely considered. Since **adhesives** play an essential role in the manufacture of advanced wood materials, special attention is dedicated

to their **synthesis and optimisation towards superior performance** and minimised environmental impact. In addition, interactions between material features and technological processes and methods are investigated.

**The research topics of this area comprise:**

- Analysis and optimisation of disintegration processes of wood composites and renewable raw material
- Drying technology (simulation and optimising industrial drying process)
- Wood and fiber modification
- Surface functionalisation and hydrophobising
- Fire behaviour of renewable raw materials
- Optimisation of production processes to reduce product variability
- Development of new adhesives
- Analysing adhesive properties (e.g. tack) as well as interactions between adhesive and wood
- Adhesive distribution on industrially manufactured wood composites
- Analytic and evaluation of VOC and odours from solid wood and wood composites
- Development of processes for VOC and odour reduction
- Function oriented wood composites by means of “Design Engineering“

**Wood & Paper Surface Technologies**

At St. Veit/Glan our research is focused on the topic **surface technology** concerning wood based products and bio based composites. In synergy with our industrial and scientific partners the work is carried out by our well educated researchers to establish a high expertise. This allows long term cooperations with larger enterprises and enables the first research steps for small size enterprises. Our offers range from foundational research up to generation of prototyping.

**The research topics of this area comprise:**

- Powder coating technology of wood based panels, natural fiber composites and composite material
- Surface modification and functionalisation using plasma activation
- Coating under atmospheric pressure conditions
- Bio-based composites made from biopolymers
- Development of long fiber reinforced thermoplastics based on wood or flax fabrics
- Laminates: surface functionalisation and functionalisation of the layer composites
- Optimisation of paper properties (décor paper, kraft paper, sack paper)
- Systematic evaluation of process data for a knowledge-based process control
- Determination of correlations und interactions between technology properties and surface appearance
- Process analysis for these surface properties
- Determination of efficient (production) processes
- Development of new surface characterisation methods
- Surface characterisation

**Sustainable Innovation and Impact Analysis**

The team Sustainable Innovation and Impact Analysis works at the interface of technology and economy with the aim of successfully shaping innovation processes by providing tailor-made information. Considering Wood K plus conducts research in three different technical areas, the context of their research is also reflected in SIIA’s tasks, e.g. **investigations on market potential of new products or technologies** and their social acceptance. Using a wide variety of analysis methods, market barriers can be identified and addressed, or market opportunities can be targeted. In addition, together with our research partners **we assess economic, ecological and social impacts** of new materials and processes alongside R&D. In this way,



we support our partner companies in their contribution to climate protection and sustainable development.

**The research topics of this area comprise:**

- Economic, ecological and social product & technology assessment
- Life cycle sustainability assessment
- Eco-efficiency analysis for new technical developments
- System Dynamics sector simulations with FOHOW
- Agent-based market modelling
- Econometric models and analyses
- Experimental designs for market-oriented product development
- Lead User Analysis, Conjoint Analysis and Analytical Hierarchy Process
- Technology foresight with scenario analyses, Delphi surveys, network analyses
- Media and content analyses
- Quantitative and qualitative methods of empirical social research, e.g. interviews, content analyses or online surveys





**Boris Hultsch, CEO**  
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## Competencies

Wood K plus is a MEMBER of the UAR Innovation Network, which consists of a total of 18 highly specialized R&D centers (as per 2023). Research on cutting-edge technologies for efficient production is one of the major fields of strength of the UAR Innovation Network.

Within the research fields Smart Systems, Digital technologies and Sustainable materials, the involved R&D centers conduct research in a variety of topics like process engineering and optimization, software engineering and modelling, high-tech materials and components, energy efficiency and many more. In addition, the available expertise is also successfully implemented in medical technologies.



# Shaping the Future, together

Contributions to a Flexible and Sustainable Production

**JOANNEUM RESEARCH Forschungsgesellschaft mbH**

## Vision

JOANNEUM RESEARCH, as the research organisation of the countries and regions, shapes the development of our modern society and economy with its innovations in a sustainable and people-centred way. As a multidisciplinary team in flexible, innovation-friendly structures, we live up to the highest social and scientific standards.

JOANNEUM RESEARCH develops solutions and technologies for business and industry in a broad range of sectors and conducts cutting-edge research at an international level. In order to do justice to the topic of flexible and sustainable production, several institutes have joined forces in the business area of production and manufacturing to serve its customers in this complex area. In the following sections, we are presenting the topic from the perspective of the individual institutes and thus examined from several sides.

### Robotics

Digitization and automation make a significant contribution to the long-term safeguarding and further development of Austria as a production location. The institute ROBOTICS has its research focus in flexible production methodologies and technologies for high mix/low volume manufacturing. Using state-of-the-art robotics technology, we develop solutions to optimize production processes, reduce costs, and improve efficiency for our clients. This particular focus on flexibility allows us to design customized robot systems that can adapt to changing production needs, resulting in faster turnaround times and improved quality control. This is in line with the

Sustainable Development Goals of the United Nations (UN-SDGs) “8 - Decent Work and Economic Growth”, “9 - Industry, Innovation and Infrastructure” and “12 - Responsible Consumption and Production”, where production should be people-friendly, based on innovative infrastructure that can be used in the long term and conserve resources. One way we promote sustainable and resilient manufacturing practices is by supporting onshoring or reshoring of production capacities in order to improve supply chain resilience and reduce carbon emissions associated with transportation. This has a particular impact for small and medium-sized enterprises (SMEs), which often operate with limited resources and face greater challenges in adapting to disruptions in the supply chain or market changes. Automation, especially robot-based automation, can be a key factor here.

- **Robotics**
- **Automation**
- **Climate Neutrality**
- **Circular Economy and Sustainable Production**
- **Decarbonisation**
- **Smart Manufacturing**
- **Data Analytics**
- **Explainable AI**
- **Process Optimisation**
- **Soft Sensor**

### Policies

The Institute POLICIES for Economic, Social and Innovation Research consults politics and enterprises in their technology and innovation strategies

based on empirical research, data analytics and model-based approaches. The primary goal in the field of production and manufacturing is applied research on databased methods to increase the quality, reliability and efficiency of technological products, processes and systems. Rapid development of smart manufacturing, Internet of Things, robotics and new sensor technologies offers manufacturers the ability to gather, store, process as well as utilize data in daily operations. Thus, the manufacturing industry is at the beginning of a data-driven revolution facing an increased need for innovative data driven solutions. Building on many years of successful application of data analytics in manufacturing, POLICIES offers databased methods and analytics helping companies to gain insights about potential improvements of products and processes, drive productivity and improve their societal and environmental impact.

### Life

The Institute LIFE for Climate, Energy Systems and Society is the leading research institution in Austria in the thematic field of climate resilience and climate neutrality. LIFE supports business and industry in the transition phase in the development of tailored strategies towards climate neutral, circular and sustainable production in the context of the European Green Deal.

### Materials

“Smart MATERIALS for a Sustainable Future” is the basic vision of MATERIALS, the Institute for Sensors, Photonics and Manufacturing Technologies. MATERIALS provides solutions in material science for manufacturing and the industry. With its focus on production and surface technologies, micro- and nanotechnology, as well as green photonics and electronics, MATERIALS is oriented towards the needs of the regional and international economy. Therefore, we offer interdisciplinary, flexible and sustainable solutions for production processes along the entire value chain. The spectrum ranges from initial concepts to prototypes using cutting-edge technologies and processes based on miniaturisation, integration and material optimisation. The core topics include generative manufacturing technologies such as laser cladding, 3D printing and vapour deposition technologies, the simulation, design and manufacturing of optics and micro-optical elements, various structuring processes such as laser lithography, the unique roll-to-roll nanoimprinting process as well as various coating and printing processes such as inkjet or aerosoljet

printing. Additionally, MATERIALS offers comprehensive expertise in the development of sensor systems for monitoring and optimising production processes

### Digital

DIGITAL's vision is to strengthen the importance of digital innovations on a regional and European level and to make the impact on the value creation of our customers even more visible. Not only but especially in the area of production and manufacturing, in order to support the digital and green transformation of the economy in the best possible way. DIGITAL is a pioneer and reliable partner in the fields of digital innovation and transformation and develops high-tech solutions that function reliably and robustly in practical use under rough conditions. The scientific and technological foundation of DIGITAL is formed by multi-sensor systems where precise measurement systems are developed employing cutting-edge sensors and where new insights are gained using artificial intelligence methods.

## Approach

### Robotics

The Institute for Robotics and Flexible Production specializes in industrial robot system technologies and production automation. We provide research and development partnership to our clients, implementing innovative, efficient, and cost-effective digitization projects. Our expertise ranges from technology development, functional modeling and simulation, economic evaluations, to cutting-edge system implementation. We focus on supporting our project partners in developing flexible production solutions, while also providing our knowledge in performance optimization and conducting comprehensive robot safety assessment and inspection. Additionally, our ROBOTICS Solution Center offers the opportunity to perform feasibility studies, allowing clients to test the latest automation and digitization technologies, and qualifying specialists through hands-on training courses. Through our overall approach, we ensure that our clients not only receive the technical benefits but also the financial and know-how advantages of our robotics and automation technologies.

### Policies

Applying the entire data-science process, from analyzing the problem, process or system, up to validation of models and results, POLICIES provides

insights, predictions and optimizations.

The increasingly distributed data, which is often collected from different sources and presented in inconsistent ways, together with their huge amounts, is challenging for manufacturers. While capturing the data correctly, companies often fail to efficiently merge, analyze and utilize it. So, based on a well-founded systems analysis, we carefully collect, select, join and preprocess appropriate data. The more the volume and complexity of data grow, the more data visualization and exploration become important. Data exploration can help to identify data or sensor failures and process anomalies as well as provide first insights of correlations and problem root causes. Aiming not only at prediction but also at optimization of processes, transparency and interpretability of models are getting as important as high predictive performance. Thus, we focus on statistical modelling approaches, physics informed machine learning and explainable AI. To help companies to draw best possible benefit from the model-based predictions and optimizations, careful evaluation and validation are key-tasks in our data analytics projects.

### **Life**

The complex challenge for the transition of the economy and production systems towards climate neutrality and circularity requires a systemic scientific approach. LIFE stands out for its interdisciplinary competences, linking deep technological know-how in all economic sectors, method leadership in sustainability impact and risk assessment along the entire production value chain, leading edge insights into EU climate policy development and frontrunner social and psychological methods for supporting the diffusion of new technologies and products.

### **Materials**

MATERIALS takes the approach of interdisciplinary collaboration among its five research groups. This allows the Institute to use the strengths of all groups with higher, critical mass effectively. These interdisciplinary teams and approaches, the technological focus on our core topics as well as the professional handling of national and European funding, from application to effective project management to successful project completion, are among the Institute's core competences. Based on a high level of scientific expertise, MATERIALS provides access to the latest technologies for implementation into innovative products and services. It is the primary contact for the development

of technologies and processes for green photonics and printed and organic electronics, structured (biomimetic) surfaces, piezoelectric sensors and energy harvesters, large scale production of microstructured organic coatings (including roll-to-roll nanoimprint lithography), (optical) chemical and bio-sensors, Lab-on-a-chip devices and microfluidics, laser production technology, aerosol and inkjet printing and laser and plasma-supported deposition processes. The systematic development of these areas of strength makes the Institute an attractive national as well as international research partner.

### **Digital**

Optical and acoustic sensors are combined into intelligent sensor systems to enable high-precision measurements and to gain new insights into the observed products and processes from the data streams with the help of artificial intelligence. Our research focuses on (i) quality assurance using intelligent sensor technology, (ii) plant monitoring, (iii) sorting waste material and (iv) human-machine interaction.

New IoT and edge-to-cloud computing technologies are enabling design and manufacturing to produce increasingly complex products in less time and improve information management throughout the product lifecycle. We focus on the application of various sensor technologies to help industry to achieve greater efficiency and conserve resources while maintaining flexibility in production.

Data-driven techniques and knowledge-based methods such as sequencing, heuristic search methods, and mathematical optimisation and scheduling techniques are being used. Knowledge graphs are relevant for the dynamic capture of structured knowledge and the use of these structures is used to support people in industrial manufacturing environments.



## Impact

### Robotics

Modern robot systems are widely used in applications where it is economically rewarding or where other significant values, such as worker's safety, can be obtained. Ultimately, robots act as direct bridges between the virtual/digital and the real environment and are thus key components in human-centered automation and digitization. The impact of JOANNEUM RESEARCH ROBOTICS focuses on research activities in industrial robot systems technologies, digitalized production automation and economy. SMEs can reduce their dependence on distant suppliers and minimize the risk of supply chain disruptions by onshoring their production capacities. Incorporating resilient manufacturing practices, such as flexible production and circular economy principles, can help to enhance their efficiency and reduce costs, while also enabling them to adapt to changing market conditions. These principles empowers us to assist SMEs in improving their competitiveness, reducing risks, and contributing to a more sustainable future. By utilizing robotics and innovative manufacturing practices, we can help businesses achieve their production goals while also advocating for sustainability and resilience in the manufacturing industry.

### Policies

Due to increasing digitalization in production and the spread of highly developed sensor technologies in industrial applications the availability of data and consequently the need for adequate data analytics and modeling methods are increasing rapidly. Data-driven manufacturing and effective use of data is becoming a strategic necessity for companies to get value with better speed and efficiency, making businesses more sustainable and more profitable. Applying innovative data analytics and developing customized process models, POLICIES can help companies to make a significant impact with data. By joining process, machine and product data with various external data sources as well as providing interpretable models and predictions manufacturers can gain insights far beyond one single process.

### Life

LIFE combines high level of scientific and methodological excellence in the nexus of climate, energy systems and society, and a strong orientation towards questions on practical relevance for national and international business and industry. This is supported through excellent national and international research networks, the constant feedback from stable business and policy partnerships, and a clear focus on the most relevant industries and their most pressing issues in achieving climate resilience and climate neutrality.

### Materials

The interdisciplinary team of MATERIALS offers their customers solutions across the entire value chain – from the idea to the prototype – using cutting edge technologies and methods based on miniaturisation, integration and materials optimisation. Combined with state-of-the-art equipment and infrastructure MATERIALS provides innovative solutions and services tailored to the needs of business and industry. More than 20 years of close cooperation with leading research institutions such as the Austrian based Graz University of Technology or the University of Leoben enables us to continuously improve and extend the portfolio of expertise. Moreover, MATERIALS has long-standing experience in managing a wide range of research cooperations, thus enabling the clients to successfully participate in national and international funded research projects. Especially relevant are the European Pilot Lines Phabulous, MedPhab and PhotonHub Europe, as well as the Open Innovation Test Beds

Next-Gen-Microfluidics and FlexFunction2Sustain.

MATERIALS is also committed to align its research activities with the priorities of the European Green Deal as well as the global Sustainable Development Goals and related EC priorities. This ranges from environmentally friendly production of materials (biomaterials, biodegradable, ...) via lower consumption of resources and energy saving through more efficient production processes and the implementation of circular economy strategies at the application level. (i.e. use of renewable energy, minimization of energy use for transportation, invest in long-living equipment, reduced use of solvents and water consumption, recycling and end of life assessment, etc.). In addition, environmental impact assessments at material, process and product level ensure the alignment of research with the Circular Economy Action Plan.

### **Digital**

DIGITAL's solutions are fundamentally aimed at saving or optimising important resources such as raw materials and energy in the production process. The earliest possible quality controls reduce product return rates and enable batch size 1 production. The classification of recyclable materials allows valuable materials to be sorted and reused. Predictive maintenance adapts maintenance intervals to actual requirements and thus saves valuable consumables.

Active membership in relevant associations such as EIT Manufacturing, the Confederation of Laboratories for Artificial Intelligence Research in Europe (CLAIRE) or the Big Data Value Association (BDVA) enables international networking with all relevant stakeholders and ensures our contribution to achieving the strategic goals at European level.

## Competencies

### Robotics

Our combination of cutting-edge equipment and research infrastructure with the wide spectrum of topics and expertise enables the development of trend-setting solutions and the provision of innovative scientific services. Our key technologies include primarily innovation-driving industrial robot system technologies for the flexible process automation in manufacturing and professional service applications.

The Research Group Industrial-Robot-system-Technologies offers a wide technological portfolio for innovative robotics with a focus on robot-based, flexible production. We work on the main fundamental technological elements for innovative robots and intelligent systems in nationally and internationally funded research projects. We design robot systems and robot system components in industrial research and experimental development for business and industry to demonstrate the systems in the appropriate environment. Furthermore, we develop optimised and safe robot-based manufacturing systems at higher TRLs (Technology Readiness Level) in cooperation with end users and system integration partners. The broad expanse of expertise in the team enables tailored solutions to be offered for the targeted use of modern robot technologies.

The ROBOTICS Evaluation Lab (REL) is a specially equipped measurement laboratory that is able to measure and evaluate bio-fidelity forces of contact situations between a human and robots both validly and traceably. State-of-the-art, calibrated measurement equipment is used and the entire testing process is executed while applying quality assurance measures according to ISO/IEC-17025. Furthermore, the REL offers supporting services for business and industry. The REL provides industry with safety services in the sense of measurement and test services, consulting activities and the development of software tools. The REL is an accredited test lab for the determination of biomechanical forces and their conformity evaluation according to ISO/TS 15066.

The targeted use of modern robot technologies requires knowledge of the latest technology available in the field of robotics and of the opportunities and limitations of their use. The establishment of the ROBOTICS Trainings Center (RTC) enables us to react to current business and industrial

requirements for qualifications in the field of robotics. For this purpose, all trainings use the unique laboratory infrastructure such as our Hands-on-Area, which offers the latest robot and automation systems ready to be used for practice- and demand-oriented training. The RTC thus supports a long-term transfer of technology from research to practical application.

### Policies

The activities of the POLICIES research group "Data Analytics and Statistical Modelling" cover the entire data-science process from problem specification to result communication. The research group stands for innovative and creative databased models and solutions, profiting from numerous research and customer projects in manufacturing and production.

We offer algorithms and models for optimization of products and processes during design phase as well as data analytics, models and optimization of industrial processes for smart production. We develop calibration models for metrology and sensor systems and build soft sensors for virtual metrology. In the field of reliability and maintenance, we perform reliability analysis and lifetime modelling for components and systems, contributing to highly efficient Predictive Maintenance applications. Customer-specific predictive models for various tasks in manufacturing and production complete our competencies. Recent examples of cooperative research projects with leading Austrian technology companies as partners comprise the FFG projects IMPROFE and LUSI-Q. In IMPROFE a digital image of a hairpin stator manufacturing process is created, by utilizing AI-based modeling and optimization approaches, combined with laser ultrasound measurement methods and optical inspection. In LUSI-Q a soft sensor technology for contactless, non-destructive detection of mechanical anomalies of chips on wafers, based on laser ultrasound (LUS) and statistical modeling for signal interpretation, is developed and evaluated.

### Life

The research group "Weather and Climate Risk Management" is specialized in the spatially high-resolution modeling of economic climate risks. The in-house developed macroeconomic models for Austria and for global value chains, the stochastic flood and storm damage models, the Typical Farm Approach for agricultural risks, as well as operational forecasting models for the energy sector define the state of the art in their respective fields.

The research group “Climate-neutral energy systems and lifestyles” transforms the impulses of the EU Green Deal and the climate protection legislation into concrete “roadmaps” for the transition of economy and industry towards climate neutral and circular production. Key competencies combine methodological leadership in life cycle-based sustainability assessment (LCA), in-depth technological know-how across all sectors of the economy and innovative approaches in social science lifestyle research and “User Experience Sustainability Assessment” supporting new technology and product diffusion.

The research group “International Climate Policy and Economics” focuses on energy markets, renewable energy and energy efficiency energy and energy efficiency technologies, sector coupling, the decarbonization of the building sector and on nature-based solutions. The combination of quantitative and semi-quantitative methods from economics, energy system analysis and environmental psychology influences and reflects recent methodological trends and thus enables. The group has a clear national USP as a multiplier for leading-edge knowledge in the field of European climate legislation.

### **Materials**

The research group “Hybrid Electronics and Structuring” develops flexible micro- and nanostructured layers with integrated components. The major application fields include organic electronics and microfluidics, printed physical and biological sensors, large-area optoelectronics, and biomimetic functional films. Its core competencies are functional surfaces, piezoelectric sensors, organic electronics and microfluidics. In these areas, the research group covers the entire value chain, from design and simulation as well as materials development via lithographic processes and printing processes to imprinting processes.

The core competence of the research group “Light and Optical Technologies” includes simulation and rapid prototyping of optical structures over a multiscale size range. The focus of their work is light in its diverse applications: Light management in complex optical applications, precision machining, patterning and characterization of optical components in the micro- and nanometer range.

The research group “Laser and Plasma Technologies” develops materials, processes and coatings using lasers (100 W to 8 kW) and plasma-based surface and coating technologies

for a wide range of industrial applications such as metalworking, power generation, aerospace, automotive, medicine. We combine in-depth materials science knowledge with extensive know-how in the development of manufacturing and coating processes for a wide range of applications. For example, in the field of medical technology, the combination of 3D printing and surface coating enables hemocompatible, antibacterial and osteoinductive components for a new generation of heart valves, spinal implants and implantable electronic actuators and sensors. The combination of different additive manufacturing processes allows the production of large components with complex details for e.g. applications in aircraft construction. Their expertise is based on the many years of experience of the team and includes the competencies in the fields of laser production technology, additive manufacturing and plasma surface technologies.

The research group “Sensors and Functional Printing” develops chemo- and biosensors as well as novel printing processes and combine these technologies, for example, into bioanalytical lab-on-a-foil systems. Their core competencies are opto-chemical sensor materials and their adaptation to the respective measurement task as well as electronics development and instrumentation for corresponding digital readout systems; the development of novel functional inks and digital printing processes such as aerosol jet or ink jet printing and microarray spotting focuses on material, process and application development in the areas of printed electronics, heterogeneous integration of different materials, optics and sensor technology; and microfluidic systems form the basis of integrated bioanalytical and diagnostic chips (lab-on-chip) and enable the production of very compact analytical and sensor systems. They pursue a comprehensive systems approach from simulation to prototyping to large-scale manufacturing methods for microfluidic structures on polymer films. This includes their functionalisation with sensor elements such as biomolecules or electrodes. The extensive expertise in the fields of material development, surface chemistry, micro and nano structuring technologies as well as sensor technology, optics and electronics enables the comprehensive development of complex systems and suitable manufacturing processes.

The research group “Smart Connected Lighting” develops innovative and

networked lighting solutions for the domestic, working and industrial worlds of today, tomorrow and the day after tomorrow. They work on the development of comprehensive light and illumination concepts including sensors, control, networking and communication. This mirrors the international trend towards connectivity and digitalisation that contains luminaires and the light infrastructure as crucial components in an overall concept. The required sensor and communication components are being increasingly integrated directly into the lighting infrastructure. This transforms it into the main artery of networked domestic and industrial worlds and into the communication centre of the Internet of Everything. Their core competencies include smart electronic systems, systems of system - connectivity and communication – and integrated lighting.

### Digital

DIGITAL's scientific competences are organised in research groups, each with about 20-30 employees, in which internationally recognised top researchers and their team advance the state of the art in the respective

field. In the area of sustainable and flexible production, these are primarily (i) Intelligent Vision Applications, which use hyper-spectral and 3D technologies to classify objects and surfaces based on decades of experience in the field of machine vision, (ii) Intelligent Acoustic Solutions, which use the analysis of acoustic and vibro-acoustic signals to determine the condition of objects and machines and also deal with the voice control of machines in the industrial environment, (iii) Connected Computing, which deals with the industrial Internet of Things, wireless sensor networks and modern cloud-to-edge architectures, and (iv) Cyber Security, which plays into all areas of networking and, in addition to protection against cyber attacks, is primarily concerned with the design of secure IT systems (Security by Design).



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# Materials







# Materials Science for a Modern Society

Christof Sommitsch, Sergio Amancio-Filho, Josef Domitner, NorbertENZinger, Cecilia Poletti

## Vision

Components in **modern mechanical engineering** must rise to a wide range of challenges, such as (i) **lightweight construction**, (ii) functional integration, (iii) excellent **processability** and machinability, and (iv) tailored **mechanical and physical properties**. Materials, material compounds and composite materials are used for this purpose. Their properties are determined by their chemical composition and thermo-mechanical processing. In the future, graded materials and structures that can be changed over time or by deformation – and thus properties – will generate requirement-optimized components. So-called smart materials react interactively to loads, providing information about their condition and thus their service life via sensors. Maintenance and replacement intervals can therefore be adjusted and optimized. Self-healing mechanisms can minimize structural errors and extend the lifetime of a component.

**Ab-initio** and **atomistic material models** can visualize representative structure sizes and complexities, predicting their properties thanks to steadily increasing computer power. This allows for the creation of new materials and alloy systems, such as high-entropy alloys.

Such properties-optimized components are manufactured using advanced and, in some cases, new production methods. In this regard, **additive manufacturing** is an enabler due to the fact that many different parent material, heat sources and heat inputs / process controls can be used. The large number of **dissimilar materials** in components requires the development and application of **new joining processes**. Especially in the field of **lightweight**

**construction**, metallic components are increasingly being combined with polymers and fiber-reinforced plastics in order to reduce weight while maintaining good mechanical properties. The use of high-strength steels and aluminum alloys for chassis parts makes lightweight construction possible, but reduces the formability of higher-strength materials and requires **new forming processes**. Integrating and connecting solid wood or plywood components could be the key to both decarbonization and lightweight construction through the integration of **renewable raw materials**. In the case of high-strength steel components, one major challenge is the **interaction with hydrogen** and possible material

- **Additive Manufacturing**
- **Welding and Joining**
- **Metal Forming**
- **Metal-Polymer Hybrid Structures**
- **Polymer Composites**
- **Hydrogen Embrittlement**
- **Modelling and Simulation**
- **AI and Steel Design**

embrittlement, especially with introduced plastic deformations. The development of hydrogen embrittlement-resistant steel grades could make a significant contribution in this regard.

In the future, **manufacturing processes** and **process chains** will overcome trial-and-error approaches in order to guarantee optimized and efficient process flows while maintaining the required component properties. For this purpose, **process simulations**

that utilize **artificial intelligence** and **machine learning** are employed. In addition to collecting, evaluating and making use of large amounts of data (**big data**), simulation data is also generated (**hybrid models**). **Digital twins** allow for processes to be visualized and increase our understanding of the impact process changes can have on the process sequence as well as the final component properties.

**Climate change** requires, among other things, an **energy transition** towards electric drives and accumulators, fuel cells, as well as the efficient production of energy sources such as methane, hydrogen and biofuels. This requires tailor-made material solutions. Due to the **electrification of mobility**, special functional properties (magnetic, thermoelectric, etc.) and structures (e.g. porous materials and highly entropic alloys) come to the fore in addition to the traditional structural properties.

The increasing mix of materials poses great challenges for the **recyclability** of components and parts. In the future, disassembling and recycling will be taken into account in the design and manufacturing phases in order to improve the **material circulation**. In addition, the increased use of recycling materials leads to changed base material compositions, which must be taken into account when developing joining processes or necessary additional materials. Impurities in particular can significantly affect weldability (susceptibility to cracking, process window) or certain properties (strength, toughness, fatigue strength), even in very small quantities. **Developing more durable materials** is in line with the **European Green Deal** agreed in 2021. Therefore, IMAT focuses on the development of highly creep, fatigue and corrosion-resistant materials for high performance operations.

## Approach

### Materials design:

One research core area is the **materials design** of high-strength, corrosion-resistant, wear-resistant and high-temperature steels. Specific subject areas include: Q&P medium manganese forged steels; body sheets for use in the automotive sector characterized by an exceptional combination of strength and toughness [1], low LME tendency in resistance spot welding and good galvannealing properties [2]; creep-resistant ferritic-martensitic steels [3]; and Q&P N-martensite with special

mechanical and corrosion properties [4].

### Additive manufacturing (AM):

**AM processes** in combination with upstream and downstream heat treatment, processing and machining processes make it possible to generate custom material properties and component structures. Powder-based processes, including the **laser powder bed process (LPBF)**, have the intrinsic advantage that a wide variety of powder mixtures, i.e. chemical compositions, can be processed. In addition to pre-alloyed powders, **in-situ alloying** can also be utilized by mixing elementary powders in the right proportions. Graded chemical structures are made possible by multiple powder reservoirs or variable powders in one reservoir. Locally changing properties (e.g. strength, toughness, magnetism) can be realized by changing process conditions (energy input, laser shape and focus, hatching distance). Our research activities focus on **printing light metals** (Ti, Al), **magnetic alloys** (Fe-Cr-Co, Nd-Fe-B) and porous structures for catalytic processes. The Fe-Cr-Co alloy system treats rare earth-free **hard magnets** with special directional magnetic and processing properties [5]. The Nd-Fe-B magnets have very good magnetic properties, but setting the optimal microstructure in the AM process poses a challenge. By producing powder from recycled old magnets, these can be transferred to the material cycle. Our research also focuses on reusing Ti64 powder for printing aerospace components [6]. AM process optimization makes it possible to create structures that are as pore-free as possible on the one hand and to create **highly porous structures** with a high specific surface area on the other in order to further develop catalytic processes for biofuel production. **Integrating sensors** during the printing process allows for measuring of pressure, temperature, humidity, flow velocity, etc. in AM components.

**Wire as a starting material** has the advantage of being easier to add and manage, as well as being available and drawing on previous experiences in the field of build-up welding. Advanced control and automation make it possible to create custom three-dimensional structures or coatings. The **wire can be melted** using an arc, laser or electron beam or in a plasma. Combined processes involving multiple wires and powders allow for complex heterogeneous structures to be printed or components to be manufactured by in-situ alloying. Here, alloys based on known filler materials are produced with variable feed rates to meet the

requirements despite the complex T-guide. Through the use of two wires or flux-cored wires, alloy development can also be specifically supported or simplified for special applications. A particular challenge is the increasing **contamination of the materials** as a result of the increasing use of recycling materials. This reduces or shifts the process window, which is why the **determination of the characteristic curves** for the processes is becoming increasingly important.

**Advanced joining and forming processes for metals:**

In addition to **gas metal arc welding processes**, which are widespread in industry, we also deal with **friction welding, electron beam welding and plasma welding**, thus creating a basis in teaching and research to promote these innovative processes in Austria. These methods form a valuable supplement to the basic processes and allow for solving of specific problems. By avoiding melting during friction welding or by processing in a vacuum during the electron beam process, it becomes possible to join an extended range of materials. In particular, research topics include **thermal, mechanical and hybrid joining of dissimilar material combinations**, such as aluminum-steel or aluminum-wood. The parent materials and the resulting compound materials are characterized under static and cyclic loads [7] and tested for their formability. For this purpose, **instrumented joining and forming machines** are available on an industrial scale, which allows for direct implementation of the research results in industry [8, 9]. The interaction of the high-strength materials to be processed with **hydrogen** is examined using methods of **diffusion modeling** and **experimental analysis** in order to determine the influence of the structure and the processing conditions on hydrogen binding and embrittlement [10].

**Advanced manufacturing of hybrid materials and structures:**

The manufacturing of metal-composite hybrid structures presents great challenges, due to their incompatibility in physicochemical material properties. The R&D approach at IMAT has the goal of mitigating these challenges by combining materials science knowledge, joining and additive manufacturing (AM) processes to produce **metal-thermoplastic composites** hybrid structures (MTC-HS). These hybrid structures have high strength-to-weight performance, improved damage tolerance and crashworthiness. Moreover, MTC-HS have good reparability (e.g., by thermal

joining or welding) and are easily disassembled and recycled since their thermoplastic composite matrix can be remelted; therefore, thermoplastic composite matrix can be returned to the material cycle. The methodology of AM of hybrid structures combines materials science knowledge, and new additive manufacturing routes, which are supported by process optimization, modelling and simulation tools. Our scientific-engineering approach is schematically presented in Figure 1. In this methodology, innovative **friction-based joining techniques** are combined with **additive manufacturing** of metals (powder bed and directed energy deposition processes) and **engineering thermoplastics composites** (e.g. via FFF/FDM) to produce MTC-HS.

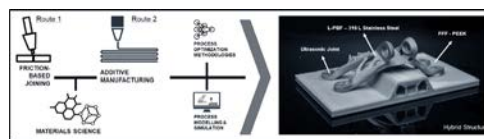


Fig. 1. IMAT's scientific-engineering approach for manufacturing advanced metal-polymer/composite hybrid structures.

Two innovative manufacturing routes to produce MTC-HS have been followed at B-EPA: a) **friction-based joining (FB-J)**; and b) **additive manufacturing (AM)**. In the friction-based joining method (a) both the metal and polymer/composite parts are produced separately, whereby formative, subtractive or additive manufacturing can be used for this purpose. A FB-J technique is subsequently utilized to join the MC-HS. In the AM method (b), the metal part is preferentially produced by AM processes (state-of-the-art metal manufacturing processes may be also applied) and is subsequently hybridized by polymer or composite by polymer/composite 3D printing. Process optimization methodologies, such as design of experiments (DoE) and analysis of variance (ANOVA), as well as machine learning are combined with process modelling and simulation (i.e., FEA, CFD, Topology Optimization) to understand and optimize the manufacturing processes and properties of MC-HS.

**Advanced tools for modeling materials and simulation of processes: Modelling and simulation tools**

support the development of new materials in terms of chemistry and processing. Particularly with the processing, microstructures are created that lately determine the mechanical, thermal and physical properties of the workpiece. In this sense, correlating

the process with the microstructure and the properties is the main goal stated here. Depending on the scale, the models are classified as **atomistic**, **mesoscale** and **macroscale models**.

IMAT is very strong in developing meso- and macroscale models. In the last decade, we have developed:

- **Mesoscale models** to describe the evolution of the microstructure during **hot working, dislocation creep** and **stress relaxation**. We used **dislocation reactions** to model creep curves in P91 steels [11, 12] and adapted for **hot deformation of Ti-** [13] and **Al-alloys** [14]. This last model was extended to describe the creep strain of **Ni-based superalloys** and stress relaxation for Al-alloys (both to be published) to converge in a unified physical model. Tertiary creep damage due to porosity and coarsening of precipitates was included in [15].
- One **physical-based model** using the same microstructural variables for all three phenomena. The motivation for developing the unified model comes from the aspiration of solving the following issues:
  - Alloys are usually modelled separately. Some previous works have shown that different alloys behave similarly during plastic deformation. We identified that the **stacking fault energy** regulates the formation and annihilation of dislocations, and thus, the hardening and restoration mechanisms. Since the stacking fault energy value depends on the chemical composition of the deforming phase and the temperature (both may vary during thermomechanical processes), we can develop models that describe the behavior of the material depending on the stacking fault energy.
  - The scientific community has identified the similarities between **dislocation creep** and **plastic deformation** phenomena for many years. We have used physical approaches and extend the concepts to **stress relaxation**. Furthermore, we consider the presence and evolution of phases and

precipitates.

- Models are developed usually for isothermal and homogeneous conditions along the workpiece and samples. We deal here with **heterogeneous microstructures evolutions** within workpieces.

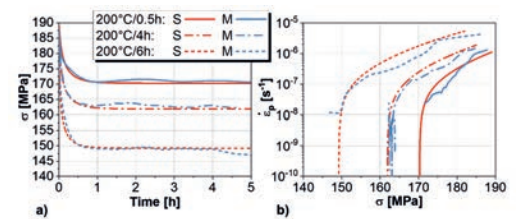


Fig. 2. Simulated (S) and measured (M) stress relaxation of an aluminum cast alloy during artificial ageing process for different precipitation conditions a) stress evolution over ageing time and b) plastic deformation rate over the stress relaxation (results presented in the LigthMat 2023 conference in June 2023 in Trondheim, Norway)

- Descriptions of **microstructural features** such as grain size, dislocation densities and precipitation state in final or intermediate products within the workpiece. Using the heterogeneous conditions at the laboratory scale, we can validate our models for large industrial products [16]. This was used to describe **forging** and **rolling processes** as well as **friction stir welding** and **thermomechanical welding**.
- Subrogate models for implementing physical mean field models into **finite element simulations** aiming at a lower computational time for forging of titanium alloys. [17]
- Integration of **CALPHAD based simulations** to describe the microstructure in terms of stable and metastable phases with mesoscale models [18]. Therefore, we could account for the interaction of boundaries and defects with different phases during plastic deformation.

## Impact

Out foundational research has a **scientific** and **socio-societal impact** in multiple ways. Topics of knowledge-oriented research are driving improvements in the field of **lightweight construction** through new high-strength steels, aluminum alloys and also hybrid materials and components. In this way, energy can be saved in mass transport in the future. **Hydrogen-resistant steels** will accelerate developments in generating, transporting, storing hydrogen. New AM devices with porous structures will accelerate and cheapen catalytic processes for biofuel production, thus enabling their uptake and supporting the **energy transition**. **Recycled magnetic powders** will improve the material cycle and reduce dependency on countries that distribute rare earths. The **functionalization of AM components with sensors and actuators** will make it possible to obtain data from components in use that was previously impossible or only possible to integrate with considerable effort. The **use of modern AI and ML methods** and **cross-scale modeling and process simulation** will enable more efficient and optimized process routes for the production and processing of smart materials and components.

**Application-oriented development** supports our business partners in optimizing their materials, processing methods (AM, joining, forming) and applications, thus generating an **economic** and **industrial impact**. In the long term, the implementation of the specific, partly unknown processes in **teaching** expands the possibility of working on certain questions in a targeted manner and applying alternative solutions. Close cooperation with research partners from national and international industry ensures that the research topics we work on are highly relevant to those industries and that research results can be directly implemented in an **industrial environment**. Furthermore, our students are well prepared for their future careers due to this cooperation in the context of research projects and theses with industry.







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## Competencies

IMAT, the Institute of Materials Science, Joining and Forming of Graz University of Technology, holds **workshops and laboratories** to conduct research tasks. These include: the **physical testing laboratory** for determining thermo-mechanical properties under static and dynamic loads; the joining laboratory with MIG/MAG welding, friction stir welding, electron beam welding, plasma welding, ultrasonic welding and wire-based additive manufacturing; the **corrosion laboratory** and **hydrogen testing laboratory**; the **metallographic laboratories** with light microscopy and scanning electron microscopy; the heat treatment laboratory; the **AddLab** with the laser powder bed process; and the creep laboratory with an industrial press, wear testing, surface inspection and facilities for mechanical joining.

IMAT is part of a **global network** of numerous scientific and corporate partners and is active in bilateral and funded research projects, including within the framework of the Austrian Science Fund FWF, the Austrian Research Promotion Agency FFG, the Christian Doppler Research Association CDG, and the EU. Austria has established itself as a hub for research and innovation by hosting numerous **congresses** in the field of materials and processing. These include **Thermec** (2016, 2021, 2023), the Esaform Conference 2015 and the triennial "**International Seminar on Numerical Analysis of Weldability**". On average, we release one peer-reviewed publication per week and supervise around 40 doctoral theses. Institute staff are active and recognized members in various national (Austrian Society for Metallurgy and Materials ASMET, Austrian Society for Welding Technology ÖGS, Austrian Standards, ...) and international committees (International Institute of Welding IIW, ...).

With more than 60 **courses** in the bachelor's and master's degree programs in mechanical engineering, mechanical engineering and business economics, advanced materials science, production science and management, and technical chemistry, we make a significant contribution to teaching the fundamentals of materials science and applied production technology. Numerous lecturers from the industry make use of current case studies and ensure that the content taught is practically relevant.

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# Advanced Materials Science & Analysis

Johannes D. Pedarnig, Kurt Hingerl

## Vision

**Advanced Materials Science** plays a pivotal role for modern industrial products and processes. It helps to develop **new energy generation technologies**, more resistant hard coatings, custom designed sensors for a specific interaction with environmental parameters, and also more **energy efficient devices**, all of them supposed to be easily recyclable and less toxic. Examples are fuel cells, advanced steels, hybride materials synthesis, wafer surfaces, corrosion and tribological coatings. The Centre for Surface and Nanoanalytics (CSNA) acts as a mediator between basic research and applied material science, serving both the in house (JKU) institutes as well as cooperating interested Austrian and European companies. It plays a primary role through support of interdisciplinary and interfaculty research, training and education. It further provides in one unit essential resources for electron- and ion beam characterization of materials, for determining optical properties, for micro- and nano-characterization, through specific analysis techniques for surfaces and interfaces.

Smarter production processes and the fabrication of smart products require **Advanced Materials Analysis** for fast and comprehensive investigation of all relevant materials at all steps in the production chain. The measurement and monitoring of the chemical composition of raw materials, additives, chemical agents, intermediate substances, by-products, and the final material and product are key points in **smarter industrial processing** and essential to **strengthen European Industry competitiveness** [1, 2]. This holds for many industrial branches, for example metallurgy, polymer

technology, electronics, chemistry, construction and building, recycling, etc [e.g., 3, 4]. The Institute of Applied Physics (IAP) is performing scientific research on the development and application of novel laser-based techniques. The current topics of research are: (i) Optical sensing for chemical element analysis, (ii) Nanophotonics and metamaterials, (iii) Laser-matter interaction processes (thin films, surface modifications). This includes measurements in the laboratory, modeling and simulations, and also field measurements, for instance in industrial environment on site at production plants.

- **Physics**
- **Chemistry and Compositional Analysis of Advanced High-Tech Materials**
- **Surface and Nanoanalytics**
- **Process Monitoring in Manufacturing of Complex Materials and Industrial Products**

## Approach

The aim of the **Advanced Materials Science task** is to understand the Physics and Chemistry, i.e. the underlying function: we put great emphasis placed on fundamental properties of materials, surfaces and interfaces rather than on applied science and product development. Naturally, application of materials is the ultimate goal, but this needs to be built on firm theoretical basis so that improvements can be made more efficiently and reliably. Particular

attention is therefore given to **understanding a material's behaviour from the atomic/nano-level via microstructure to macrostructure levels** using advanced analytical techniques and computer modelling. This strategy is applied to both the improvement of conventional "bulk" materials, such as steel, and to new functional materials for increasingly smaller, "smarter" devices", e.g. MEMS.

The aim of the **Advanced Materials Analysis task** is to develop laser-based measurement techniques for compositional analysis of "technical materials". The interaction of intense laser radiation with the relevant materials and the optical response of samples (e.g. the emission of laser-induced plasma, LIBS) are studied to develop measurement systems for fast and accurate analysis without time-consuming preparation. The LIBS method can be applied to materials in

form of solids, liquids, gases, powders, etc. **Multi-component industrial materials are quantitatively analyzed** by calibration-based and calibration-free methods (trace/minor and major elements) in the laboratory and on-site / in-line / at-line in industrial environment [5 - 7].

The Materials Science and Analysis work is performed in national and international research projects and in **co-operation with various industrial partners from different branches** (e.g., Austrian industries such as Fronius International, OMV, voestalpine Stahl, Lenzing, EVG, Kraiburg Austria) and with innovative start-ups (SMEs). Our partners provide scientific and technical challenges to our specific blend of competences, facilities, and we contribute with our research approaches in strategic national/ international R&D partnership activities.

## Impact

With our **Advanced Materials Science and Analysis activities** we are addressing scientific and technological issues as well as societal needs.

We are aiming for a detailed understanding of all physical and chemical processes relevant for the development, fabrication, optimization, and production of novel, functional high-value materials. Besides fundamental scientific investigations we are aiming also for technological advancements to cope with the requirements for different industrial applications, e.g. the development and integration of sensing systems.

We expect our RTD activities to **contribute to the development of novel tailor-made materials**, the optimization and production of high-tech materials, the in-line process monitoring etc. and to have significant impact in various branches such as metal, chemical, and polymer industries. Furthermore, large societal impact is reached by the education and training of young scientists on modern topics that are relevant for our industries. This includes scientific and technological topics and conjunct topics such as resource-efficient production processes and sustainability.



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## Competencies

Our operational research units (JKU Institute of Applied Physics IAP, JKU Center for Surface and Nanoanalytics ZONA) are well interwoven with national and international R&D projects. Besides skilled and creative scientists, the research units ZONA and IAP offer a broad range of analytical facilities for co-operation:

- SEM/EDX – Scanning Electron Microscopy / Energy dispersive X-ray spectroscopy
- FIB/SEM – Focused Ion Beam / Scanning Electron Microscopy
- TEM – Transmission Electron Microscopy
- FT-IR – Fourier Transform-InfraRed spectroscopy
- XPS – X-ray Photoelectron Spectroscopy
- AES – High Resolution Auger Spectroscopy
- XRD – X-ray diffraction system for structural analysis of solid materials
- AFM – Atomic force microscopy
- TG – Thermogravimetry
- OM – Optical microscopy (bright field, dark field, fluorescence)
- 3D-OM – White light interferometric 3D optical microscopy
- Various types of laser sources (continuous wave and pulsed from nanosecond to femtosecond)
- Various types optical spectrometers
- Materials synthesis equipment (incl. evaporation, sputtering, laser deposition, sintering, spin coating)

In addition, the following techniques are especially useful for optimization and for process monitoring in-situ and in real time, e.g. in production processes:

- SE – Spectroscopic Ellipsometry for determining the real and imaginary refractive index (NIR-VIS-UV, laboratory based)
- IR-SE – Infrared Spectroscopic Ellipsometry for chemical analysis (laboratory based)
- Raman – Raman spectroscopy for chemical analysis (laboratory based)
- LIBS – Laser-Induced Breakdown Spectroscopy: Mobile and transportable systems for element analysis out-of-laboratory
- Full-field Optical Coherence Microscopy

All these analytical techniques are accompanied with our expertise down to the shop floor, through consultancy for process monitoring [8 - 10]. Further analysis techniques are available in cooperation with Chemistry Institutes of JKU Linz.



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# Optimizing Material Applications

Udo Pappler

## Material Analysis and Quality Assurance

Since its foundation in 1946, the vision of the Austrian Research Institute for Chemistry and Technology (OFI) has been to support companies in material selection and **quality assurance**. With testing, inspection, certification, consulting as well as applied research and knowledge transfer, OFI supports different industries in their innovation efforts with **interdisciplinary expertise**. Start-ups and SMEs in particular, which do not have their own research departments, benefit from OFI's know-how and its wide range of RDI services. The unifying element is the examination of materials in the broadest sense - from the investigation of new materials to the development of alternative methods for analysis and the optimization of concrete applications. Sustainability, recycling and recyclability are aspects that are becoming increasingly important in production and thus also in product design. These aspects are consistently reflected in the current research focus areas that the approximately 120 OFI experts are currently working on.

plastic(s), paper and aluminum - in the most diverse designs - are not recyclable in most cases. Up to now, the individual materials or layers can hardly be separated from each other with technical solutions and, accordingly, cannot be recycled with the same quality. Based on this initial situation, OFI is conducting intensive research into sustainable solutions.

- **Materials Technology**
- **Applications**
- **Analysis**
- **Recycling**
- **Circular Economy**
- **Sustainability**
- **Method Development**
- **Quality Assurance**
- **Life Science**
- **Health**
- **Photovoltaics**
- **Safety in Use**
- **Product Durability**
- **Applied Science**

## Research Focuses

### Recyclable packaging

Packaging today must be modern all-rounders in order to be considered sustainable. This also means that they must be as recyclable as possible. A great deal of **research and development** work is currently required to ensure that this succeeds. After all, what has proven to be a safe, material-efficient packaging solution in recent years rarely meets the requirement for recyclability. Combinations of

In addition to developing new solutions that already take **Design for Recycling** criteria into account, it makes sense to review existing packaging for its recyclability. Results of an independent analysis can not only serve as a basis for optimization, but also provide a valuable advantage over the competition. To assist in this regard, OFI, in cooperation with the cyclos-HTP Institute (CHI), offers a **comprehensive assessment of the recyclability of packaging**. This assessment system is an established industry standard,

compliant with the German minimum standard, and also integrates Austria-specific sorting, recycling and recovery structures. OFIs' long-term knowledge with the optimization of packing solutions adds an extra value to that research focus.

### Use of recycled materials

In addition to designing recyclable solutions, the packaging industry has to overcome another hurdle on the way to a functioning cycle. With the exception of PET, recycled plastics are currently not approved for food contact. In the absence of concrete data, the European Food Safety Authority (EFSA) has so far assumed a worst-case scenario and that any contamination in a recycled plastic is a mutagenic substance, potentially carcinogenic even at the lowest concentrations. Since it is not possible to determine all substances in a recycle using chemical analysis alone, this stipulation means that many recycled plastics have so far completely been excluded from reuse in the food sector. In some cases, this means that materials are taken out of circulation because of a single component that may not even be hazardous.

As part of the "PolyCycle" research project, the project consortium, which includes OFI, has succeeded in **developing a novel test strategy** for the comprehensive **safety assessment** of plastic polymer recyclates. This involves a biological method known as the Ames test. This makes it possible to determine whether or not a plastic contains a potentially carcinogenic substance on the basis of its effect on a bacterial culture. In the follow-up project "SafeCycle", the focus is now on identifying the origin of detected mutagenic effects in recyclates.

### Animal-free test methods

For a long time, there was no way around animal testing for the **biological evaluation of medical devices**. There was a lack of reliable alternatives. As part of the "BioRelation" project, an interdisciplinary research team has addressed the issue and developed a strategy for risk assessment of complex materials and medical devices using bioassays and chromatographic methods that can be used to characterize biocompatibility. Specifically, cell systems will be used for this purpose. In vitro tests can be performed at an earlier stage of **product development**, so they help with **product optimization** and provide faster results than animal testing.

In the meantime, non-animal approaches to risk assessment, such as the methodology developed by OFI

as part of the "BioRelation" research project, have also found their way into the ISO 10993 standard. Animal testing is still part of the standard, but in vitro methods are listed as a recognized alternative. The **use of bioassays** for other product groups can also lead to new insights there. Currently, OFI is conducting research in the "LEIFS" project on **new test strategies for menstrual products** in order to obtain a scientific basis for the safety assessment of disposable and reusable articles.

### Hygiene processes in healthcare facilities

Hygiene concepts play an important role, especially in hospitals and care facilities. Nevertheless, so-called nosocomial infections caused by hospital germs are on the rise. In many cases, these are germs that are resistant to antibiotics and can be particularly dangerous for immunocompromised people. To prevent the emergence and spread of infections, it is crucial to further **optimize hygiene practices and the underlying processes**.

In several research projects, the OFI is therefore addressing **different aspects of cleaning and disinfection** and the special requirements that healthcare facilities place on hygiene processes. In the "SaferTex" research project, for example, OFI has focused on the interaction of cleaning agents and disinfectants with textiles. Currently, within the framework of "RobiDES", the development of an autonomous hygiene robot is being pursued, which is to reduce infection germs by means of **UV/LED**.

### Real-life testing of filters

Even before the outbreak of the corona pandemic, experts at OFI were already working on the topic of **air hygiene** and - at that time still with a focus on allergy sufferers - researching ways to improve **indoor air quality through the use of filter systems**. As part of the "Aeropore" research project, a simulation system was set up at OFI that allows filters to be assessed according to biological risk. With the aim of making life easier for allergy sufferers in the future, the research project focused on allergenic particles such as pollen, fungal spores and fine dust. With the emergence of the coronavirus, the method was quickly adapted. As a result, OFI is one of the few places in Europe where filter modules can be realistically tested for **the separation performance of viruses and bacteria**. This service benefits not only plant engineers and ventilation manufacturers, but also vehicle manufacturers and the travel industry. In order to be able to carry out analyses

independent of location in the future, further research is being carried out in the “Aeromobil” research project.

### Identification of microplastics

The most important function of packaging is to protect consumers by maintaining the quality of food on its way from production to the consumer. Many of these packaging solutions are made of plastic. Therefore, until now, when microplastics were suspected in food, it was automatically assumed that these plastic fragments came from the packaging. However, without a serious, established methodology, this is merely conjecture.

The international research project “microplastic@food” starts here and focuses on the **development of methods and research into microplastics in food**. It is part of the CORNET (COLlective Research NETworking) initiative, which promotes international research projects for the benefit of small and medium-sized enterprises. The aim is to develop a reliable, reputable detection methodology to find out whether microplastics are present in the human food chain, and if so, in which foods. In the case of particle detection, potential sources and pathways of microplastics can then be investigated. For this purpose, both the quantification and the identification of the detected particles are carried out.

### Design of PV modules

Photovoltaics is considered a sustainable option for energy generation, the importance of which is set to increase even further in the future. In order to make the best possible use of their potential, photovoltaic modules and their possible applications are constantly being developed further. The goal is to make them reliable and stable over decades. With applied research & development, OFI supports this goal step by step. Research projects are currently focusing on the topics of **long-term durability, recyclability and end-of-life management**.

PV modules are multi-material composites. It is difficult to recycle them. Therefore, usually only the glass is recycled, the rest is considered electronic waste or plastic waste and is disposed of. In order to be able to put as many components as possible back into a material cycle, it is necessary to know the material composites and to be able to separate the materials from one another, preferably layer by layer. The project “PVRe<sup>2</sup> - Sustainable Photovoltaics” has dealt with this initial situation and looked for solutions.

This has not only resulted in an **initial scientific basis for follow-up projects**, but also in the development of a repair option for backsheet cracks, which can increase the service life of PV modules.

## Impact

What the research projects have in common is their objective: by means of **applied research & development**, the **quality of products** is to be increased, the **use of resources** is to be made more sustainable, and **novel methods** are to be developed so that the **safety of products and processes** can be measured in the future as well. In addition to sustainability, recycling and recyclability, increasing digitalization also plays a role for manufacturing companies. As an **independent research and testing institute** that, among other things, supports SMEs in their **innovation efforts**, OFI is part of the European Digital Innovation Hub (EDIH) Applied Cyber Physical Systems (CPS) together with ACR (Austrian Cooperative Research) and other project partners. Together, the aim is to professionally advance the development and operation of cyber-physical systems (CPS) for SMEs, start-ups as well as the public sector in Austria and to efficiently implement them for the construction, mobility and industrial sectors. In doing so, the entire value chain of CPS is covered.

In order to (even) better exploit the potential that digitization and sustainability efforts in production hold, the creation of interfaces is necessary. Applied research that not only includes different expert voices, but also **directly involves the manufacturing industry and users**, is an important piece in the mosaic for positioning Austria as an **innovation partner** in the European research landscape. As an independent testing and research institute and member of the ACR research network, OFI works together with Austrian start-ups, SMEs and large companies to address current challenges and research forward-looking solutions.



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## Progress in good hands

As a testing and research expert, OFI supports its customers in product development and accompanies them all the way to market launch.

120 employees test and confirm the reliability of materials, whether for use in automotive engineering, packaging or in the healthcare sector. To make sure that products are fit for the market.

OFI assess constructions and plans renovation measures, to ensure the safety and sustainable use of houses, bridges, streets and monuments.

Under an umbrella, OFI offers: individual consultancy, trendsetting solutions to complex questions, securing quality and safety.

OFI is a founding member of Austrian Cooperative Research (ACR), a network of private research institutes that support SMEs in their innovation efforts.





# Modelling mechanical Properties of Engineering Materials

**Bernhard Sonderegger, Gerold Zuderstorfer, Florian Riedlsperger, Bernhard Krenmayr**

## Vision

Metals and alloys are the second largest category of structural materials following concrete, and traditionally play a vital role in Austria's industrial landscape with its focus on mechanical engineering. Semi-finished products, parts in automobiles, aircraft components and energy plants, medical implants – applications are plentiful. In high-tech applications, excellent, precise and reliable mechanical properties are the key for new materials to be accepted in an increasingly competitive global market. Depending on the specific material and application, mechanical properties of interest are as diverse as elastic limit/ yield strength, stress-strain curves (at various temperature regimes and deformation rates), ductility, cyclic behavior, toughness etc. Looking at the most prominent alloying groups for structural applications, we are mainly (but not exclusively) looking at steel with its diverse properties, Nickel-base alloys for high temperature applications and Aluminum alloys for lightweight constructions.

“Better” and more reliable properties of materials generate positive side effects for manufacturers and societies such as:

- Reliability/safety/quality of components
- Less energy and CO<sub>2</sub> consumption during production due to optimized production routes
- Less consumption of resources due to optimized chemical composition
- Less consumption of resources due to higher strength of the materials, enabling more efficient lightweight constructions

- Lower production costs.

Within a competitive global market, the design and development of new/ improved materials demand for time-efficient routines beyond “trial and error” approaches. This can be achieved by actually “understanding” and predicting the material behavior. Since the engineering properties of the structural materials result from thermal, mechanical and/or thermo-mechanical loads during production and service, we need to understand the impact of these external parameters on the properties. In order to understand the material properties, one has to uncover their underlying physical roots. In general, any macroscopic property is based on phenomena on micro- and nanoscale. This suggests a modelling concept

- **Metals and Alloys**
- **Physically based Modelling**
- **Microstructure**
- **Material Simulator**
- **Thermodynamic Modelling**
- **Dislocations**
- **Precipitates**

including the relevant microstructural constituents and their interactions, and deducing the macroscopically observable properties from this point of view.

Currently, we are in the process of setting up an according easy-to-use online “material simulator” software with integrated microstructural models. The software includes the interaction of relevant microstructural constituents, such as dislocations, (sub)grains and precipitates. Micromechanical models enable establishing microstructure-

property relationships. Once critical parameters are identified (e.g. those responsible for a drop of strength or toughness), materials can be **virtually** optimized. This implies cheaper and faster development routines and/or safer and longer operation of components which depend on the longevity of their structural alloys (power plants, engines etc). The software features a user interface running on an ordinary internet browser. This interface lowers the entrance barrier for new users and is ideal for disseminating our research within the scientific community, thus initiating an international database of modelling approaches.

The medium-term vision is to set up an online-platform containing executable interactive microstructural material models, serving industrial partners as well as the international scientific community. However, the long-term scope goes beyond that, since a myriad of scientific/technical tasks can be formulated by our simulation tool (see approach section). The framework can bring together experts from scientific fields ranging from material scientists, physicists, chemists, environmental scientists (any field where the experts can formulate their models as differential equation systems) and experimentalists, who want to test their results against the included models. The implementation will make testing and comparisons simple. New models can be uploaded, edited, tested online and shared within the community, reaching significant impact a lot faster than by current means of conventional information exchange.

Last, but not least: we select models not only according to their capability of including the underlying physical phenomena, but also by their capability of providing reasonably short computing times. This feature fosters strategies such as parameters studies or systematic variations of side conditions in complex systems (backward engineering to finding optimized production routines).

## Approach

From a scientific point of view, the mechanical response on external loads is governed by the microstructure (evolution) of the material, the interaction between the microstructural constituents, and the manifestation of these interactions on a macroscopic level. These interactions have to be understood on a fundamental physical level, formulated

into models and then applied for optimizing the material in parallel to actually answering the scientific questions on the very nature of the phenomena.

In addition, experiments can be very costly and time-consuming (e.g. creep tests may take over a decade). Modelling the microstructural changes occurring over such long periods of time is a good alternative to substitute for experiments and speed up the development of new alloys. By understanding the underlying physics, materials for specific applications can be optimized by tuning process parameters or initial microstructure. In this context, modelling approaches with statistical representation of the microstructure have a huge advantage over spatially resolved simulations: their calculation time is much shorter and the results can be interpreted more straightforwardly.

This general situation suggests the 4 complimentary approaches of our institute:

**Approach 1:** Identify/improve/develop/interconnect physically based microstructural models of complex structural alloys, which are suitable for predicting macroscopic engineering properties within reasonable computing times.

This aim demands following side conditions of the respective models:

- Target results are yield strength, various stress-strain curves, deformation rates, ductility, high temperature behavior etc.
- Target loads are constant loads, variable loads or cyclic loads. Broad range of deformation rates, broad temperature regimes. Loading schemes should be able to represent production routines and service conditions.
- Microstructure evolution and microstructural interactions.
- Physically based sub-models (as opposed to phenomenological models, which lack predictivity)
- Results have to be representative on a macroscopic level
- Models are fast enough to allow for short computing times for inversion techniques and/or FEM representation of components

Keeping in mind reasonable computing times, this task can best be achieved by models containing a statistical representation of the microstructure (spatially resolved information can be

included from a statistical point of view) by “representative volume elements”.

Prominent examples of these model types are the MatCalc model for phase transformation, precipitate evolution and generally microstructural evolution in complex alloys [1], the 3IVM model for a detailed look on dislocation interactions [2], and derivatives of the Ghoniem model [3], which have been developed for steel [4], Ti-alloys [5] and Aluminum [6]. These models can also integrate sub-models for specific microstructural phenomena such as dislocation climb-and glide, grain boundary mobility, phase boundary energies etc.

Of course, simulation results have to be validated by actual experimental investigations, leading to our second approach:

**Approach 2:** Validate the results by mechanical tests and microstructural investigations considering various thermo-mechanical exposures

The thermomechanical exposures are aimed to either mimic production and service conditions, or provide standard material conditions for easier model validation. The engineering parameters of interest are then either tested in-situ during the thermomechanical exposure (e.g. by our quenching & deformation dilatometer), or/and a-posteriori by instrumented stress-strain experiments, tensile tests etc. Standard light optical investigations can be carried out in our lab as well. For more elaborate investigation including SEM and TEM techniques (precipitates, matrix boundaries, dislocations) we rely on close cooperations to ZONA (JKU) and FELMI (TUG).

All modelling and experimental results are to be combined into one general simulation tool. This leads to our third approach:

**Approach 3:** Development of a “material simulator” which is combining/merging the individual models and providing a simple-to-use device for testing of a model against experimental data.

The prototype of the material simulator is currently developed in our institute (present name is “CreeSo” due to its first application on modelling creep deformation rates). It combines an easy-to-use interactive user-interface for operators of the software (for simulating the material behavior), with developer tools for implementing material models. We would like to point out that even the developer tools

do not require the knowledge of any programming language. The software is able to create solutions for complex coupled differential equation systems (DEQs). In the context of material models, the DEQs are representing the governing physics of the microstructural evolution of complex alloys, whereas the parameters in the equation systems are either indicating microstructural constituents (and their respective time evolution) or physical constants. Macroscopically observable properties of the material (such as deformation rate) are calculated on the base of the microstructure applying according micromechanical models.

“CreeSo” has a HTML5 frontend and a C++ backend. This allows us to produce a desktop and an online version with only little extra effort on one hand. On the other hand, we can use the maximal computational speed of the hardware by the use of C++. Current tests on a complex creep model suggest calculation times roughly 10 times faster than equivalent MatLab code. Both HTML5 and C++ are platform-agnostic (which means a change of the operating system is relatively simple).

The software, however, is not limited to the description of creep - very general DEQs can be solved. Currently we are working on the descriptions of other physical material properties (relaxation, creep-fatigue, high-temperature strength). In the future, the software does not even have to be limited to the scientific field of mechanical engineering. Other applications in research and engineering are conceivable and planned (but probably not under the name “CreeSo”).

With the use of an internal DSL (Domain Specific Language) it is possible to compile the models into DLLs (dynamic link libraries) and also to produce a mathematical display of the equations. However, the DSL allows for many features in the nearer future, as checking the units of measurement and other constraints of the equation systems. The DSL also allows for the exchange of models within the scientific community and a better comparison of different models. The further aim is to expand the models from sets of differential equations into an ontology, a wider digital representation of knowledge in a database.

The capabilities of the material simulator suggest our fourth approach:

**Approach 4:** Distributing and providing a framework of online-executable models and complementing experimental data

The capabilities of the software and its HTML5 frontend allow us to provide an online version with integrated executable material models. Partners can either test the built-in models against their experimental data or formulate their own models and test them online. The platform is also planned to act as exchange hub for executable material models as well as experimental data.

## Impact

The potential impact of our work is plentiful. On a very basic level, we are going to continue our work in setting up material models depicting the plastic deformation (rate) of complex alloys under various temperature- and stress loading conditions (constant, cyclic, random, slow, fast, high and low temperatures; steel, Ni-base alloys, aluminium, others). In addition, we are combining these frameworks with physically based models on the individual microstructural constituents (e.g. models on phase boundary energies, line tensions of dislocations, mobility of matrix boundaries, atomistic modelling of nano-segregation effects etc.). In the near future, we aim at generalizing our current (Ghoniem based) model to a point where it can be combined with alternative approaches such as 3IVM – reaching a point where we can handle a wide range of plastic deformation (and related) phenomena with several aspects of one single unified model.

These individual models (and networks thereof) are continuously implemented into our material simulator software. This implementation kicks-off a number of positive side effects: first, it elevates “inactive” models (such as journal publications) to interactive experiences, which can be tested immediately by the user. Second, complementary models can be directly merged and combined. Third, users can upload experimental data and can test competing models against them. In total, representative digital twins of a complex alloy (including its microstructural evolution and plastic response to loading) can be set up.

These features open the powerful opportunity to create a universal online-tool and information exchange platform for material models, which is open to the scientific community and industrial partners. An online test-version is planned for late 2023. The platform will be continuously fed by our own (interactive) models and experimental data, and will be open for extension, testing and online-calculations by any registered user. The feature which is setting this tool apart from established communication platforms is its interactivity – models are not merely stored, but ready to be applied and tested immediately, and thus lowering the barrier between developers (basic science) and adopters (applied science and industry).



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## **Competencies**

The members of our institute have a long ranging experience in microstructural-, micromechanical- and thermodynamic modelling of complex alloys as well as mechanical and thermomechanical testing.

With respect to software, we are currently developing a material simulator (“CreeSo”) which includes various extensions of the Ghoniem model and is able to simulate plastic deformation rates of complex steels under high temperatures and creep load. This software is continuously extended to wider fields of application (see sections “Approach” and Impact”). For testing purposes, we code the according models in MatLab as well.

In addition, we work with MatCalc software and are experienced in setting up precipitate kinetic simulations during heat treatments and service, Scheil calculations and equilibrium simulations.

Apart from operating software packages, we are keen on designing physically based models for microstructural constituents in complex alloys. In the past, we have set up novel concepts for martensitic transformation, phase boundary energies [7], nucleation theory (latter two are implemented in MatCalc software), 3D atomistic Monte Carlo [8], and general frameworks of interacting microstructural constituents (coupling of dislocations, matrix boundaries and precipitates) [4].

Within our lab, we are equipped with a quenching & deformation dilatometer, which can reproduce a wide variety of heat treatment and production routines plus in-situ mechanical testing during these routines (Linseis L78 RITA Q/D/T). In addition, we provide standard mechanical test equipment (Universal testing machine Hegewald & Peschke UTS 100 kN, Charpy impact test, Hardness testing machine Zwick/Roell Durascan G5), light optical microscopy and a metallographic preparation line for further external electron-microscopical investigations (carried out externally at ZONA/JKU or FELMI/TUG). We furthermore provide a heat treatment furnace (Nabertherm LT 15/14) for heat treatments up to 1400 °C.



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# Embedded Sensors and Actuators in Microsystems

Wolfgang Hilber, Bernhard Jakoby

## Vision

**Sensors and actuators**, also referred to as **transducers**, can be found in **virtually all areas of life**, either directly visible or doing their work hidden in the background. Major fields of application are the automotive industry or, more generally, transportation, intelligent buildings and smart textiles, environmental monitoring and control, communication and information technologies, industrial process and quality control, aerospace and defense (i.e., security), smart consumer products in general, and health care. **Modern automobiles**, as an example, represent familiar as well as **highly complex sensor actuator systems**. Automotive manufacturers employ a steadily increasing number of transducers, for instance, for engine control, recently also for hybrid, fuel cell and fully electric engines, for vehicle control, crash avoidance, passenger comfort and convenience, and safety as well as security issues [1]. A typical vehicle nowadays contains over 30 electronic systems and more than 100 sensors which continually communicate with the on-board computer or possibly even with a data center in the world wide web (www). In this context, a modern vehicle can be seen as a **mobile resource of sensory data and sensor-related services** [2]. This very same concept, utilizing the vehicle as a mobile sensor, opens up new and exciting possibilities for urban sensing, with advantages not only for the driver of the automobile, but also for third parties and the society as a whole. In general, a **tendency** can be recognized towards **smart or intelligent sensor actuator systems integrated and embedded into objects of the daily life** around us, which are not only designated to collect raw data, but which are also able to perform self-

diagnostics, self-calibration and which are capable to communicate with each other with the help of wireless networks like the World Wide Web. This vision of a world, where virtually everything communicates with everything over wireless networks, also known under the catchword **IoT (Internet of Things)**, has the potential to improve and promote life together in our society by providing new and innovative ways to connect, communicate, and collaborate. For example, in **healthcare IoT devices** can be used to monitor and track health conditions, allowing for **better management and treatment**: wearable fitness trackers can help people stay active and track their progress, while connected medical

- **Miniaturized Sensors and Actuators**
- **Printed Electronics and Transducers**
- **Functional Composite Materials**

devices can monitor vital signs and alert healthcare professionals if there are any concerns. Or in the above discussed field of **transportation, IoT devices** can be used to improve transportation, making it **more efficient and safer**: connected vehicles can communicate with each other and with traffic lights to optimize traffic flow and reduce congestion, while also providing real-time updates on road conditions. However, regardless of the actual field of application, for the **technical realization** of the **IoT** there is **substantial need for intelligent mechanical sensor systems** (e.g., tactile sensors, gyroscopes and

accelerometers) and smart chemical/biological sensor systems (e.g., microfluidic systems, electronic nose/tongue) [3].

## Approach

For the realization of the sketched vision of IoT it will be inevitable to equip objects around us more and more with transducers for data collection, system monitoring and user interaction. Resulting therefrom, to **meet** the ever-increasing **need for cost- and resource-saving methods** for fabrication of specifically devised transducer concepts, cost- and resource-saving **additive production techniques** such as printed electronics have gained considerable attention in the recent decade.

Originally developed as a method for realization of electrically conductive interconnections in the early 1940s, the technology has proven also as a suitable technique for processing newly developed, so-called **functional or stimulus-responsive nano-composites**, the base material for modern **embedded transducers** [4]. Though in the main applied to flat substrates such as printed circuit board (PCB) based materials, polymer, ceramic or glass sheets, the technique can, in modified form, also be applied to objects with a **three-dimensional surface topography**, facilitating the integration of transducers into the surface of unusual objects such as **metallic machine parts** or **everyday necessities** that are nowadays in the main made of polymers and related materials. For this purpose, in order to achieve reliable functional coatings with uniform and reproducible physical properties, the conventional **thick-film deposition processes** must be **adapted**. The main issues in this context are technological issues related to (i) surface roughness and porosity of a possibly pre-existing protective coating into which the transducer is to be integrated, (ii) compatibility between the solvent system of the functional ink and the protective coating, which is related to the surface energies, (iii) the actual deposition and masking process, which must be adapted for three-dimensional substrates, and finally (iv) sophisticated schemes for control and/or readout of the embedded transducer, in particular if the substrate is metallic or, more generally, electrically conductive. Typical additive printing techniques utilized in this context are **screen- and stencil print, ink-jet, airbrush** and **water transfer print**, just to name a few

methods that can also be used at the industrial scale.

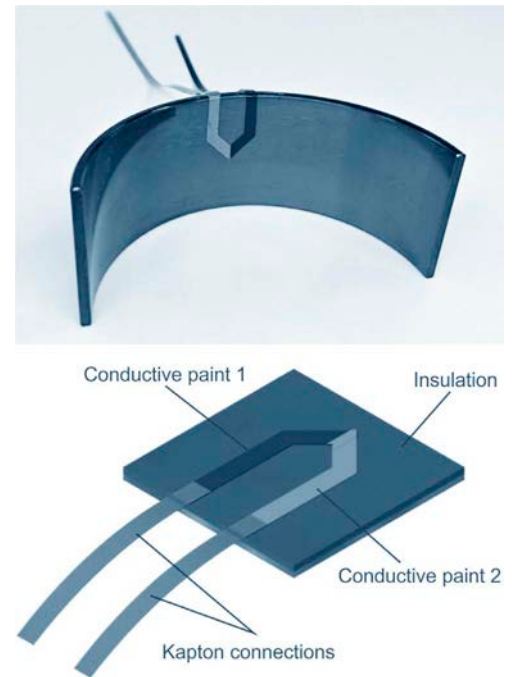


Fig. 1. Integration of a spray-coated temperature sensors into the organic surface coating of a plain bearing shell (top) and the underlying sensor concept utilizing the thermo-electric Seebeck-effect (bottom).

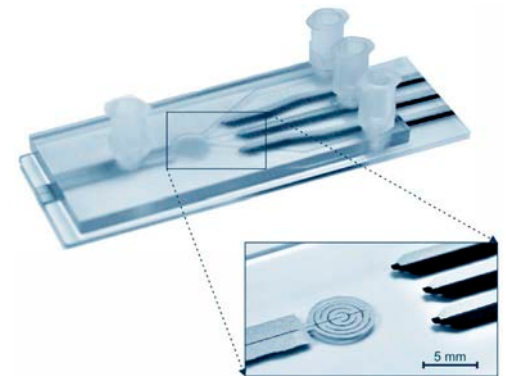


Fig. 2. Screen-printed sensor for thermal flow velocity measurement in a microfluidic chip: picture of the fabricated device with 3D printed channel featuring fluid connections and the sensor geometry printed on the bottom slide [6].



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## Competencies

The **Institute for Microelectronics and Microsensors** at the JKU operates a well-equipped **technology lab** with cleanroom section for material development and realization of specifically devised transducer concepts with conventional and enhanced thin- and thick-film techniques. Here, in recent years resource- and waste-saving additive techniques became a major focus, such as, for example, screen, stencil and 3D printing of polymers and related functional composites, particularly suitable for realization of embedded sensor systems in surface coatings. For testing and characterization of devised sensor concepts the institute operates an **electronics lab**, also equipped with special equipment for long-term measurements under defined environmental conditions.

The main research competences comprise (i) **modeling and simulation** of miniaturized sensors and actuators, (ii) investigation, design and **fabrication** of demonstration devices with focus on **novel functional**, i.e., **stimulus-responsive nano-composite** materials that are specifically suited for additive production techniques, (iii) design and implementation of **control** and **readout electronics** at the demonstrator level, (iv) **system integration**, and (v) characterization of **performance** and accuracy.

Recent funded research activities are allocated in the area of embedded and printed transducers based on functional nano-composites for environmental monitoring and user interaction, miniaturized sensors and sensors systems for assay of complex fluids, as well as microfluidic lab-on-a-chip concepts for system integration.

## Impact

Here, in order to **demonstrate versatility** and **adaptability** of our technological approach, we mention briefly **two niche applications** of printed and embedded transducers, that cover the range from possibly **very large metal parts** to **tiny polymer chips**.

When it comes down to increasing functionality and added value of industrial products based on sheet steel, a possible approach may be the integration of sensors and actuators into the organic surface coating, typically already present for the sake passivation and corrosion protection, by additive printing and embedding of functional inks and pastes. In doing so, elements for user interaction like switches and touch pads, for measuring and recording of environmental parameters, or for monitoring of the structural health and condition of the mechanical construction around may be implemented. Also, the measurement of physical parameters at locally defined positions that would otherwise not be accessible with discrete sensor elements represents a potential field of application [5]. A particular example of this approach is the integration of **printed temperature** and **pressure sensors** into the **organic surface coating of bearing shells**.

On the other hand, the very same sensory evaluation scheme may also be of interest for completely different objects, so called lab-on-a-chip (LOC) or micro-total-analysis-systems ( $\mu$ TAS), tiny, mostly polymer based, chips with integrated microfluidic structures for the use in bio-chemical assays. In these microscopic fluid streams, the physical parameters like temperature or flow velocity are hardly accessible using standard MEMS transducers without disturbing the experimental conditions due to the particularly cramped conditions. To this end, the embedding of printed transducers based on functional composites on the side walls of the microchannel is an appropriate way to assess the desired parameters of the fluid sample under investigation [6]. These two examples illustrate the capability of functional nano-composites for the integration and embedding of transducers into the **surface of objects** that are **usually not considered** for equipment with sensors and actuators, or **at positions** that are **difficult** to access with classic measurement techniques utilizing discrete sensor elements. In this context, embedded sensors in microsystems may foster the implementation and dissemination of transducers in everyday life, thus contributing to the proclaimed vision of IoT.

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# Novel Surfaces and Electrochemistry: Key Elements for Sustainability

Markus Valtiner, Tanja Singewald, Philipp Fruhmann

## Vision

Innovations in energy and surface technologies are required to advance industry toward much-needed sustainable solutions. Solving these problems will lead to drastic carbon use reductions and radical new profit opportunities for the industry leaders delivering these solutions. The Center for Electrochemical Surface Technology (CEST) is at the nexus of this much-needed research and its vision is to set the future standards for electrochemical surface and interface engineering needed to create solutions for a circular and sustainable world & economy. Companies need to operate more efficiently, effectively, and sustainably to remain competitive - Novel surfaces and electrochemical methods lead the way through CO<sub>2</sub> reduction, capture and conversion technologies by three core visions:

- **Solutions for CO<sub>2</sub> reduction, capture, and conversion**

CO<sub>2</sub> and the related climate change, is probably the greatest challenge and has great social and economic importance. Beside our liability to find solutions for upcoming generations, CO<sub>2</sub> also has a huge economic potential since the recycling pathways have the combined potential to abate 6.8 gigatonnes of CO<sub>2</sub> per year worldwide when displacing conventional production methods [1]. The potential market growth for Austria alone is expected to be around 20-40 Mio €/year and is not even including potential revenues by valorization of CO<sub>2</sub> derived valorization products.

- **Solving crucial problems in long-term energy storage**

The need for energy storage systems and solutions is crucial to achieve a sufficient degree of energy autonomy and price stability for the industry. We are aiming to improve redox flow batteries, which come with a current market size of about ~170 Mio €/yr. and are expected to reach ~700 Mio. €/yr. on a global scale by 2028 [2]. To fully unlock this potential, novel materials for broad, economic, and long-time use are needed.

- **Surface Technology**
- **Electrochemistry**
- **Coatings**
- **Sustainability**
- **Energy Conversion**

- **Material life cycle prolongation by new solution for corrosion protection**

The globally costs of corrosion are estimated with 2.5 trillion €. By closing the corrosion problem, annual savings of \$375-875 Billion €/year are expected. For Austria alone, this is a 12 billion € problem and novel surfaces with improved corrosion resistance are essential to prolong material lifetimes and achieve prolonged lifetimes [3].



## Approach

To ensure applicable solutions with respect to the complexity of the topic, the **approach can only be based on a high degree of independence and cross-sector partnerships throughout the entire value chain to provide solutions which can be immediately used in industry.** Although the development of novel functional surfaces is the key element within the efforts to improve sustainability, they are not limited to a specific use case and are essential in nearly aspect related to the energy transition and green solutions in industry. Starting with the currently hyped field of Hydrogen (H<sub>2</sub>) together with carbon capture, utilization and storage (CCUS), impressive progress is made on an

fundamental level of understanding. Both are critical technologies for decarbonization efforts and a transition from the fossil fuels to sustainable solutions.

However, huge challenges come with their future widespread implementation in industry and energy supply. Beside insufficient amount of green energy for such processes, a giant lack of suitable H<sub>2</sub> and CO<sub>2</sub> compatible infrastructure (pipelines, transport, storage...) as well as downstream infrastructure (turbines, engines, suitable pioneer plants) are heavily hampering the practical transformation in a reliable energy ecosystem [4]. This especially accounts for the fast material embrittlement due to H<sub>2</sub> corrosion.

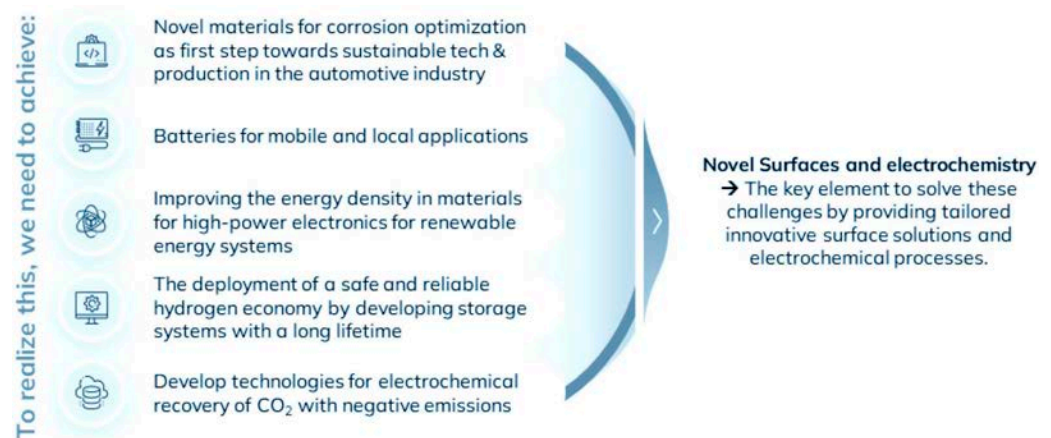


Fig. 1. Short overview about the Important role of novel surfaces and electrochemistry to achieve sustainable solutions for (I) decarbonization, (II) materials for the energy production and (III) novel energy store materials.

### The core approach to overcome these issues is the development and optimization of suitable electrochemical processes and materials which can withstand the resulting conditions.

Although energy storage seems not directly related to these issues, the know-how related to these challenges are immediately applicable to storage systems, since the requirements are often closely related. Starting with the decarbonization by capture and conversion of CO<sub>2</sub>, novel electrochemical systems are key systems [5], since they usually directly rely on electrons as reactive species, which are accessible by conventional as well as green technologies. In addition, their high efficiency and the lack of toxic chemicals and waste are outstanding properties, which makes them highly attractive for the implementation in a wide range of different processes. Although

these systems can generate value added chemicals and potential substitution products for oil, novel materials for the fabrication and storage of the intermediates and products are required. All mentioned aspects can perfectly be tackled with electrochemistry and surface technology, but the implementation of developed solutions for suitable large-scale infrastructure will require years for its implementation. For this reason, battery technology is essential to store excess energy as buffer system for a high degree of flexibility and autonomy. In addition, new energy materials and improved storage systems are highly demanded due to the raising energy prices, which started an explosive growth in the exploitation of renewable energy resources.

Considering that the globally existing electrical grid systems are not suited to handle the mass integration of these intermittent energy sources without

serious disruptions, the importance of storage systems with increased energy density, prolonged lifetime and a fundamental understanding of the relevant working and degradation processes on a fundamental level is demonstrated.

In addition, it is worth to mention that on a global level there is only about ~170 GW installed storage capacity, whereas 96% comes from the pumped-hydro sector which is site-constrained and not widely available [6]. All these facts are clearly pointing out the need for novel and improved energy storage systems.

To tackle this challenge, it is necessary to focus on redox-flow batteries, where the energy is provided by two liquids which are separated by a membrane. The liquids are pumped through the system and can be easily exchanged anytime to regenerate the whole setup. Although different redox flow systems are already described, the remaining way towards widespread use is difficult, due to non-optimized system components ranging from the electrolyte and the membrane to the not fully understood electrochemical processes in the system. **For this reason, the approach to achieve a solution will be development and improvement of new materials for energy generation and storage.**

In addition, the fundamental understanding and related surface characterization with high-end equipment, such as e.g. low energy ion scattering (LEIS), are the required crucial parts, to provide a holistic solution and to **enable a sustainable energy transition tailored for the specific needs in industry.**

We therefore focus on the development of novel materials and electrochemical processes to create sustainable solutions with partners which comes with collaborative patents and a thriving cooperative work environment.

You're invited to join CEST on this journey!

## Impact

The holistic approach towards new materials and improved electrochemical processes bears the unique potential to **provide solutions for the energy transition and decarbonization along the whole value chain**. Although the impact based on the already ongoing improvements in the three (sub-)areas is remarkable, the impact in each of the three fields are perfectly matching each other:

**(I)** Suitable materials and electrochemical methods for CO<sub>2</sub> capturing and conversion offer the unique possibility to generate value added products out of CO<sub>2</sub>, which technically is an “end of life product”. Considering the current legislative situation requires payments for CO<sub>2</sub> certificates, a huge impact on industry at the industry can be expected upon wide availability.

**(II)** Novel materials and improved electrochemical understanding in corrosion mechanisms are essential to establish the necessary network for the widespread use of hydrogen and related decarbonization products. The availability of inert materials towards embrittlement are a fundamental requirement for an industrial scale use of H<sub>2</sub> and have a crucial impact.

**(III)** Similar materials and electrochemical processes can be used to develop and optimize energy storage systems, which are crucial to achieve a sufficient degree of energy autonomy and reliable economic energy supply in industry. Considering the easy scalability of redox-flow batteries (e.g. ship container size), the impact towards energy autonomy is huge, especially when in industrial scale is required.



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## Competencies

Our operational research units (Center for Electrochemical Surface Technology, Wr. Neustadt & Linz) are equipped with high end analytical equipment such as SEM or LEIS and is completed by state-of-the-art electrochemical equipment. In addition to our nearly 50 well trained scientists, we have several running EU and national projects and several universities as close cooperation partner [7], which allows PhD students and easy university access in cooperative projects.

For details, please visit [www.cest.at](http://www.cest.at) or contact us directly.

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# Reliable Electronic Products

Bernhard Czerny, Thomas Walter, Golta Khatibi

## Vision

In the global competitive market of electronic industry, the emerging technologies are confronted with challenging trends of higher functionality, smaller feature sizes, increased packaging density, and capability of **performance at harsher operational conditions**. Realization of advanced devices involves implementation of novel material systems and fabrication technologies. Moreover, fulfillment of mandatory safety and environmental restriction leads to a further limitation of the material choice. Along with technological innovations, the business trend is characterized by cost reduction and **shorter-time-to-market**. Reducing the technology time cycle is one of main keys to success and market leadership in the electronics sector.

The complex structures of microelectronics which involve combinations of materials of different properties with sizes ranging from several millimeters down to few nanometers is highly susceptible to fatigue and failure throughout the service life. The major causes of failure in electronic devices and components are due to thermo-mechanical, vibrational and electrical loading during the production and service. **Thermo-mechanically induced stresses** caused by **thermal mismatch** between the constituent materials, are considered as one of the main reliability concerns and a **bottleneck in the development** of present and future microelectronic components. Considering the vulnerability of the established technologies to failure, significantly higher number of critical sites with still unknown failure modes may be expected in advanced devices which operate under more severe conditions.

Keeping up with the rapid technological advancements and market demands requires application of **highly accelerated** and practice relevant **reliability assessment methods**. Reliability tests are commonly designed to simulate typical applications of electronics in an accelerated manner to obtain the required results in a reasonable time. There is an urgent necessity for new and **reliable accelerated testing procedures** especially for qualification of new products and implementation of new process parameters. For example, assuming five years warranty for electronic devices, variation of only two chip geometries and ten production parameters in an interconnected device result in a variety of unknown interconnect properties. Determination of the influence of these parameters on the quality of the interconnect requires performance of numerous test series resulting in unrealistic testing and development times and encountered costs.

- **Electronics Reliability**
- **Accelerated Testing**
- **Fatigue of Interconnects**
- **Material Modelling**

In industrial practice, the majority of thermal and electrical or combined reliability testing procedures are based on pass /fail criteria. If necessary or required, encountered failure mechanisms are evaluated by a subsequent **failure analysis**. The recent reliability trends demand physically meaningful and rapid testing procedures which also provide “**end-of-life**” data of the devices. Accelerated



tests are commonly conducted by excessive changes in variables such as temperature, humidity, load, current, and voltage resulting in degradation and failure in a short time. These provide information about the **global reliability of the devices** and probably onset of failure. Yet there are limitations to thermal stress test due to physical characteristics of the electronic devices. Further acceleration by exceeding a critical temperature or excessive time reduction may result in occurrence of failure mechanisms other than those encountered in real application or even result in a suppression of these failures. For these reasons, manufacturers of electronic products are continuously seeking **alternative efficient, cost-effective and trustworthy accelerated test (AT)** methods to keep up with the today's market demands. On the other hand, **physics-of-failure (PoF)** has become an integral part of the design and development cycle of all electronic products, whether they are consumer items with a design life of 3 years or safety-critical systems with a **design life of 30 years**.

## Approach

Recently **accelerated mechanical fatigue testing (AMT)** has been proposed as an alternative reliable and time-saving method for qualification of electronic devices [1]–[4]. The principal idea is simulation and **substitution of thermally induced strains** in the components by means of equivalent mechanical strains, by using suitable experimental set-ups. The duration of testing can be efficiently reduced by increasing the testing frequency. Based on a PoF approach, the relevant failure modes are specifically induced to the **material interfaces** or critical connections enabling fast detection of weak sites of the devices.

The schematic principle of the occurring thermomechanical stresses during operation, failure modes and critical interconnects and accelerated mechanical fatigue testing set-ups are illustrated in Fig. 1. An AMT testing set-up consisting of a oscillating system, which **induces forced cyclic vibrations** in a micro-component or device. Depending on the direction of oscillation of the sample to the system, different loading modes e.g. shear, tension-compression or mixed mode loading can be induced. The value of **stress in the interconnect area** can be adjusted by selection of the displacement amplitude of the vibrating system, which also depends on the interconnect area and on the

mass of the component. The oscillation amplitude can be measured contactless by differential laser Doppler vibrometer (LDV), which are also applied for detailed modal analysis of the sample and the test set-up.

Finite element simulations can be applied for calculation of the complex state of **stress in the multi-layered structures** and lifetime modeling by using realistic time and temperature material data and experimental boundary conditions. As an additional feature, **in-situ modal analysis** can provide information on the **degradation behaviour** of the samples during the vibrational testing. Different loading frequencies and amplitude ranges are achieved by using experimental set-ups consisting of various shaker systems or high frequency transducers for excitation of the samples. **Ultrasonic resonance fatigue testing systems**, and piezo- and electromagnetic shakers working in a broad frequency range starting from few Hz to several kHz are applied.

Using different configurations of this set-up allows testing of model test structures as well as samples out of production with different scales and material combinations and determination and evaluation of their critical interfaces or interconnects. **Life time curves** are obtained as a function of strain / stress amplitude versus loading cycles to failure in a very short time. **Cyclic shear fatigue or bending fatigue** configuration can replicate the most significant **failure modes in interconnects** (heavy wire bonds used in high power semiconductor modules, fine thermosonic bonds used in power chips, solder joints in surface mounted devices, chip or substrate solder, multilayered thin films, multilayered substrates etc ... [5]–[10]).

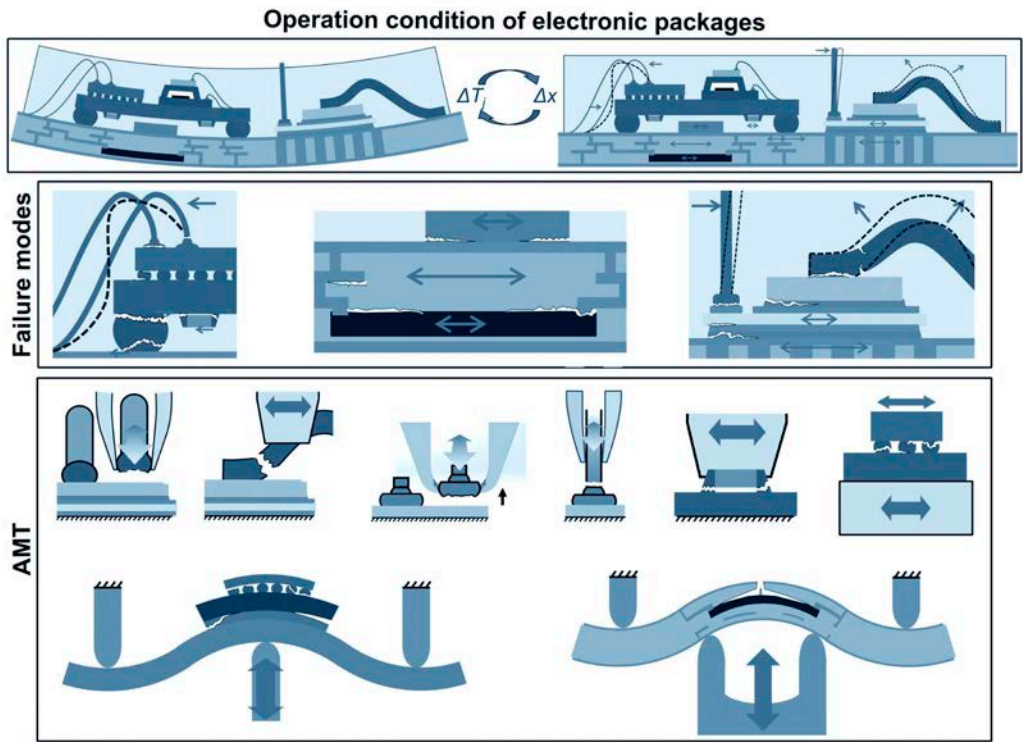


Fig. 1. Schematic diagram showing the conditions of electronic packages under thermomechanical stress, the resulting fatigue failure in a joint due to combination of temperature cycling and CTE mismatch and schematic principle for a variety of accelerated mechanical fatigue testing set-ups for specific components and interconnects.

## Impact

A remarkable advantage of AMT is the possibility of **decoupling of thermal, mechanical and environmental stress factors** for a more effective investigation and diagnosis. Considering that the reliability problems are often caused by various **thermal and mechanical loadings** associated with design and processing steps of the devices, the approach by AMT methods can be used for screening and evaluation of a large number of design and production parameters in an **extremely time saving** manner. Implementation of adequate temperature and frequency dependent acceleration transform functions allows establishment **reliable lifetime prediction models**.

The approach of **implementing highly accelerated mechanical fatigue testing methods** provide manufactures of devices with a tool to **enhance the reliability** of their products and **improving the manufacturing processes** within the **short time to market** parallel to the development and production stage. Combining such experiments with simulations for virtual prototyping in a **Design-for-Reliability** approach can provide rapid evaluation of the lifetime for novel material systems and design innovations.

The impact to the competitive electronic industry is time to market and ability of innovative designs without uncertainties of reliability concerns. This approach enables **proactive product design** which expedites advancements and pushes novel product solutions due to the **timely advantage** and leads to a ruggedized products for a **sustainable electronics** equipment. Implementation of AMT allow companies to outperform their competition on a global scale in terms of **process reliability, quality and durability** and secure and expand their frontrunner position.



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## **Competencies**

**Bernhard Czerny** is program director for the bachelor program applied electronics and photonics at the university of applied sciences Burgenland. As a physicist his area of research is specialized on reliability of electronic packaging and developing novel accelerated fatigue testing methods, in close cooperation with industrial partners over several research projects at the UNI Wien, TU Wien and FH Burgenland over the last 15 years (FFG K-Project “micromat”, CDL “RELAB”). His development of BAMFIT fatigue tester with BONDTEC and INFINEON won the productronica Innovation Award 2019 for future market clusters. Current research projects (FFG “semicond4buildings”) focuses on electronic and photonic packaging and reliability in building applications in a living-lab environment within the department Energy and Environment and the center for building technology at the FH Burgenland.

**Thomas Walter** is a physicist specialized in design and development of test equipment in accelerated mechanical testing and micromechanical material testing and characterization. His expertise of more than 10 years has lead to numerous academic research projects in the field of adhesion of thin film in semiconductors, and to close cooperation with semiconductor partners in the power electronics industry. He has patented qualification methods for coating adhesion of hard protective metal coatings. At present he works on the development of non-destructive methods for early failure detection of multilayer electronic packages.

**Golta Khatibi** is a materials scientist with a PhD degree in technical chemistry. She is a professor at TU Wien leading the research group Mechanical Response of Materials. The main field of her research is studying physical and thermo-mechanical properties of materials and structures in small dimensions. A special focus of her research group is design and development of novel diagnostic tools for investigation of fatigue lifetime and long-term reliability of electronic components. With a long-term experience in this field, she has been project leader and key researcher in several international scientific and industrial projects including a Christian Doppler Laboratory for Lifetime and Reliability of Multi-Material Electronics. She with her research team was awarded the prestigious Houskapreis 2021 in the category higher education for the project “high reliability power electronics”.

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# Integrated Computational Materials, Process and Product Engineering (IC-MPPE)

Werner Ecker

## Vision

In the coming years, humankind will probably face its greatest challenges to date – addressing the issues related to climate and environment and securing prosperity in the face of changing geopolitical constellations and a continuously growing world population. To meet these challenges, the European Commission has defined the so-called Green Deal in 2019, a new growth strategy that will transform the European Union (EU) into a fair and prosperous society with a modern, resource-efficient and competitive economy whose growth is decoupled from resource use, including the goal of reaching zero net emissions of greenhouse gases by 2050 (European Commission 2019, The European Green Deal).

**Materials** and materials production inherently consume raw materials and energy, making them the **key to a successful implementation of the Green Deal goals**. Hence, in the production sector issues such as energy and resource efficiency in manufacturing as well as circular economy become central in addition to the classical development goals of realizing new, innovative, reliable and cost-efficient solutions and functionalities.

The second major challenge is the digital transformation of industry. Key topics such as big data, Artificial Intelligence (AI), robotics, the Industrial Internet of Things (IIoT) and high-performance computing are transforming the very nature of work.

The rapid development of computing power, the availability of high-performance computers in combination with suitable algorithms

and software opens up previously unknown possibilities to introduce AI in engineering and production (European Commission 2020a, WHITE PAPER – On Artificial Intelligence). AI is a possibility to accelerate materials and process design [1, 2] and knowledge discovery [3, 4]. The recent developments in AI-based technologies, e.g. applied for chatbots, have demonstrated the enormous possibilities of AI to a wide audience.

Essential components of the digital transformation are platforms, standards and technologies for data processing, data storage, data exchange and data analysis: in this way, existing research results can be used more efficiently in the long term. **Digital platforms** will play a crucial role in future materials science and technology as they **have the potential to change**

- **Materials Design Platforms**
- **Circular Economy**
- **Sustainable Materials**
- **Multiscale Simulation**
- **Materials Characterization**

### **the paradigm in the engineering of materials, processes and products.**

Such platforms provide a powerful basis for combining data from experiment, simulation and literature, enabling entirely new approaches to both (i) integrated computational and AI based engineering, and (ii) multiscale simulation and modelling of materials, processes, and products (i.e., components and systems).

Manufacturing plays a critical role in the economy of industrialized countries.



In Europe, the manufacturing industry is seen as one of the backbones of the European economy and the combination of materials and process engineering (often supported by advanced simulation) with smart mechatronics is seen as one of its key elements (EuropeanCommission2020b, Made in Europe). Because materials are involved in every step of the manufacturing process chain, **innovations in materials science and engineering are essential to the technological advances required for next-generation manufacturing.**

European production industry is, both, a driver and a subject to the ecological and digital transition. The challenges of this twin transition are great and include the integration of AI, the use of industrial process data, the transformation to a circular economy and the need for agility and responsiveness. And, manufacturing system capabilities need to follow product and material roadmaps to enable viable and sustainable manufacturing of these high-tech products. The program “Made in Europe” will exploit the possibilities offered by advanced materials, digital and manufacturing technologies to achieve a considerable reduction of the ecological impact and CO<sub>2</sub> emissions. On an ecosystem level, recycling and reuse of materials and components will be increased while still raising the performance of the manufactured products (EuropeanCommission2020b), which is in principle a contradiction in terms and therefore a major challenge.

**The Integrated Computational Materials, Process and Product Engineering (IC-MPPE)** research program of MCL as well as of our COMET-K2 Center IC-MPPE go in line with the vision of a Common Digital Materials Data Space of the Materials 2030 Roadmap published in 12/2022 by the Advanced Materials 2030 Initiative and **comprises**

- **sustainable computational engineering of local product properties**, tightly integrated into the **circular economy lifecycle** chain
- industrial data science for **model-based condition monitoring** and for **autonomous systems** using the IIoT and allowing for **Predictive Maintenance and Reliability of structural components and electronic systems** and for **Smart Process Control and Predictive Quality in manufacturing processes** of metallic components and microelectronic systems, and

- **AI-driven Materials Acceleration Platforms (MAP)** enabling a radically **accelerated development of novel functional materials, respecting the Green Deal goals** (e.g. circular economy, zero-emission, zero-waste, avoidance of critical raw materials).

## Approach

The IC-MPPE approach of MCL has pronounced similarities with **Integrated Computational Materials Engineering (ICME)** (TMS2013, ICME; NASA2018, Vision 2040). The goal of ICME is to enable the optimization of materials, manufacturing processes, and component design long before components are actually fabricated, by integrating the computational processes involved into a holistic system. ICME has reached a level of maturity that allows it to be used fruitfully on an industrial scale, solving problems that were unattainable a decade ago [Doghri2020, Whitepaper: ICME for beginners]. It allows engineers across all industries to use the optimal combination of materials and manufacturing processes to innovate and maximize product performance while reducing cost and lead time. It enables **new design paradigms** by modelling the strong coupling between materials, manufacturing, and product performance.

Examples of our research approach applied to **computational multiscale materials design** [5, 6], model based process design [7, 8], as well as hybrid modelling and AI-based **digitalization and virtualization of manufacturing** [2, 3, 9] can be found in literature. MCL's research approach is supported by the Materials 2030 Roadmap (AMI2022), highlighting the importance of a holistic computational approach in materials research as such:

*“The combination of digital technologies such as high-performance computing, big data management, knowledge engineering based on ontologies and artificial intelligence (AI) revolutionises research and development methodologies that enable this digital transformation by merging computational (modelling, simulation) and experimental materials data (high throughput characterisation). They are supporting the screening of materials properties, materials development, and production processes.”*

With our approach, we contribute to the accelerated development of new and improved materials,

processes, parts and components for green mobility, green energy technology microelectronics, and tooling. To this end, **we develop and use fundamentals, experimental methods, simulation tools, software and workflows required for IC-MPPE.**

From a methodological point of view, we address the following key topics:

- Further development of **physics-based material models**, simulation tools and software on all relevant length and time scales.
- Integration of the different material models, simulation tools and software that predict phenomena at different length and time scales.
- **Integration of multiscale material models** and simulation tools into engineering software to simulate material phenomena in manufacturing processes and in products during use.
- Development of a **digital materials design platform** to utilize data from physical modelling, experiments, and literature in a new integrated computer aided materials design workflow.
- **Development of automatically searchable libraries** of structured, labelled FAIR (findable, accessible, interoperable, reusable) data including property, production, and microstructure data (images) from simulations, experiments, and literature for use with our digital materials design platform.
- Use of AI technologies for the **simultaneous development of materials, processes and products.**
- Development of **novel material characterization techniques** focusing on (i) validation of material models, (ii) determination of parameters for material models, and (iii) in situ characterization methods
- Development of expertise to effectively construct hybrid models (i.e., combined physics-based and data-driven models) for (i) **model-based** materials design, (ii) **process design, monitoring, and control**, and (iii) condition monitoring and predictive maintenance of components and products.
- Targeted development of new, **resource-efficient and climate-friendly materials, manufacturing processes** and products using the new validated simulation tools.

## Impact

With our activities we contribute to all “common R&D needs” related to materials processing and scale-up which are defined in the Materials 2030 Roadmap, namely: **1) process optimisation, 2) decarbonisation, 3) mass customisation, 4) zero defect production, 5) circular economy, 6) multi-materials processing, 7) new materials processes.**

The innovation potential includes **material-based innovations along the circular economy chain**, such as **new and significantly more sustainable materials, manufacturing processes and products**, but also new models, simulation tools and software for computer-aided design and planning processes, as well as the **realization of smart processes and products with embedded intelligence**. The implementation of these innovations in practice is ensured via cooperative R&D projects primarily with Austrian and European companies, which are often international leaders in their business fields.

The impact of the IC-MPPE approach is manifold and it has high impact in accelerating the green transition. Within our COMET K2 center devoted to this topic we published 134 papers in 2022, thereof 99 in international peer-reviewed journals. The set of experimental and numerical methods developed over the years and its integration to holistic workflows, software packages and platforms leads to a significant speed-up of research and development processes.

The **holistic and simulation-supported approach** provides detailed knowledge of the microstructure evolution during production as well as of the corresponding local material properties within the product. A thorough understanding of the material behaviour and of how it may be beneficially modified throughout the whole circular product life is crucial for the development of processes and products following the paradigm of the Green Deal. Examples for such improvements are localized heat treatments instead of energy intensive full component treatments, substitution of natural gas heating by hydrogen or induction processes, through-process-chain optimization of sheet steel cores for electric drives for optimized efficiency, or low-defect, high-yield single crystal growth processes for microelectronics applications.

The automated AI-based workflows (e.g. active learning) integrated in our Materials Accelerator Platforms (MAPs) in combination with the combined utilization of FAIR data from experiments, physics-based models and literature allow for a radical acceleration of materials and process development. MAPs are favourably applied for new materials design in a large design space which is yet very little explored. An example for such a use case is the development of perovskites, a material class with an impressive array of interesting properties (e.g. ferroelectricity, superconductivity, magnetoresistance). Other examples are **the substitution of critical raw materials** while maintaining the materials' properties (e.g. for battery or fuel cell components) or the design of bainitic steels combining high strength and high ductility.

The **application of industrial data science** to build condition-monitored and autonomous production systems using the IIoT adds another quality to process engineering and control. The condition monitoring system can either rely on pre-existing data sources or on retrofitted production equipment. Since the lot sizes of many metallic products are rather low, purely data-driven methods often fail due to a lack of training data. For those cases we follow a **hybrid semi-parametric approach combining physical modelling and machine learning (AI)**. A well-established IIoT system for manufacturing processes has beneficial effects on the tool, the production process, and the product. For example, an in-line tool health monitoring system helps to use tools and assets more efficiently on one hand, and to avoid scrap on the other hand. **Smart process control and predictive quality systems**, which have the workpiece in its focus, play a crucial role in



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## Competencies

**MCL has about 170 employees.** Our strategic business areas cover research, development and services. The research activities are structured in three departments focusing on **Materials Technology, Multiscale and Multiphysics Simulation and Materials for Microelectronics** each with about 50 researchers, respectively. **MCL runs the COMET K2 IC-MPPE** with more than 40 scientific and more than 30 company partners. **MCL is partner and coordinator in many national and international research projects.** We also offer our competencies as a service and in form of trainings within our MCL Academy.

Circular economy is a key competence of MCL: we aim at improving the performance and extending the lifetime of materials and products, we develop sustainable manufacturing processes and solutions to up-cycle materials. Through **computer-aided technologies based on high-end characterisation, measurement data, physical models and AI**, we accelerate the development of new and improved materials, parts and components **for green mobility, microelectronics, energy technology and tooling.**

Our condition monitoring, process control and predictive maintenance solutions enable adaptive, property-optimised manufacturing and maintenance-efficient assets and products. With all of this, we are driving the twin, digital and green, transformation of the production industry and are ensuring its sustainable competitiveness in an international context.

We have **laboratory facilities for materials characterization and testing on all length scales**, ranging from mechanical testing, through scanning electron microscopy, thermal analysis and heat treatment to dedicated microelectronics test methods. For more details see [www.mcl.at/en](http://www.mcl.at/en). MCL is also **ISO 9001 certified** and offers a large and continuously increasing portfolio of **ISO 17025 accredited testing methods**. In the field of **numerical modelling** and simulation we cover and integrate **all length scales and many different physical domains**: basic material properties can be calculated with atomistic modelling, e.g. Density Functional Theory (DFT), and subsequently integrated via CALPHAD (CALculation of PHase Diagrams), thermo-kinetics or phase field models in order to solve higher-scale problems; on the higher scales we also use the Finite Element Method (FEM) and Computational Fluid Dynamics (CFD).

Furthermore, we combine these physics-based models with data-driven models to so-called **hybrid semiparametric models** allowing optimum use of knowledge and data for improved model accuracy. AI is used as one of our standard tools in all our fields of activities, **ranging from digitalization of experimental materials characterization to optimization of manufacturing processes.**

In the context of I4.0 and IIoT, we develop sensor solutions for retrofitting of processes and products and have a dedicated research group for **embedded computing**. Many of our projects lead to **custom-tailored software solutions** for different material-oriented problems, ranging from simple visualization tools to complex AI-driven development platforms integrating multiple data sources.

A more detailed overview on our competencies can be found on our homepage ([mcl.at/en/](http://mcl.at/en/)). Our latest research output can be found in the publication and the success story sections of our homepage.

energy and resource-saving production processes. An example is the flexible handling of materials with greater compositional fluctuations caused by the increased use of scrap. As the chemical composition varies with each lot, depending on the available scrap composition, a predefined process with fixed parameters would lead to quality issues causing downcycling of the material. However, a custom-tailored condition-monitored and autonomous production system allows for automated process adaptation, based on a digital twin updated in real time by in-line measurements, in order to achieve the targeted properties. IIoT systems for smart process control also enable flexible production processes down to a lot size of a single piece. On the product side, similar systems are central for condition-based predictive maintenance allowing longer maintenance intervals and extended product lifetimes at increased availability and reliability (e.g. for cutting tools or railway turnouts), thereby providing an important contribution to the circular economy.

In summary, the **IC-MPPE** research program of MCL is a **game changer for resource-efficient extraction, processing, and use of materials. This will be critical to achieve the goals of the Green Deal, i.e., zero net greenhouse gas emissions and decoupling economic growth from resource use.**

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# Production Process Effects in Fatigue Design

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## Vision

Traditional production processes, such as welding and casting, as well as modern techniques, such as additive manufacturing (AM), can significantly affect the **local material properties** of metallic materials. To ensure a safe and reliable operation of engineering structures and components, fundamental knowledge of **production effects** on the fatigue performance is of utmost importance. [1]

In general, the structural durability can be defined as a cross-disciplinary science incorporating the interaction between mechanical and environmental loading, technological influences due to manufacturing, and geometry. The shape of a component may be restricted by the production process-dependent boundary conditions finally affecting the local fatigue properties. To ensure a sound **product design** and achieving the postulated in-service life, it is of utmost importance to consider operational, environmental and technological aspects.

As the **fatigue assessment** is mainly performed by small-scale specimen test data, one main challenge is to properly incorporate size and production influences in the design process. Additionally, special load cases, such as under- and overloads, instabilities like buckling of structural elements as well as dynamic impacts need to be respected. As mentioned, **operational and environmental effects** also significantly influence the fatigue performance; hence, multiaxial load conditions as well as elevated temperature, wear, corrosion and creep must be considered as they impair structural durability. The total fatigue life includes the initiation stage, which

implies the development of cracks that are substantially longer than intrinsic microstructural features such as grains or phases, and the lifetime spent for further crack propagation. Compared to the crack propagation stage, especially crack initiation mainly depends on the local microstructure involving production process-based phases and defects. Hence, a **defect-tolerant design** incorporating surface and bulk material imperfections needs to cover both the crack initiation and subsequent short-crack growth to properly assess the local fatigue resistance. Further, also residual stresses fundamentally affect the

- **Fatigue Design**
- **Engineering Structures**
- **Production Process Effects**
- **Material Properties**

### **structural integrity of engineering structures.**

Thermal, thermo-chemical and mechanical manufacturing and post-treatment processes, such as welding or surface hardening, produce significant residual stress states, which majorly influence the fatigue strength and crack growth. Especially for post-treatments causing fatigue-beneficial compressive residual stresses, the knowledge of their (cyclic) stability is crucial for a safe fatigue design. The combined consideration of all these effects acts as superior vision in order to facilitate a **holistic fatigue design enabling reliable lightweight products.** [2]



## Approach

Various **standardized approaches** exist to assess fatigue strength of engineering structures and components, which mostly lead to a conservative design. However, the FKM guideline [3] provides a sound basis for fatigue strength assessment, but also reveals certain limitations. In case of welded components, the IIW-recommendations [4] act as well-proven fundament, but, especially for modern high-strength steel structures incorporating post-treatment methods, further research is ongoing to improve design methods.

Additionally, the weld quality and impact of local imperfections, such as undercuts at the weld toe or

gas pores, are crucial for the use of higher steel grades, which need to be continually investigated. Additional research on these topics may enable the consideration of elaborated fatigue approaches in international standards in the future. Especially **production process effects**, like residual stress states, and variable amplitude loads covering special loads and load history effects **are important for fatigue crack initiation and propagation**, which can be determined based on small-scale specimen tests and transferred to the real application considering size and crack shape influences.

Further background to state-of-the-art fatigue approaches and corresponding assessment models are provided in [2].

## Impact

Based on the described approaches and the further ongoing research to assess the fatigue performance of engineering structures, the following selected topics can be stated as up-to-date impact to consider production process effects in fatigue design [2]:

- Application of X-ray computed tomography to assess micro porosity of cast and **additively manufactured products**: Different scanning and evaluation procedures can be utilized in order to ensure a proper statistical assessment of micro porosity as basis for a further **imperfection-based fatigue design**. [5-7]
- Influence of interior filler material and exterior weld toe imperfections on the fatigue resistance of welded mild and ultra **high-strength steel** joints: Assessment of manufacturing process induced gas pores within the filler metal and undercuts at the weld toe to consider the impact of weld imperfections in the production process-based fatigue design. [8, 9]
- Determination of effect by **beneficial residual stress states** induced by post-treatments in the production process: Increase of fatigue performance due to High Frequency Mechanical Impact (HFMI) treatment influencing the local effective stress ratio at the weld toe of welded joints. Moreover, superimposed thermal and mechanical post-treatment reveals remarkable benefit to enhance the fatigue life of mechanical engineering steel components. [10, 11]
- Cyclic stability of production process-induced compressive residual stress conditions and **effect of variable load spectra**: As the cyclic stability of beneficial residual stresses is crucial for the structural performance, numerical tools are able to analyze these impacts. Further, the lifetime under variable amplitude loads based on damage sums is assessable. [12, 13]
- Evaluation of additional influences, such as environmental conditions or numerical effects: As not only the production process or loading condition impacts the fatigue strength, additionally **environmental influences**, like elevated temperature, or also **numerical effects** in the course of a finite element analysis is crucial and needs to be considered in fatigue design. [14, 15]



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## Competencies

In the course of the **research activities**, the Institute of Structural Durability and Railway Technology at Graz University of Technology deals with the **following topics** [16]:

- Structural durability assessment of lightweight mechanical engineering structures
- Mapping of production process steps for the development of elaborate design methods
- Set-up of advanced simulation concepts as basis for the fatigue design process
- Development of experimental test methods for representative specimens and real systems

A development of **innovative components** is essential to implement new design concepts in mechanical and rail vehicle engineering. Research at the Institute, in **close cooperation with partners from industry and science**, contributes to a development of elaborated engineering structures and components, and provides methods for the fatigue design considering production process and load aspects.

The **holistic testing infrastructure** at the Institute facilitates tests on several size scales, starting from representative specimens over real components up to whole complex systems. A significant aspect in the research activity of the Institute is the **development of new digital tools** as basis for an elaborated engineering design process, which enables a sustainable production of modern components. As best-practice example, the design, production and commissioning of a lightweight bogie frame for rail vehicles is presented in [17].

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# Digital Transformation in Polymer Processing

Gerald Berger-Weber

## Vision

The **importance** of **plastics** in reaching the United Nations Sustainable Development Goals (SDGs) is beyond any doubt. The sustainable development in many industries such as the building and construction, mobility, health, and green energy sector is mainly associated with the **versatile property profiles** of plastics materials – plastics grades are made of base polymers and additives to specifically tailor to the respective applications. Furthermore, their low weight, durability, and **advantageous carbon footprint** considering the overall process chain from manufacturing to end-use to recycling, **makes plastics to the materials of choice for many sustainable solutions**, as evident by the ever-increasing world-wide annual production rates. Though, photos of marine littering, proof of microplastics particles in food and human bodies, and landfilling of plastics waste adversely affect the image of the overall group of artificial polymeric materials.

Furthermore, **plastics conversion processes**, also named **polymer processing**, and its respective equipment are frequently not optimized for a certain application and often designed on the basis of experience and simple analytical models. Consequently, there is **still a need in** (i) **finding the optimum balance** between **throughput, product quality, and energy efficiency**, (ii) **minimizing process rejections** due to long start-up times, offline process control, and process instabilities, (iii) **increasing the continuity of product quality**, (iv) **reacting to process fluctuations** (e.g., due to temperature controls or dosing) **and input stream variations** (as commonly observed **from** mechanically

**recycled fossil-based plastics, in processing of bio-plastics**, or between different batches of raw materials), (v) generally increasing process know-how (e.g., for **troubleshooting**), and (vi) **optimizing maintenance** intervals.

**Our vision is sustainable polymer processing. Our mission is to address these major challenges, i.e. sustainability by advanced technology) in the field of plastics** – no matter if bio-based, fossil-based, or recycled – **by driving forward the digital transformation in polymer processing**. We are deeply convinced that **this transformation requires** a combination of **various key elements**: **First** of all, live evaluation and characterization of process and final

- **Polymer Processing**
- **Process Modelling and Simulation**
- **Hybrid Modelling Approach**
- **Model-Based Control**
- **Process Analysis Technologies**
- **Self-Optimizing Machinery**
- **Circular Economy**
- **Technology for Sustainable Development**

product by means of **inline, online, and in-situ measurement technologies** is essential. This may include acquisition of process pressures and temperatures, optical spectroscopy, ultrasound technology, rheological measurements, color spectroscopy, any type of soft sensors, and others. Thus, input parameters for subsequent

process modeling steps are obtained and the time gap between quality assessment and potential interventions, and hence process reject is reduced drastically. Furthermore, the **key component of digital process twins are process models** that are (i) precise and accurate, (ii) stable, (iii) fast in execution (ideally real-time capable), (iv) generalizable, and (v) know the physics behind the process.

#### Therefore, a hybrid modeling strategy

– combining experimental, analytical, numerical, and data-based methods effectively in a holistic approach, and described in detail in the next section – **has been developed at the Institute of Polymer Processing and Digital Transformation**. We are not satisfied with generating the digital model of a process, **in the end, the crucial step will be the back-connection between the outputs of the models and the process itself** often referred to as digital trigger. This can **range from** basic actions such as **warning the machine operator** via a dashboard up to more sophisticated actions: **predicting future behavior** or events of a process (e.g., predictive maintenance), providing additional guidance to the operator (**assistance systems**), or even taking actions autonomously by means of a **model-based control loop** implemented into the system (**self-adjusting and -optimizing machines**).

## Approach

For decades, modeling and simulation in polymer processing have been of particular interest for design purposes and gain more and more attention in the context of digitalization. We **always** have to **balance** between **accuracy** of a model or a simulation, the **assumptions** and **simplifications** considered, and the **effort** (i.e., the evaluation time and computational power), **to cope with** the complex **rheological behavior of plastics melts** (shear-thinning, pressure- and temperature-dependence, and viscoelastic behavior), **complex flow geometries** (e.g., wave and energy-transfer screws, die and adapter systems), a wide range of **size scales, phase transitions** (melting, solidifying, and crystallization), and **multiphase systems** (co-extrusion, free surfaces, fillers). The **hybrid modeling approach** developed at IPPD is an elegant way to address this optimization problem and has proven efficient in modeling numerous polymer processing problems [1]-[6].

The term “hybrid” is referred to the fact that **expert knowledge** as well as **experimental, analytical, numerical, and data-based modeling strategies** are **coalesced into a holistic approach** employing each of their individual benefits.

**Developing a hybrid model** includes the following main steps: (i) analysis of a **specific problem** and target parameters (outputs), (ii) physical and mathematical **description** of the **problem** (e.g., definition and simplification of the governing equations), (iii) conducting a dimensional analysis to identify the set of independent influencing parameters of the problem, (iv) **numerical model generation** (e.g., implementation of a numerical solution) **or an experimental setup** and (v) conducting a **parametric design study** under variation of the independent influencing parameters within ranges of practical interest, (vi) **data analysis**, and finally, (vii) a **data-based modeling step** employing **symbolic regression** analysis based on genetic programming [8].

The **outcome** of this approach **is** a rather **simple** and **continuous algebraic relationship** between a given target parameter and the set of independent influencing parameters. This **enables real-time solutions** for mathematically complex problems that initially needed numerical methods to be handled. Furthermore, hybrid modeling is not an exclusively data-driven approach, but **also considers** the **fundamental physics** behind the process, and thus, achieves **excellent prediction accuracy**. Additionally, analyzing the problem in dimensionless space **creates a general model** applicable to any combination of material properties, geometry size scale, and processing conditions considered within the parametric design study.

To describe the process of a **whole machine** or **plant**, it is common to model individual sub-processes separately and then **link** the **sub-models to a more global process model**. For instance, accurate modeling of the conveying behavior within the metering zone of a grooved single-screw extruder has to take into account (i) local variations of the screw geometry (as present in high-performance wave screws), (ii) the

flow within grooves machined into the extruder barrel, (iii) and the leakage flow through the small gap between screw flight and extruder barrel (i.e., clearance). We have developed symbolic regression models perfectly predicting the flow through channel sections of infinitesimal size. These sub-models were then linked – in analogy to electrical networks – applying a circuit diagram in which currents and voltages were replaced by flow rates and pressure drops [9], respectively.

**In the future, the hybrid process models will fundament digital process twins.** Due to their mathematical simplicity and execution time, any machine control (such as programmable logical controllers) can handle the **models**, which **can act as a soft sensor** or **be part of a model-based control loop** in combination with inline monitoring of processing conditions (e.g., rheology) and product quality.





## Impact

The proposed research approach aims at a countless number of **applications** and **use-cases** in **polymer processing**, ranging from plastics grade development, further compounding and material tuning, conversion machine and process design, in-line product quality monitoring, model-based closed-loop-controlled processes, and closing the material cycle together with plastics converters for recycling.

From a **scientific perspective**, our smart polymer processing approach may create tremendous **synergy effects** and novel opportunities by **coalescing** knowledge and research from **different disciplines** as (polymer) chemistry, measurement technology, mechanical engineering, polymer engineering, control technology, informatics, and machine learning. **Interdisciplinarity** aids the knowledge development on transport phenomena in polymer processing at various scales.

Building the fundament for future **industry-ready tools**, our hybrid process models offer further opportunities for (i) **smart, software-aided design** of product, equipment, and process, (ii) implementing **digital process twins** for process monitoring, process performance prediction, and assistance systems, as well as (iii) reaching maximum levels of **process automation** in terms of model-based process controls for self-optimizing conversion processes.

**Addressing the three dimensions of sustainability** – environmental, social, and economic: The potential **economic impact** for the polymer processing industry includes benefits as increased **overall equipment efficiency** (OEE), cost- and time-optimized design procedures, **reduction of energy demand** and process **rejects**, faster process start-up, **minimizing wear**, and **enhanced process reliability**. All of these help to **reduce the carbon footprint of conversion processes and machinery**, to **lower the use of fossil-based raw-materials**, and to **allow more plastics into material cycles**, i.e. fostering the **environmental impact**. Our research is also an **investment** into **education** – the foundation for an informed and intellectual civilization. Driving the JKU mission statement “**Re-Thinking Plastics**”, IPPD majorly contributes to three new **academic study programs at JKU** for educating future, **sustainable-solution-oriented-thinking engineers for industry, science, and society**:

- Sustainable Polymer Engineering and Circular Economy (bachelor’s degree program)
- Plastics Management and Sustainability (master’s degree program)
- Polymer Engineering and Science (master’s degree program)

**Finally**, our research will contribute to **orchestration**, i.e. **reaching far more when humans and digital technologies collaborate**: by providing (i) better design guidelines for products and equipment, (ii) allowing valuable feedback to the operator (i.e., assistance systems) for start-up or troubleshooting, (iii) a higher level of automation while lowering the cognitive load on the human operators.



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## Competencies

Research activities at the Institute of Polymer Processing and Digital Transformation span across a wide range in polymer processing, including different **products** and **applications, machinery** (processing technologies such as different extruder types and shaping methods), **and material types** (fossil-based plastics, bio-plastics, and recycled plastics). In our **cooperation network** – including **notable** Austrian and international **partners from polymer processing industry and academia**, for instance, Leistriz, Erema, GAW Group, SML, Poloplast, Greiner Packaging, Battenfeld-Cincinnati, Senoplast, Soplar sa, Pro<sup>2</sup>Future, CHASE, SCCH, TCKT, Wood K-Plus, KTP, and many others – **a multitude of research projects** (e.g. FFG projects Coex\_ABS, circPLAST-mr, Pro<sup>2</sup>Future Cognitive Production Systems, CHASE Process Digitalization; FWF projects HetGroMelt, NewWave) **have been handled**. IPPD plays also a major role in the research activities at the **LIT Factory**, the **Austrian pilot plant** for education, learning and researching smart polymer processing and digitalization. The IPPD provides a world-wide unique, **state-of-the-art research infrastructure**, which is **industry 4.0 ready** and structured into **three main labs**: (i) the **Extrusion Technology Lab** includes numerous single- and twin screw extruders (for plasticating and compounding purposes) and processing technologies (e.g., co-extrusion of films, sheets, and pipes, extrusion of unidirectional fibre-reinforced thermoplastic tapes, comprehensive equipment for all essential process steps in mechanical recycling) from lab-scale to pilot-scale. This enables efficient developments that can be directly transferred to industry-scale processes. The (ii) **Modeling & Simulation Lab** employs common commercial CFD software packages, software for self-development of numerical solution procedures for particular flow problems in polymer processing, machine learning tools, and corresponding server infrastructure. Finally, our **Measurement Technology Lab** includes state-of-the-art technology for characterization of polymeric materials and melts (e.g., inline and offline rheometers, measurement devices for thermodynamic properties) and numerous technologies for inline, online, in-situ or offline assessment of process and product quality, such as optical coherence tomography, color measurement, fluorescence spectroscopy, and laser-deflection based extruder torque measurement.

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# Smart Sustainable and Degradable Polymers

Oliver Brüggemann

## Vision

One of the world's most imminent problems is the **increasing global plastic crisis**. In the past decades, plastics production constantly increased having reached a level of 368 million tons per year in 2019 [1] with additional 36 million tons of polymers in liquid formulations [2]. The **recycling rates of plastic materials are far too low**, also in western countries, with only 33% (collected post-consumer plastic waste [1]) and 42% (collected post-consumer plastic packaging waste [1]) in the European Union (2018) and 32% (plastic packaging waste) in Austria (2018 [3]). In comparison, the recycling rate of plastic waste in the USA was even lower with only 8% in 2018 [4]. This leads to a **severe loss of valuable materials**.

Europe-wide, in 2018, beside the recycled 32.5%, 24.9% of the plastic waste ended up in landfills, 42.6% were used for energy generation [1]. But these are only the figures covering the collected waste. **What about the unaccounted plastic waste ending up in the environment?** In a National Geographic publication, it was stated that "without drastic action" the annual amount of plastic trash flowing into the oceans will increase to 29 million metric tons per year in 2040, adding up to an estimated total amount of 600 million tons in the seas by 2040 [5]. It becomes quite clear that **with such low recycling rates and millions of tons of non-degradable plastic waste accumulating in rivers and oceans, new approaches are of urgent need**, in order to reduce the environmental impact of plastics and to dramatically improve the circular economy of them. Within the last decades, the primary focus of research and development

has been on improving the mechanical and chemical stability of polymers. Thus, they degrade slowly and potentially remain and accumulate in the environment for a very long time. Far too many plastics end up as insoluble macroscopic and microscopic particles (microplastics) causing environmental pollution, because their end-of-life options in the context of defined degradation have not yet been sufficiently explored [6]. All polymers, biological as well as synthetic, are degraded in an undefined way and/or

- **Polymers**
- **Functional Polymers**
- **Plastics**
- **Sustainability**
- **Degradability**
- **Recycling**
- **Plastic Waste Crisis**
- **Polymers in Medicine**
- **Polymers in Liquid Formulations**

the nature and fate of their degradation products is often unclear. Here, further research and development in the direction of polymers **that show tailored degradation behavior are urgently needed**.

On the one hand, **polymers ending up in the environment shall degrade as fast as possible**, leading to harmless degradation products. On the other hand, in terms of an efficient circular economy, it is necessary to **develop new chemical methods that degrade recycled polymers and plastics in a**

**tailored way**, and by this means, **keep the materials in the system for as long as possible at their highest utility value**. And beyond that, **renewable resources for such degradable polymers** have to be included in the research, since the world sooner or later will run out of fossil raw materials.

## Approach

We, together with our cooperation partners at Johannes Kepler University Linz and at other Austrian and international universities, are aiming on substantially contributing to solving this global plastic problem by

**I: Developing new classes of biodegradable polymers with intrinsic, naturally triggerable breakage points for single use & short-term applications, as envisaged for most functional polymers** (with a focus on packaging plastics and polymers in liquid formulations):

A major aim is to develop macromolecules with **intrinsic, naturally triggerable switches for single use applications** allowing a defined **environmental decay** of the polymeric chains shortly after reaching the end-of-life status. This project area focuses, on the one hand, on **plastic packaging and container materials** that today are responsible for the millions of tons of plastic waste contaminating our environment and showing far too low degradation rates. On the other hand, **polymers in liquid formulations and other functional polymers** [7-8] pose a major, but still underestimated threat to our biological life as well, since they are in all their different applications mostly non-degradable. Polymers that, after a short application life, are expected to end up in nature in the future must be provided with tailored biodegradabilities.

**II: Developing new classes of polymers with intrinsic, physico-chemically triggerable breakage points for medium-/long-term applications** followed by subsequent tailored depolymerizations using novel catalysts and processes for reutilization purposes:

All polymers that are designed to be **applied for a longer period of time** are typically **more durable** contradicting the idea of degradability and complicating the idea of a chemical reutilization. In order to allow defined depolymerizations of such plastic product polymers, they shall

be equipped with intrinsic, **physico-chemically triggerable breakage points** that are not bio-sensitive allowing the polymers' environmental survival during their applications, however, that **enable the defined chemical break-up of the polymers in chemical processes**. Beyond that, **catalysts or novel transition metal complexes** shall be developed to cut polymers into molecular pieces in highly defined ways, leading to chemically reusable fragments. This will be combined with **optimization, modelling and simulations of the processes and reactors** used for the tailored chemical degradation of these macromolecules reaching yet unseen levels of control of the depolymerizations, and thus, an improvement of the quality of the polymer fragments and their values for reutilization.

**III: Developing new ways of using renewable resources and recycled polymers** for a sustainable polymer production:

Fossil raw materials are limited and valuable, but still the major resources for producing hundreds of millions of tons of commodity and other polymers. This simply has to be changed, in a way far beyond that what we see today. One major aim is on **using bio-waste as a polymer resource**, as well as **artificially derived bio-mass stemming, e.g. from artificial photosynthesis**. Another focus will be on **CO<sub>2</sub> as a raw material for forming new monomers and resulting polymers** using novel catalysts and processes, combining that with areas I and II, closing the loop leading to a fully circular economy.

**IV: Developing characterization and modeling methods to investigate and predict (bio)interactions of polymers and their degradation products:**

This fourth area will support the other three areas in terms of **characterizing the polymers with intrinsic breakage points newly designed in areas I and II, investigating and predicting the stability** of such novel polymers, their **degradation behavior** and **the fate of their degradation products**. Consequently, a major focus of this area will lie on the investigation of polymer-derived **microplastics in the environment** and reflecting how to prevent them or **how to redesign the polymers in order to make these microplastics biodegradable**.

## Impact

A major focus of our research will be on the design and synthesis of **thermoplastic and crosslinked polymers with tailored and controllable (bio)degradabilities based on internal breakage points** which, after reaching the polymers' end-of-life status, shall be **activated by natural or chemical triggers**. Such completely novel linear and crosslinked polymer structures would be ideal future components not only for plastic materials **designed for single and short-term use and polymers in liquid and medical formulations**, probably ending up in the environment, where a fast degradation into harmless fragments shall be evoked by triggers such as salt water, light, enzymes, or pH-changes, to name only a few, but also for **polymers with extended lifetime**.

Beyond that, **new types of catalysts and processes** shall be developed **allowing a controlled disintegration of collected polymers** and plastics which are intended to be **kept in the circular economy**, leading to defined and useable fragments for high-quality reuses. Based on this, an understanding of the precise molecular degradation mechanisms of existing and newly developed polymers that goes beyond previous knowledge will be used to adjust and/or redefine the design of degradable polymers. The listed approaches will advance this field of research by also investigating the effects of additives and processing conditions on the degradation behavior of the new polymers with inserted breakage points.

Our research also aims at **advancing the use of biomaterials** as resources for the production of new degradable polymers and plastics, with special **emphasis on biowaste** neglected so far, **degradation products from chemical recycling** and **CO<sub>2</sub>**, in **combination with implementing degradabilities** in such macromolecules. Finally, interactions of **(newly developed) polymers and their degradation products with organisms, cells and humans** shall be investigated in detail.

Only such a wholistic investigation will allow a **transformative change of the world of polymers and to contribute to solving the plastic waste crisis for the benefit of man and nature**.







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## Competencies

The Institute of Polymer Chemistry (ICP) has more than 20 coworkers and has been established in 2007. ICP focuses on the chemical synthesis, structure, chemical and physical properties of polymers and macromolecules, as well as on the development of functional polymers and polymeric hybrid materials. Prof. **Oliver Brüggemann's main focus of research is the design, synthesis and characterisation of functional polymers**, but also hybrid materials and composites (wood-polymer, silica-polymer etc.) **for technical, medical, pharmaceutical and biological applications**. His **work also includes aspects of biodegradability and biomimetics**. Prof. Brüggemann has specific knowledge and experience in the development and characterization of different kind of molecularly imprinted polymers and nanomaterials, from organic to inorganic systems for **biomedical applications** [9-18].

At ICP, some projects are focused on multifunctional polyphosphazenes and derivatives, which are mainly led by Prof. Ian Teasdale, deputy head of the ICP. These **polymers are designed and synthesized for later applications as drug carriers for drug delivery** [9, 10] or as **scaffolds for tissue engineering** as well as **curable inks in 3D-printing for manufacturing biocompatible and biodegradable scaffolds and implants** [16, 17] (EU-project 953134 INKplant).

In the projects earlier performed in co-operation with Competence Center Wood, the development and characterization of **degradable polymer-based composite materials** were addressed. Furthermore, **industrial collaborations** played and play a major role at ICP, e.g., in the current **developments of novel and optimized polyimides and degradable polyurethanes**. The projects performed over the years at ICP will be a good foundation for the envisioned future research, since the already acquired **knowledge of (bio)degradable** [9-17] **and industrially relevant polymers** might be in part transferable to the novel materials we are aiming on.

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# Polymer Products

Zoltán Major, Umut D. Cakmak

## Vision

- To develop industrial and commercial polymer products for a circular economy
- Application of polymers for green energy – green hydrogen technologies: production, storage, transport and application
- Support locomotion in all situation of the human life – from childhood growth up to old age decay on one hand and from competition level to various degree of handicap on the other.

## Approach

The characterization of the material constitution-processing-material structure-property-component performance relationships. The present but even more the future product development will not only be an engineering and economic activity. For the majority of the products it is essential the integration of a comprehensive life cycle analysis into the product development process.

### Methodology:

- Design WITH materials” combined “design THE materials”
- Practical engineering molecular dynamics simulations combined with processing simulations
- Engineering molecular dynamics –micromechanics – macroscopic component performance simulations and
- Life time/reliability assessment prediction

The main activity of IPPE is the adaptation and implementation of various modules of the methodology “Integrated Computational Materials Engineering (ICME)”.

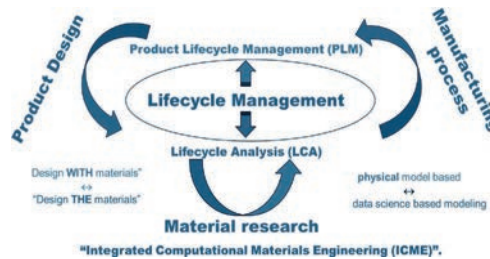


Fig. 1. The integrated life cycle management in the product design process

- Polymer Matrix Composites
- Thermoplastic Elastomers
- Integrated Computational Materials Engineering (ICME)
- Life Cycle Analysis

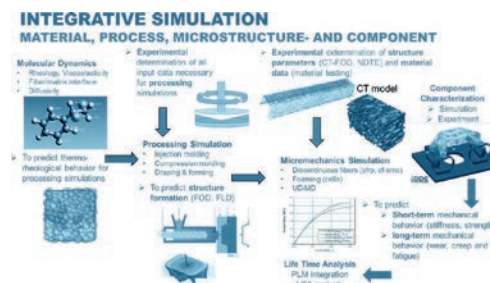


Fig. 2. Integrative multiscale simulation methodology

### Laboratories of IPPE

The design and development of engineering components for complex demanding applications using above mentioned computational tools and experimental characterization results. Special focus lies on the thermoplastic composites with different fiber reinforcement architecture.

In addition, the manufacturing and application of medical products will also be supported by simulations. The focus lies on endoprostheses (knee) and medical models for training and maneuver planning (aneurysm treatment). Special focus is dedicated to the contact and the long-term wear behavior of polymers under real dynamic and physiological loading conditions.

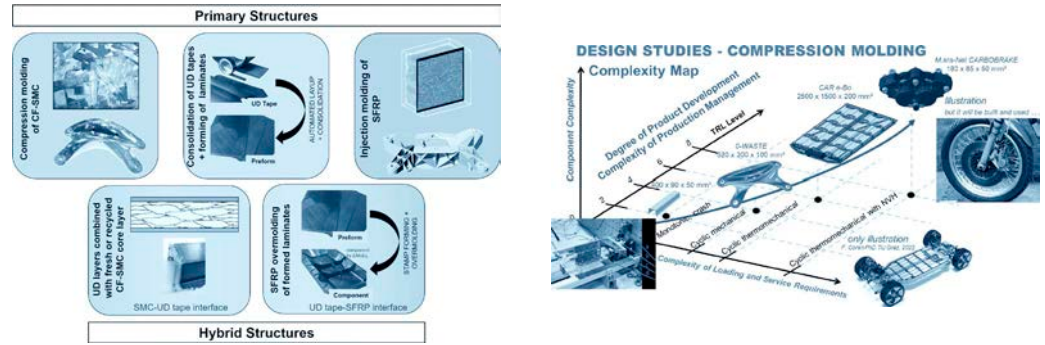


Fig. 3. Engineering components; (a) from primary to hybrid structures and (b) complexity management



Fig. 4. Medical engineering (a) knee simulation (b) hand supporter, (c) skull model with cerebral arteries and (d) aneurysm model

Hydrogen-based traffic and transportation requires also new material solutions both for the vehicles and for the auxiliary systems of the entire infrastructure. The focus lies on

the application of various polymer and polymeric composites for the storage and transport of pressurized hydrogen for vehicles (e.g., seals, hoses, valves and pressure vessels).



Fig. 5. Application of polymeric materials for hydrogen technologies; (a) seals, (b) hoses and (c) pressure vessel.



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## Competencies

Though my research group has been just formed in late 2022, I am bringing my past experiences in Japan, US, and Germany to my group. My most recent project on supercritical geothermal energy was funded by Deutsche Forschungsgemeinschaft – **DFG** and Japan Society for the Promotion of Science – **JSPS**, partnering with the Helmholtz Centre for Environmental Research – **UFZ** (Germany), Technische Universität Bergakademie Freiberg (Germany), The National Institute of Advanced Industrial Science and Technology (Japan), Kyoto University (Japan), and Tohoku University (Japan). An ongoing project on development of crack simulation tool in rock is currently funded by Japan Organization for Metals and Energy Security - **JOGMEC**, which funds another project on numerical modeling of wormhole partnering with Waseda University (Japan). Another project on chemo-mechanical aging of cementitious materials is funded by European Joint Program on Radioactive Waste Management – **EURAD** and is partnered with Belgian Nuclear Research Centre (Belgium), the Helmholtz Centre for Environmental Research – UFZ (Germany), and the Spanish National Research Council (Span).

Furthermore, I have been part of the development team for an open source project, **OpenGeoSys** (<https://www.opengeosys.org>), which is maintained at the Helmholtz Centre for Environmental Research - UFZ in Germany and is led by an international consortium of academic and research institutions.



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# Layered and Lithomimetic Material Design

Florian Arbeiter, Gerald Pinter

## Vision

Polymeric materials are a pillar of modern society. Due to their broad property portfolio, easy processing and cheap base chemicals they have found their way into every corner of appliances, from packaging, to transport of water and gas to medical products. However, due to their broad availability, and insufficient ways to re-use or recycle them, they have also become one of the main problems of modern society. Tackling this issue will be one of the major tasks in the years to come. Therefore, also regulations by the EU are put into place which enforce the **re-use of plastic materials** to avoid further pollution. However, this does not solve the current problem of polymers already existing on landfills, the oceans, etc. An ideal case would be to simply re-use these materials in the same or even better category (up-cycling) as the initial product.

In **mechanical recycling**, which is the most used procedure using recycled material still poses the risk of introducing unwanted particles and impurities into your material, possibly **degrading properties** far below what's expected or needed for safe application. Structural integrity is of utmost importance in engineering applications. Hence, so far recycled polymeric materials have not been used extensively in such applications. In order to be able to re-use polymers safely in engineering components, it is necessary to find means of creating highly **damage tolerant materials** which do not suffer from a great loss of other **important** properties, such as stiffness or strength. Strength and ductility are usually mutually exclusive. This indicates, that usual methods of increasing ductility to ensure damage tolerance in polymers, such as simply

blending with soft components or using additives and fillers to change the micro-structure usually leads to a **significant decrease** of the other mechanical **properties**.

Another **promising** and recent approach is the use of **layered structures** to provide outstanding damage tolerance in polymers by tailoring the macroscopic structure, e.g. the introduction of soft layers between recycled material. Layered polymers can provide **outstanding damage tolerance**, while still being rather cheap and easy to manufacture.

By combining **materials of different mechanical properties**, it is possible to influence the overall toughness of a layered material via the so-called material inhomogeneity effect (MIE). Based on the mismatch of properties,

- **Layered Materials**
- **Lithomimetic Materials**
- **Architected Material Design**

such as stiffness, strength or hardening behaviour of the materials, the local **crack driving force** (CDF) can be influenced. For example, the CDF is increased if the modulus or strength are lower in the direction of crack growth and decreased, if the modulus or strength are higher. While this basic concept is not new, the application of the so-called configurational forces (CF) concept has provided a tool for a more general description. Using this approach, it is possible to describe the CDF of a crack growing towards and through a soft interlayer. While initially increased due to the soft phase of

the interlayer, the CDF drops very low at the back face of the soft interlayer due to the increase in mechanical properties of the matrix. Subsequently, the global load has to be increased drastically to overcome this minimum in CDF, **effectively increasing** the overall **toughness** of the composite significantly.

**For polymers**, this **topic** is still **new** but it has been proven **possible** to apply this toughening strategy also to polymers to some degree [1–5]. However, compared to metals and ceramics, the **necessary difference** in properties is **much higher** in polymers in order to trigger aforementioned positive effects [2]. Thus, it is necessary to further decrease the mechanical properties of the interlayer. Very “soft” materials, indicating low stiffness and low strength, have to be used to stop cracks effectively in polymers, which in turn leads to a high stiffness loss [4]. Exact knowledge of the interaction of material properties, layer thickness and position enables to overcome this drawback to a significant degree (Fig.1) [5]. However, in many cases there is still a significant drop in stiffness. In application where stiffness loss is tolerable, this method can be applied directly. In case a decrease of stiffness is not acceptable, another approach can be added on top of the layered structure.

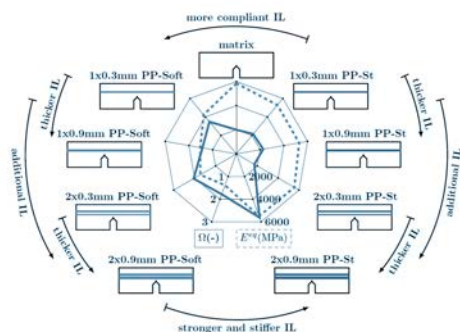


Fig.1. Layer architecture dependent comparison of specimen stiffness versus fracture toughness of multilayered composites. [5]

**Architected material** design is an **emerging trend** in materials science. Contrary to classical material design, the inner structure (e.g. atomic constitution or exact phase composition) is not the main target of optimisation. Rather, by influencing primarily the material's meso-scale, bridging micro to macro, exciting new property portfolios are designed. As shown in Estrin et. al. [6] architected materials can be classified into several sub-categories, such as topological interlocking materials, lattice structures, biomimetic materials and several more. With regard to mechanical properties, **biological materials** even manage to shatter the stiff and **strong OR tough**

**paradigm**, which is one of, if not THE hardest barriers for material scientists to overcome. Subsequently, scientists have focused especially on biomimetic materials in the last decades. Based on findings from literature, nacre appears to be a promising blueprint to promote high strength, stiffness and toughness at a first glance. Due to its brick and mortar structure it utilizes several mechanisms to increase the toughness of its otherwise brittle main constituent. Many researchers have tried to replicate its structure. However, as proven by many, it is necessary to not only copy the large-scale structure of nacre, but also its micro- and nano-scale. For example, mineral bridges keep the platelets together and avoid shearing. Only by incorporating these details as well, is it possible to create materials with outstanding properties. Due to the complexity of these **hierarchical structures**, for now this type of architected material is mainly realised via additive manufacturing or other **complex processing** routes, which are limited to rather small amounts of material. Thinking of the scale necessary to actually being able to decrease the ecological burden of used plastics, this type of material and manufacturing methods are simply not feasible. Contrary, **layered structures**, either with **straight layers or lithomimetic** (meaning designs copied from earth's lithosphere) patterns are comparably **easy to produce** with polymers, also on a larger scale. Co-extrusion techniques are available which are capable of producing structures between the  $\mu\text{m}$  and  $\text{m}$  scale.

## Approach

In order to produce **tough and strong** layered **materials** it is important to comprehend a multitude of interwoven aspects. Therefore, the following main topics have to be understood to approach this topic successfully.

### 1. Material selection

To produce cohesive layered materials, chemical affinity between the chosen constituents is necessary. Additionally, a difference in mechanical properties is essential to create a material inhomogeneity effect that is large enough to significantly improve the overall toughness of a layered structure. This can already significantly decrease the pool of potential partner materials and material selection becomes quite challenging. An auspicious approach is the combination of the same base polymer with vastly different molecular weight distributions, different co-

monomers, or also reinforcements via fibres or platelets [5]. Thus, suitable candidates can be found for the targeted material.

## 2. Processing of layered materials

In order to trigger a positive effect in layered materials, it is necessary to have continuous layers, to avoid cracks growing around separate phases [4,7], which would cancel out most of the positive effect. Thus, precise process control, e.g. during co-extrusion, is necessary. This becomes increasingly challenging, with bigger differences in the viscosity of the combined materials, as well as smaller layers and with the intentional creation of disturbances or the creation of lithomimetic patterns. Therefore, it is possible to apply easier, but batch-wise, processing techniques for a pre-screening of the potential of material combinations, as well as patterns. Two promising techniques can be of course processing via additive manufacturing, as well as compression moulding of precursor layers.

## 3. Material inhomogeneity effect

The material inhomogeneity effect is the main driving factor of toughness increase in layered polymers (assuming no delamination between layers, which would increase toughness but reduce stiffness and form stability to unacceptable levels). For the quantification of the MIE there are two possible approaches – a theoretical and an empirical one. The theoretical approach is based on the so called configurational forces concept, which enables the mathematical and mechanical description of the local CDF [8] at an interface. This way, the effectiveness of material pairings can be estimated before going into manufacturing and testing. This approach has proven reliable for the description of layered metal and ceramic sheets. In detail, it is possible to describe the local CDF in terms of energy-based fracture mechanical parameters, such as the J-integral values at the crack tip ( $J_{tip}$ ) as well as of the whole specimen ( $J_{far}$ ) and corresponding inhomogeneity terms ( $C_{inh}$ ) to account for spatial variation of properties at interfaces. The empirical approach is the measurement of energy uptake which is necessary to drive cracks through the material. Usually, this is done for nonlinear homogeneous materials via the so-called experimental J-integral ( $J_{exp}$ ) on produced specimens. While this requires the fabrication of actual specimens of every configuration, the results directly reflect reality, which also accounts for the high time dependency of polymers. This is an aspect, that has not yet been dealt with in sufficient

detail in the theoretical approaches.

## 4. Time dependent properties of polymers

As previously mentioned, the effect of time is not neglectable in polymers. Contrary to metals and ceramics, mechanical properties of polymers are highly dependent on stress relaxation, as well as retardation even at ambient temperatures and moderate loading rates. As the MIE strongly depends on the mechanical mismatch, which is susceptible to change over time for polymers, this has to be integrated as well. Especially for the case of applications under long-term loading, the precise change of material properties has to be integrated in both theoretical, as well as empirical analysis.

## Impact

The current and future work is expected to provide significant **scientific impact** within the area of architected materials. We plan to combine the impact of the MIE on the local CDF, and thereby overall fracture resistance, with the change in material properties over time due to creep and relaxations processes. With the exception of a few preliminary studies, there is not much research work available in literature regarding this crucial topic. Empirical studies will provide evidence of the proposed methodology and calculations to better understand the exact impact of spatial deviations of properties on the local and global behavior of both layered and lithomimetic materials in combination with the extension into time dependent, ergo visco-elastic properties of polymers. With regard to the processing of lithomimetic materials we expect large advances and to pioneer new methods of production. Subsequently, we aim to significantly advance the current state-of-the-art of architected polymers.

The **industrial opportunities** for both tailor-made layered and lithomimetic polymers go way beyond of what is currently possible. By providing guidelines on how to produce materials of outstanding mechanical and fracture mechanical properties, as well as, possible manufacturing routes, industry can push their current portfolios into the next level. Possible applications may range from automotive sector, construction, ballistic protection, and even recycling.

The **societal impact** possibilities are numerous. One very significant possibility of both layered and lithomimetic materials is the possibility to apply them towards recycling of materials. By producing layered products with outstanding damage tolerance, it is possible to reuse polymer recyclates of lower quality also in structural- and/or long-term applications. Thereby, it will be possible to reuse formerly "unusable" polymers in a second or third life cycle, thus decreasing the overall burden on the planet significantly.



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## Competencies

My team focuses on several different aspects and areas of the performance of polymeric materials, such as additive manufacturing (FFG K Project CAMed, FFG Production of the Future Project eFAM4Ind), reliability and long-term mechanical performance (FFG Bridge Projects BioMimicPolymers and Methusalem, FFG K1 Comet Project VI-3.S1, VII-3.S4), material and structural development for optimized performance in special environments (FFG VIF Projects PolyDrain and DrainRepair), mechanical performance of recycled materials (PCCL Comet VII-3.S5, FFG LightCycle). Translational research cooperation with industrial partners range from infrastructure producers (AGRU, Poloplast, Pipelife, HILTI), infrastructure providers (ASFINAG & ÖBB) to classical OEMs (automotive, aircraft industry).

The chair of materials science and testing of polymers has a state-of-the-art laboratory, necessary for the characterisation of architected polymeric materials. The equipment consists of the mechanical lab (universal testing machines, fatigue machines with testing forces between  $10^{-3}$  and  $10^6$  N, impact and creep testing facilities, digital image correlation techniques for normal and high-speed cameras), the morphology lab (light and digital light microscopy, SEM, AFM, micro-IR and nano-IR, in-situ tensile testing machine) and the thermo-mechanical lab (DSC, DMA, TMA, TGA)



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# Responsible Materials

Lorenz Romaner, Daniel Kiener, Christian Mitterer

## Vision

Today's world is characterized by **environmental stresses** to an extent never seen before. In fact, and not much different to other highly industrialized countries worldwide, Austria passed its World Exhaustion Day just before Easter, on 6th of April 2023. All anthropogenically induced negative Earth system trends have accelerated in recent decades, including biodiversity loss, terrestrial biosphere degradation, temperature rise, or land domestication [Steffen 2015]. The reasons for this can be simply summarized as a **significant growth** in global population and global wealth. The demand for **raw materials** corresponds directly with population growth and gross national incomes [Krausmann 2018]. Globally, the consumption of raw materials increased from 6 billion tons per year at the beginning of the 20th century to 84 billion tons per year in 2015 (biomass, fossil fuels, metallic and non-metallic minerals). Each material has a specific **environmental impact** due to the way it is extracted, refined and transformed into products, as well as how it is (re-) used and disposed of in the post-consumption phase. A stated target of the UN Sustainable Development Goals is to decouple the production of materials from its environmental impact, as well as the required material use from economic growth.

So far, materials, materials systems and products have primarily been designed and produced to achieve certain functionalities. Only rarely **sustainability aspects** during the use phase and the re-phase (re-use, re-pair, self-healing, re-cycling) have been included in design considerations [Korhonen 2018]. Radically **new and holistic solutions** are urgently needed to decouple materials production from

environmental impacts [Grubler 2020], and at the same time create **material cycles** that require as little material and energy input as possible [Raabe 2023].

As a visionary step-change, the proposed **Responsible Materials** concept aims to create a sustainable system based on a rigorous holistic design of products and services that use as little materials as possible (e.g., by substituting digital for physical service), maximizing service provisioning per end-use device while minimizing its embodied material footprint. Likewise, this concept also aims to **re-design material** supply systems that use only single or several (combined) elements/materials/functionalities that, because of their "responsible behavior" in production, use and re-phase, create planetary impacts so low that – even in situations

- **Sustainable Materials**
- **Responsible Consumption and Production**
- **Circular Economy**
- **Materials Design**

of significant volumes of "material flows" – the planetary boundaries are well respected in the long run. Ideally, the materials should even "pay back" to the planet, by harvesting energy or binding CO<sub>2</sub> during continued use.

Key aspect of the Responsible Materials concept is, in distinct opposition to current trends [George 2019, Oses 2020], the **substantial reduction** of the number of natural elements and their compounds used in products, functionalities and services, based on their responsible behavior including

(i) long-term and, thus, sustainable availability in geological or bio-sphere deposits; (ii) **low planetary boundaries impact** during the primary production phase and (iii) ability to form products of desired functionalities with low planetary boundaries impact during the service and use phase, the re-phase and responsible restoration capabilities.

## Approach

**General approach:** The general approach is to design a universal, **artificial intelligence supported toolkit** that will develop materials with an awareness of their footprint within a circular economy and aim to minimize it. With this enabling toolbox, “simple” materials can be created together with systems that are optimized in terms of property and function through intelligent materials design taking into account physical, chemical and structural principles, while simultaneously avoiding critical materials, complex chemistries or composite structures that may deteriorate recyclability of sustainability.

Approaches for tailored structure design include, for example, creating nanostructures and tailored defect configurations, optimizing interface design (toughening/adhesion of interfaces or grain boundaries, topological design of interfaces), exploiting order-disorder phenomena (pattern formation in disordered systems or (local) frustration and (dynamic) fluctuations in complex systems, hetero-structuring through nano- or cluster structures, inducing phase transformations locally (complexion engineering) or globally through external fields (transformation-induced plasticity, twinning, field-driven migration properties etc.), or creating hierarchical/graded structures. These sophisticated strategies should result in **intelligent and responsible materials** or structures with tunable functional and mechanical properties. Moreover, advanced fabrication techniques, for example additive manufacturing or thin film deposition techniques, not only allow building geometry optimized structures and complex architectures, but also enable localized materials synthesis/phase formation/ transformation in hierarchical structures that can be tuned on different length-scales, all the way from atomic size (clustering, nucleation) over nano- to micro- and meso-structures. Furthermore, additive manufacturing, cryo-forming or plasma-assisted thin film deposition enable realization of previously inaccessible microstructures.

Therefore, by an adequately processing-adjusted microstructure, a leaner more environmentally friendly alloy can excel over conventional highly alloyed systems.

Structure design approaches can be supported by **computational methods**, which allow predicting structure and property of materials utilizing hierarchical modelling concepts, combining ab-initio modeling for basic materials quantities, molecular dynamics for defected and nano/structured materials, phase-field or CALPHAD methods for microstructure evolution and homogenization schemes to extend length scales towards macroscopic dimensions. Simulation methods will enable to scan the periodic table to identify alternative chemical compositions for materials with comparable performance, but with reduced or no critical (undesired) chemical species. In a similar way, this can be performed for property scanning and through consideration/ implementation of mechanisms-based descriptions used for determining specific structure-property-property/function correlations. In this course, **optimization concepts** from machine learning (Bayesian optimization, genetic algorithms) can be used to follow an efficient and consistent workflow. In particular, active learning approaches as outlined recently [Lookman 2019] can be utilized. Surrogate machine learning models shall be developed to accelerate physics-based materials model evaluations and to speed up property or composition scanning, while techniques of uncertainty quantification and uncertainty propagation are applied to support decision-making processes.

The toolkit will communicate with databases storing materials data as well as data from experimental analysis and simulations. The databases shall obey fundamental principles, such as the **FAIR data** principles, to guarantee a maximal re-usability and exploitation of information implicit to the data.

**Examples / Applications:** An example of a necessary **re-alloy design for steels** is the substitution of non-responsible alloying elements, such as e.g. Co. This requires re-thinking tooling alloys. Such novel strength-ductility-toughness optimization can be achieved using ab-initio guided interface engineering by modifying grain boundary motives or structures [Leitner 2018], or via an artificial intelligence (AI) guided replacement of critical elements by more responsible alternatives. At the same time, it is important to ensure that these lean

alloys can be produced from low purity recycling materials, thus possessing a high chemical tolerance window. In this context, it is also inevitable to re-think common materials testing and validation schemes. Rather than a conventional work- and cost-intensive assessment of the close to final piece, already in the development stage highly localized and high-throughput screening methods must be employed, in conjunction with AI schemes to predict and advance the respective material structure and property information along the subsequent value chain.

Another prominent example concerns **aluminum**, which due to its low density helps saving energy in transport and mobility applications, but its extraction from ores is energy-intensive. Recycling shifts this balance towards higher sustainability, since only about 5 % energy is needed. This requires understanding how multiple scrap-related contaminant elements act on aluminum alloys and how they can be designed upfront to become scrap-compatible, a property that equips these materials with a gene of recyclability. However, the basic science behind is still an underdeveloped field. Aluminum alloys have been developed for almost a century for specific high performance with a narrow and complex chemical composition. This multi-material mix diminishes recyclability, since the ignoble character of aluminum hampers metallurgical refinement. Conceptually, crossover alloys recently showed that several advantageous properties can be combined in one “broadband alloy” [Stemper 2021], which could become a general pathway for other metals as well. Furthermore, employing completely new design strategies such as **complexion engineering**, novel interface states can be achieved in very lean alloys by proper processing, opening novel windows for resource efficient yet extremely stable alloys. While demonstrated for Al recently, these concepts are generally applicable and well suited for computational guided design [Balbus 2022, Singh 2023].

In the field of shaping, existing tooling concepts can be enhanced by hierarchically, compositionally modulated, damage tolerant **hard coatings** instead of the current complex-alloyed coatings to minimize tool wear and machining times for energy efficiency. This should also be seen from the point of longevity of responsible materials and products. Furthermore, such shaping strategies must be combined with novel material

adaptation concepts such as hardening upon annealing for nanostructured metals [Huang 2006] or complexion engineering on an interface or atomistic defect level [Kuzmina 2015] length scale. Thereby, after machining the rather soft materials, the strength of the final piece is adapted via a simple short time annealing at rather low temperatures, while at the same time preserving the adjusted microstructure, thereby simultaneously improving the piece performance and minimize tool wear. Advancing even beyond this, direct net-shaping concepts can be involved to alleviate machining completely or at least to a large amount, while adjusting local heating and cooling rates enables tailoring local microstructure to achieve the required properties.

### **Materials simplification concepts**

are also required to enhance the level of responsibility in micro/nanoelectronics. Transparent electrode coatings are facing increasing demands but require replacement of rare elements like indium. This can be approached through band gap and/or defect engineering in abundant transition metal oxides ( $\text{MoO}_2 - \text{MoO}_3$ ) using advanced thin film deposition techniques [Pachlhofer 2017]. Furthermore, with the Internet of Things gaining more and more importance, there is an increasing demand for self-powered functional devices, e.g. sensors, which are able to harvest or generate energy from mechanical motion. There, nanogenerators based on tribo- and piezoelectric [Wang 2006] or magnetoelastic effects [Makarov 2021] have been suggested, but again without including responsibility measures. Storage of the produced electrical energy could be accomplished in thin film batteries or capacitors, however, all presently commercially available thin film ceramic capacitors contain the critical element lead. Besides replacing lead in such storage systems before they widely enter the market [Kölbl 2023], we aim for novel design concepts for 3D printed biodegradable and disposable batteries. Last but not least, one way of mitigating the limited recyclability is provided by enhancing the lifetime of existing and future microelectronic devices. Envisaged here are smart stimuli-responsive self-healing concepts such as exploiting electromigration phenomena for metallic interconnects [Putz 2015], or the development of intrinsically flexible 2D materials towards “unbreakable” flexible devices [Cordill 2022].

## Impact

The Responsible Materials concept opens the pathway towards a **highly responsible design of structural and functional materials**, including all aspects of circular economy, to ensure that their impact on the planetary boundaries is well respected in the long run. The main impact of the proposed holistic approach is foreseen in three sectors (i) Mobility - Transport - Structural Applications, (ii) Sustainable Energy Solutions & Processes, and (iii) Communication Systems. **Novel alloys** will become available that reverse the current trend from increasing complexity (superalloys [Wu 2020], high entropy alloys [George 2019, Oses 2020]), where the final alloy contains up to a dozen partly critical elements (e.g. Co), towards new lean material systems that can fulfill the same application requirements while concurrently own a gene of recyclability already implanted. The complete re-design of classical structural materials' development and production schemes towards a responsible approach will reduce the planetary burden, while still enabling personal mobility, transport of necessary goods, and construction of necessary infrastructure for safe, healthy and affordable living.

A combination of **interdisciplinary sciences**, starting from geology and mining, to production, processing, usage, and recycling will enable the development of responsible structural materials (steel, Al, Ni and Ti alloys, including crossover alloys and intelligent/smart materials exploiting phase and structure transformations under external stimuli). A sustainable steel production will have to **drastically reduce CO<sub>2</sub> emissions** emerging by the current carbon based production. Hydrogen shall be used as an alternative agent to reduce iron ore, thereby averting the creation of CO<sub>2</sub> while producing H<sub>2</sub>O instead [Spreitzer 2019]. In 2050, less than 20 % of the overall steel production shall rely on carbon as reducing agent. This transformation will involve a shift from classical crude steel production to new routes, involving major consequences for subsequent secondary metallurgical processes and the quality of the crude steel in terms of nitrogen and sulfur levels. Furthermore, the effects of tramp and trace elements shall be controlled, as they significantly influence material properties and further steel processing.

Hydrogen is considered as the ideal carbon-free energy carrier, but its application still suffers from environmentally and economically viable methods for production and storage [Kostoglou 2017]. The production of green hydrogen necessitates catalytically active materials, which are often based on the use of noble metals like platinum. **Responsible design approaches** will help identifying noble metal-free catalysts with optimized porosity and functionalized surface. Environmentally friendly nanoporous carbons with ultrahigh surface area for hydrogen storage can be produced either from organic waste materials (lignins, orange peels, coffee waste [Stock 2022]) or from side products stemming from the pyrolysis of methane needed for the production of blue hydrogen. The backflow of such side and waste materials into the circular economy represents a novel approach, where up-cycling can be performed by modification of the porosity and surface chemistry of carbons. Application scenarios of these up-cycled waste and side products include their use as carbons in the cement industry (representing together with the steel industry a major emission source of CO<sub>2</sub>), as building material, as nanoporous carbons for hydrogen storage, or for filtering of nanoplastics from waste water. Another highly responsible approach could be the up-cycling of carbons for use as artificial soils for agriculture, with optimized storage capacity for rainwater and fertilizers.

Additional functionalities will be imposed to the materials and

materials systems, most prominently by adding multifunctional nanostructured surfaces. Such responsible **material enhancements** encompass self-cleaning, anti-fogging, anti-icing, as well as antibacterial/-viral/-microbial films for mobility, health and space applications. Considering the end of product life cycle of flexible electronics/communication devices rapidly increasing in volume, concepts to reduce hazardous microelectronic waste and facilitate recyclability should be pursued, such as using biodegradable or bio-based polymer substrates for wearable electronics and sacrificial layers to trigger detachability of composite structures. Novel approaches in the design and manufacturing of functional substrates, such as printed circuit boards (key elements for a variety of high-tech applications), should emerge with a focus on the use of recycled materials.

To summarize, the potential **societal impact** of the proposed Responsible Materials concept is countless, covering all aspects of materials design and development, processing, application and recycling, with the goal to keep as many as possible of the needed resources within a circular economy.







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## Competencies

At the Department of Materials Science of Montanuniversität Leoben, research is conducted at the highest international level, in order to achieve **a detailed understanding** of the structure and the properties of materials and materials systems. The international visibility of the Department stems from a supercritical size, and the completeness in methods available to us and in the materials classes covered. The Department operates a unique portfolio of facilities and methods for the design, synthesis, characterization and testing of advanced materials and materials systems, with strong emphasis on **bridging length scales from atomistic to macroscopic**. This includes top-down and bottom-up routes to synthesize nanostructured materials, a multitude of high resolution methods for nanoscale characterization of microstructure and chemical composition, in-situ structural and functional characterization, also in harsh conditions, and testing under near in-service situations up to extreme environments. Strong emphasis is laid on scale-bridging computational materials science, ranging from density functional theory and molecular dynamics to thermodynamic calculations and macroscopic multi-physics simulations.

The Department runs a huge network of national and international partners, both from academia and industry, enabling us to focus on a well-balanced relation between basic and applied research of industrial relevance. We have a long tradition in applying for third-party funding – with several highly visible Christian Doppler Laboratories, ERC and START grants, and many national and European projects undertaken. Furthermore, the COMET Center Materials Center Leoben nucleated within the Department, where many members are actively running projects within the COMET funding program.

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# Analytics



# Intelligent Systems in Production

Franz Pernkopf

## Introduction & Motivation

Data-driven approaches have transformed the landscape of **intelligent systems in production environments** by exploiting the power of sensor and network technologies to gather vast amounts of information from various components and processes [1,2,3]. This data is then converted into actionable insights, enhancing the efficiency and effectiveness of production systems. One of the most significant applications of data-driven models in the context of intelligent systems in production is health (condition) monitoring, which plays a crucial role in optimizing performance and ensuring operational reliability.

**Data-driven machine health monitoring** systems signify a fundamental shift from traditional top-down modeling based on physics to bottom-up, data-centric solutions for detecting faults and inefficiencies. By predicting future conditions and estimating the **remaining useful life** (RUL) of equipment, these systems facilitate the move from time-based maintenance to condition-based maintenance. Physics-based models are often tedious to design due to several real-world challenges such as complexity, difficult boundary conditions, expanding operational state space, and noise. Fortunately, recent advancements in digitization – such as innovative sensors, sensor networks, and computing systems – address these challenges and lay the groundwork for data-driven machine health monitoring systems.

As machine learning (ML) continues to gain prominence as a pivotal technology in the 21st century, it becomes increasingly crucial to

leverage its capabilities for data-driven health monitoring in industrial settings. ML has driven significant improvements in fields such as computer vision, natural language processing, speech recognition, and signal processing. While many traditional ML applications have focused on the „virtual world“ (e.g., recommender systems, stock market prediction, and social media services), there is an increasing need for ML solutions in industrial and commercial applications. We are now witnessing the integration of ML systems into real-world environments (e.g., autonomous navigation for personal transport and delivery services, the Internet of Things, and Industry 4.0 applications). This transition presents numerous challenges for machine learning engineers to bridge the gap between the virtual and physical worlds. Current

- **Machine Learning**
- **Edge AI**
- **Resource-Efficient Machine Learning**
- **Uncertainty Estimation**
- **Explainable AI**
- **Representation Learning**
- **Domain Adaptation**
- **Transfer Learning**

ML methods excel when given access to large data sets and substantial computing resources. This impedes the application to many real-world problems in two aspects: First, the ongoing trend towards data-intensive, evidence-based decision making poses new demands on computational efficiency, information collection in the data, and privacy concerns regarding



sensitive information. Second, in many real-world scenarios, data may be scarce, often unlabeled, and the available computing infrastructure during the operational phase is limited. In our work we aim to tackle these challenges to pave the way for the application of machine learning methods for the purpose of health monitoring in industrial environments.

The current success of ML is driven by deep neural networks (DNNs) that are trained on vast amounts of (usually labelled) data and that have huge compute and memory requirements. The expressiveness of these models has come at the cost of fragile models that are easily misled, for instance by adversarial attacks or noise [4]. Moreover, today's deep learning algorithms often fail to provide interpretable predictions, to represent the underlying uncertainty, and to account for the uncertainty within the input data; thus, these methods fail to meet many essential requirements for deployment in real-world applications. Methods following the Bayesian view – such as Bayesian networks [5] or Bayesian neural networks [6] – can represent the uncertainties in the models. The problem with the Bayesian treatment however is that it requires reasoning about distributions, which often comes with the need to evaluate intractable integrals.

ML-based **health monitoring** systems must meet several fundamental requirements to receive widespread acceptance. Besides providing sufficiently accurate results, we require that the **systems work robustly and reliably in diverse situations** and environments; provide **uncertainty measurements**; and **allow for solid interpretability** of the model's behavior. In real-world applications, models are often exposed to a myriad of unknown disturbances and environmental influences. Robust and reliable models need to be aware of adverse influences (e.g., triggered by outliers, domain shifts, or corrupted data) and counteract them accordingly. If a model fails to do so, it should at least recognize that its predictions are possibly wrong and activate an emergency routine. We can prepare a model to detect its faulty behavior by providing consistent uncertainty estimates. Furthermore, especially for safety-critical applications, it is essential to understand precisely how the ML model came to its prediction. This is the aim of research on **explainable AI** that tries to determine the decisive factors for the model's behavior. Methods for instance-wise and population-wise explanations provide insights on both

– the subset of salient features for predictions on sample/instance level and the optimal feature subset for all samples/instances. Moreover, real-world applications in industrial environments often come with heterogeneous – possibly incomplete – data with a high degree of class imbalance. **Feature imputation methods** as well as **data augmentation techniques** can be used to approach these limitations. Additionally, **transfer learning** enables us to utilize representations among related domains. **Continuous learning** and **semi- or weakly-supervised learning** are important techniques for combining all the available data and extracting the relevant information. All these techniques help to improve the generalization ability of the models in case of limited, unlabeled, and noisy data from harsh environments.

As discussed above, there is a range of complex requirements that are not only at the center of the current research in machine learning but are also of central importance for ensuring a smooth transition of machine learning technology into modern production environments and industry. In particular, the aim is to fuel the areas of intelligent process automation and health monitoring by utilizing the full potential of current machine learning research. There is a mutual benefit at the intersection of basic research and industrial applications as real-world challenges inspire the improvement of machine learning methods which in turn serve as an enabler in the relevant applications.

## Research Challenges

Dependable intelligent systems are necessary to facilitate real-world industrial applications in harsh environments such as health/condition monitoring for process optimization. Although ML has already been commercially successful in the past, there are still many under-explored research challenges (RCs) that need to be addressed for a successful deployment of ML methods in these data-driven industrial applications. In the sequel, these research challenges are introduced in more detail.

- **RC1:** How can we establish data-driven condition monitoring systems with minimal required human interaction (e.g. without manual feature engineering)? How can we build sufficiently structured models and systems allowing for accurate and tractable reasoning?

Just applying classical machine learning algorithms to the raw data will often fail to achieve sufficient prediction quality for a reliable detection of imminent failures. Therefore, one often relies on manual feature engineering for determining useful features that provide a good indication of any degradation in the process. It is, however, often not obvious at all, what characterizes good features for the task at hand. This holds true even if process experts are involved in manual feature engineering. As informative features are hard to come by, typically many potentially useful features are considered. Then the most important features for health monitoring are either determined automatically by feature selection methods or manually by domain experts. As the quality of the extracted features strongly influences the health monitoring performance, there is an interest in moving from hand-crafted feature engineering towards an automatization of this process. Considering the capability of DNNs to learn **hierarchical representations**, deep learning can be beneficial and is a promising approach for replacing manual feature engineering and feature selection.

In addition to purely data-driven DNNs, **hybrid models** including physical models are beneficial. Data-driven DNNs are highly dependent on the amount and quality of training data. For instance, they exhibit low robustness and generalization capabilities when data is noisy, incomplete, or scarce. To alleviate those limitations, new branches of deep learning have developed, including **physics-enhanced machine learning**. In addition to observational data, prior knowledge about the underlying physical system is incorporated.

- **RC2:** How can we empower ML systems to ensure continuous improvement through incorporating insights from related situations? How can we exploit **transfer learning** and **data augmentation** to compensate for limited, noisy and partially labeled data sets with potentially strong class imbalance?

Most deep learning approaches require large amounts of labeled data to attain sufficient performance. Unfortunately, in health monitoring applications, most of the data samples belong

to the healthy category while faulty data samples are rare, very costly, or even impossible to obtain. This typically leads to strong class-imbalances. Furthermore, it can be difficult and expensive to obtain labels of the data. The performance and generalization ability of deep learning models greatly depends on the amount of data and the quality of the target labels. To ensure well-performing models in the industrial setting **we advocate the use of data augmentation and semi-supervised learning** techniques. In addition, we aim to combat data limitations by transferring knowledge between different application domains and operating conditions. This research direction is of fundamental importance since some machine health monitoring problems have sufficient data available while other application areas do not.

- **RC3:** How can we handle distribution shifts between training and test situations? Can we guarantee safe model adaptation over the model exploitation phase?

Deep learning methods assume that training and test data have the same underlying distribution. In many applications, however, noise is ubiquitous and diverse; this can often lead to complete failure of machine learning systems as they fail to cope with mismatches between the data distribution during training- and test-time. For health monitoring applications, the models shall be **robust against environmental noise** or in the case when shifting the prediction model from one machine to another similar machine. Especially for the case of deploying a model to several similar machines, this model transfer should not lead to a degradation in performance or require data and labels from the target machine for retraining. **Unsupervised domain adaptation** is currently a highly active research area to improve model robustness against distribution shifts.

- **RC4:** Can we reliably detect abnormal behavior and outlier patterns in the data in an unsupervised fashion?

One specificity of the real-world applications is that the process can change abruptly. This can happen because of abnormal sensor and/or system behavior, breakdowns, or abrupt novel changes of the machine/process

state. These situations are often highly safety relevant and have to be detected reliably as human intervention and feedback is often required. Nevertheless, outliers are extreme patterns that deviate from conventional data. An outlier is an observation that diverges from the overall pattern of a sample. These outliers have to be reliably identified and reported. For industrial health monitoring applications, unsupervised approaches are of particular interest. These include **outlier detection** methods based on statistics and probabilistic methods, information theoretical approaches, cluster analysis, and generative machine learning models.

- **RC5:** How can we guarantee robust performance bounds and provide uncertainty measures over the predictions?

A desideratum for any intelligent system for real-world application is to be aware of its uncertainty over its predictions. This greatly supports the trust in the predictions and can be exploited in process optimization. **Safety-relevant aspects can be guaranteed as an uncertainty bound** is provided with each prediction. The **Bayesian** framework has several appealing properties. It is less prone to overfitting, it naturally handles the online setting where data samples arrive in an indefinite sequence, and it provides a well-justified means of obtaining prediction uncertainties. However, exact Bayesian inference requires solving integrals that are often intractable. As a consequence, the field of approximate Bayesian inference is a very active research area devoted to developing effective approximations in various contexts.

- **RC6:** How can we provide conclusive explanations and insights for ML model predictions of safety-critical applications?

Successfully explaining ML models depends on having effective means of communicating the inner-workings of these complex models. In certain domains, the explicit need for interpretable models prevails over the advantage of better performance of black-box ML methods. For safety-critical applications it is essential to understand exactly on what basis a ML model comes to its prediction. **Explainable AI** can be used to provide the influencing factors

justifying why a model performed a specific decision. The implications of this information is three-fold: (i) it is in particular important in machine health monitoring to support domain experts in the industrial environment and to ensure confidence in the ML algorithms; (ii) this insight into model behavior is in turn also important for the design of the ML methods as it supports the algorithm development; (iii) the main influencing factors in deterioration of particular components provide useful information for development of those components.

- **RC7:** How can we build computational efficient methods running on limited compute architectures?

Machine learning is traditionally a resource intensive task. It is often the case that in industrial environments, compute resources are limited. This requires a carefully chosen **trade-off between prediction performance and resource consumption** in terms of **computation** and **energy**. The development of such approaches is among the major challenges in current machine learning research and key to ensure a smooth transition of machine learning technology from a scientific environment with virtually unlimited computing resources into every day's applications. In [7] we provide an overview of the current state of the art of machine learning techniques facilitating these real-world requirements with the focus on deep neural networks. The main approaches can be summarized into (i) quantization of neural network parameters, (ii) pruning of neural networks, and (iii) efficiency by the network architecture. These techniques can be applied during training or as post-processing.

## Impact

Each solution addressing the research challenges presented in this work will contribute significantly to the scientific community and broaden the scope of intelligent systems in production.

For industry, the implementation of condition monitoring and health management techniques not only helps to identify potential problems before failure, but also enables timely maintenance, reducing downtime and increasing the lifespan of monitored equipment.

Proactive maintenance strategies promote safer operation and mitigate safety risks to employees and the general public. Ultimately, the integration of intelligent systems in production optimizes system performance, enhances productivity and efficiency, and fosters a safer working environment.



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## Competencies

The Intelligent Systems Group at the Signal Processing and Speech Communication Laboratory is hosted at Graz University of Technology. The applications of the developed methods range from signal and speech processing, industrial applications to computational medicine. The aim is to bridge the gap between basic research, applications and intelligent systems. Particular interests are in probabilistic graphical models, belief propagation, deep neural networks, resource-efficient and budgeted machine learning, and sequence modeling.

Graphical models unite probability and graph theory and allow to efficiently formalize both static and dynamic, as well as linear and nonlinear systems and processes. They provide an approach to deal with two inherent problems throughout applied mathematics and engineering, namely, uncertainty and complexity. The interest in deep learning is nourished by the remarkable performance boost in many image, signal and speech processing problems. This is particularly true when having big amounts of data and almost unlimited computing resources available. Particularly interests are in (i) scale-able semi-supervised learning to exploit huge amounts of unlabeled data during learning; (ii) robust learning in the presence of domain shifts; (iii) resource-efficient deep learning for constraint computing infrastructure of real-world applications; and in (iv) uncertainty modeling using Bayesian neural networks.

The research focus of the Christian Doppler Laboratory for *Dependable Intelligent Systems in Harsh Environments* (2023-2030) is on health monitoring applications with the associated research challenges.

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# Cyber-Physical Products

Alois Ferscha

## Vision

Among the most profound socio-technical phenomena of the past decades of technological evolution is the increasing **blurring of boundaries** between the **digital** and the **physical world**. Continuing trends in (i) **miniaturizing** Information- and Communication Technology (ICT) (microelectronics, system-on-chip technologies, quantum computing, ultra compact memory systems, micromechanics, nanowires and nanotubes, etc.) and (ii) the **exponential growth** and **globalization** of a planet-wide **communication infrastructures** (out of the estimated world population of 8.2 billion people some 5.35 billion are internet users (Statista, 2024)), and more than 17.08 billion “things” are reported to be interconnected in an Internet of Things (IoT) – when considering the broader ecosystem of connected devices, which includes computers and smartphones alongside IoT devices, is projected to exceed **207 billion** by the end of 2024 (Statista, 2024). **Digitalisation**, and consequently virtualisation have opened an unexpectedly wide spectrum for possible future scenarios of a “**co-evolution**” of **society** and **ICT** in general, and **commodities** (goods, products, consumables) and consumption in particular. This is fundamentally changing the way how people act, communicate, or even think, and consequently also how human desires, wants and needs emerge, and how they are announced and satisfied. Foreseeably, future notions of “**products**” (anything that is made available for sale, including commodity services) will redefine the principles of demand and supply, and reverse traditional supply chains from a “**produce then sell**” to a “**sell**

**then produce**” paradigm. Indeed, we evidence already today **demand driven supply chains** and batch size 1 production, mediated via the WWW.

To address such future notions of products with appropriate micro- (life cycle of an individual product) and macro-level (manufacturing, use of resources, energy, markets, environment protection) processes and policies, we have to extend the body of today’s supply chain frameworks beyond the pure physical existence of a product. The process coverage has to

- **Self-organised Products**
- **Internet of “thinking” Things**
- **Collective Adaptive Systems**
- **Embedded AI**
- **Federated AI**
- **Streaming AI**
- **Green AI**

spawn from the very **immaterial state** of a product being just a customer “idea”, or “desire” or “need” at the lower end of the spectrum, to a sequence of **physical states** throughout its life-cycle, up to the possibly **again immaterial state** of a product recycled back to raw material at the upper end of the spectrum. In a metaphoric language we could say that **products co-exist** in the **immaterial** and in the **physical world**, with the immaterial lifespan (usually) extending far beyond the material lifespan. This perspective suggests a “cybernetic” integration of both the material and immaterial sides of a product, embracing the whole product lifespan.



In the scientific literature, **Cyber-Physical Systems (CPS)** – a term coined by Helen Gill (NSF, 2006), and later discussed along design challenges by Edward Lee (UC Berkeley, 2008) – are referred to as interrelations of computations (digital world) with physical entities (physical world): *“Cyber-Physical Systems (CPS) are integrations of computation and physical processes. Embedded computers and networks monitor and control the physical processes, usually with feedback loops where physical processes affect computations and vice versa. ... To realize the full potential of CPS, we will have to re-build computing and networking abstractions. These abstractions will have to embrace physical dynamics and computation in a unified way.”* [7].

Borrowing from CPS, we understand **Cyber-Physical Products (CPPs)** as physical products (commodities, things) that are **linked** to their **abstract presentations** and control processes in the “digital world” via embedded ICT electronics. The embedded sensors, computers, actuators and communication technologies monitor and control the physical processes the product is engaged in, usually with **feedback loops** where physical processes affect control processes and vice versa. CPPs **interact locally, spontaneously and autonomously with other CPPs** in the physical and the control domain. Groups, flocks or large collectives of CPPs potentially exhibit a behavior that does not trivially follow from the behaviors of the individual entities, indicating properties typically observed in **complex systems** (i.e. condensed matter systems, the immune system, road traffic, insect colonies or social networks on the Internet).

This vision proposes research on CPPs as (i) a **new paradigm** for understanding the emergence of human needs and demands, (ii) the **close coupling** (ICT mediated) of product related data and control processes to physical products and physical process, and (iii) the **self-management** of all kinds of interactions of physical products (manufacturing, logistics, self exposure, self explanation, process embedding, life cycle management, recycling) throughout the whole product lifetime. Specifically the latter is supposed to embody a (iv) local (artificial) intelligence, that explains, manages, operates and represents the respective physical product, and connects and interacts with other products via “intelligence streams”, the AI superimposed version of data streams.

We aim at the design and provisioning of **key enabling technologies** allowing for the development of **self-organizing products**, including mechanisms to implement (i) markup languages and ontologies for **product self-description**, (ii) multi-sensor fusion and machine learning based collection and synthesis of a **local (artificial) product intelligence** including a **product memory**, (iii) collective adaptive **intelligence mechanisms** based on interacting CPP **federates** and the **intelligence streams** connecting them, (iv) **goal oriented reasoning**, self-configuration and self-management of products in **complex systems ensembles**, and (v) **P2M** (product to machine), **P2P** (product to product), **P2C** (product to consumer), **P2B** (product to business) and **P2E** (product to environment) interactions.

## Approach

Very early visions of opportunities for next generation products have already been created in the context of EU research strategies (FP7, H2020, Horizon Europe): *“Products with totally new capabilities will become available for general use, dreams such as intelligent cars, non-invasive health monitoring and disease prevention, homes sensitive and responsive to the needs of the persons living in it will become available to everybody. We will get better control of our health and environment, and over the quality of our food and our air, ensure better utilization of energy and other basic resources, we will be able to recognise diseases even before symptoms appear, and we will be able to be fully mobile and at the same stay constantly in touch with everybody...”* (ENIAC, ISTAG 2009). Although ambitious European research has addressed many of the issues raised, we are far from the reality envisioned by the ISTAG group.

About almost two decades of Pervasive Computing research since those early visions have created a critical momentum towards both the technological feasibility, as well as the industrial viability of CPPs [1]. This is evidenced by the evolution of **autonomous ICT systems**, and a remarkable advance in **AI technologies**.

The **first generation** of ICT aiming at autonomous system behavior was driven by the availability of technology to connect literally everything with everything (wired and wireless data communications). **“Networks of connected Things”** emerged, forming communication clouds of

miniaturized, cheap, fast, powerful, “always on” systems, enabled by the massive availability of miniaturized computing, storage, communication, and embedded systems technologies. Special purpose computing and information appliances, ready to **spontaneously communicate** and **opportunistically interact** with one another, **sensor-actuator systems** to invert the roles of interaction from human to machine (**implicit interaction**), and **organism like capabilities** (self-configuration, self-healing, self-optimizing, self-protecting) characterized this generation - popularly referred to as the “**Internet of Things**” (IoT).

The **second generation** of autonomous systems inherited from upcoming **multi-sensor based machine learning, recognition and knowledge processing** technologies, making systems e.g. situation-/context-aware, self-aware, activity-/user-aware, energy-aware or even socially-aware [6]. This generation reframed autonomous behavior to be based on **knowledge** (knowledge based sensing/monitoring of the environment, knowledge-based planning, knowledge-based acting), and today to be based on **empowerment** via **AI**. One result out of this course of research have been autonomic elements, autonomous entities able to recognize context, to build up knowledge, to self-describe, self-manage, and self-organize. The notion of “**Ecosystems of aware Things**” emerged, i.e. **collectives** autonomic elements interacting in spontaneous spatial/temporal contexts, based on **proximity, priority, privileges, interests, offerings, environmental conditions**, etc., giving raise to “**Aware Products**” [3,4].

A **third generation** of autonomous systems emerged, building upon connectedness, knowledge and awareness, and attempting for a **semantic interoperability** of entities in large scale, **complex, orchestrated, cooperative configurations**. Such systems are also referred to as “**Ensembles of Digital Artefacts**” (FP7 FET), or “**Socio-technical Fabric**” [5]. Ultimately, CPPs of the future are supposed to exhibit properties of social systems like **collective awareness, attraction, repulsion, flocking, foraging, morphogenesis** and **chemotaxis**. Indicative to such complex socio-technical systems is (i) their scale beyond  $10^6$ - $10^7$  entities (individuals, things, agents, objects), (ii) **continuously acting** and **reacting** to what the other entities are doing, (iii) the **system control** being highly **dispersed** and **decentralized**, and

(iv) (coherent) **behaviour arising** from **competition** and **cooperation** among the entities, so that (v) the **overall behaviour** of the system is the result of a huge number of **decisions** made and **interactions performed every moment** by **very many individual asynchronously**.

We understand CPPs as being constituent parts of such **socio-technical fabrics** of **dynamic, complex interaction ensembles** during their whole lifetime (demand/needs ensembles, manufacturing ensembles, logistics ensembles, sales ensembles, consumption ensembles, use and maintenance ensembles, recovery and recycling ensembles, etc.), within which they have to **sense, reason** and **act autonomously**. The manifestation of a rational for autonomous “reasoning and acting” is not trivial, as products may find themselves in (i) **self-adaptive ensembles**, which evaluate their own global behavior and change it whenever the evaluation indicates that they are not accomplishing what they were intended to do, or do so only at low levels of quality/performance, or in (ii) **self-organizing ensembles**, typically composed of a large number of entities that interact locally according to typically simple rules, in order to attain a certain “desirable” global behavior. In both cases, strategies leveraging **micro-level behavior** that is indicative to yield desired **macro-level outcomes** are in charge, but very hard to find.

In order to implement **CPPs**, a “stick-on” [3], networked embedded systems approach is proposed, linking physical real world objects (things, products, etc.) to digital representations and control processes by attaching a (physical) “**Smart Label**” to the object. We refer to a Smart Label as a low-power, low-weight, tiny scale, low-cost, extremely miniaturized microelectronics platform. On the **hardware** side a Smart Label integrates computing, storage, wireless networking, and versatile sensor and actuator components. On the **software** side it executes a low memory footprint, virtual machine like runtime environment, implementing (i) mechanism of **adaptive self-description** in standardized meta-data format (including the product memory), (ii) a **proxemic interaction** engine (spontaneous interaction), (iii) a **multi-sensor, multi-purpose, machine learning** based recognition framework (sensing), (iv) an **opportunistic, goal-oriented reasoning** engine (planning and decision making), and (v) a **self-adaptive, self-managed behavior control** unit (acting). Our reference implementation, the “**IPC token**”, supports (i) reliable, secure, trustworthy

and real-time **identification** and **authentication** mechanisms (to surpass the limitations of RFID, NFC, AutoID based systems, etc.), (ii) **miniaturization** and **embedding** of sensors like positioning units, accelerometers, gyroscopes, magnetometers, seismometers, thermo- and hygrometers, anemometers, gasmeters, MEMS microphones, olfactometers, radar-, lidar- ultrasonic detectors, doppler radars, geiger counters, etc. and **actuators** like photo switches, tilt switches, Reed switches, piezo- and pyroelectric actuators, etc., (iii) contains a multi-sensor based **embedded AI recognition frameworks** for localizing and positioning, environment and situation recognition, use-pattern recognition, attention and emotional state recognition (active learning, reinforcement learning, transfer-learning to surpass the limitations of unsupervised methods), novelty detection and context prediction, (iv) supports **semantic modeling**, markup languages (e.g. PML, SensorML, schema.org/thing), ontologies (e.g. GoodRelations, eClassOWL) and standards (EPCglobal, GS1), (v) **product memory** management and **goal oriented decision making** (GRL, extending traditional PRS and BDI based reasoning engines towards more anticipatory mechanisms of action control), and (vi) the **disentanglement** of the complex relationships between local interactions and global effects, in order to obtain **operational controls** to induce behavioural change.

Part of this vision of **next generation products** has been shaped as the entanglement of (intelligent, or) **cognitive products** and **cognitive production systems** as the **next generation of machines** in production processes [8] within Pro<sup>2</sup>Future. We attempt for next generation products and machines equipped with **cognitive capabilities** as to **perceive, understand, interpret, learn, reason** and **deduce**. **Cognitive systems** exceed established smart or intelligent systems by evolving from (i) **sensing to perceiving** - interpretation of semantic background of gathered sensor data, (ii) **analysing to understanding** - identification of causal connections between semantic data representations to create a fundamental, context-based understanding of input data, (iii) **relating to reasoning** - evaluation of critical aspects for decision making, and (iv) **adapting to learning** - evolution from pre-programmed system behaviour to automatic adaption of behaviour models according to changing environmental contexts. In popular science terms, cognitive products

could be referred to as “**products that think**” and “**production systems that think**”. In general, Pro<sup>2</sup>Future develops **Cognitive Industrial Systems (CIS)** by **embedding cognitive capabilities** into **products** and **manufacturing systems** so as to enable them to **perceive, understand, comprehend, interpret, learn, reason** and **deduce**, and **act** in an **autonomous, self-organized way** - together **with humans**.

#### CPPs based on Streaming AI

Recent assessments of the role of AI in industrial innovation trends capitalize the potentials of **Applied AI** against any other game changer candidate. **Conventional AI technology** in industry typically involves **centralized, edge** and **cloud-based back-end AI**, with **very resource aggressive machine learning** algorithmics, as far as **processing power, memory**, and **compute energy** is concerned. Evidently, **massive ecological impact** (greenhouse gas emissions) for model **training** and **inference** is induced, and **intricate collection, generation** and **handling of huge training data sets** is required. Recent observations on the advances in conversational AI (like OpenAI GPT-4, Bard, LaMDA, Bedrock, etc.) for example have evidenced, that the application of **AI** -aside from creating advance and value- can also **significantly harm the environment**. **Contrasting** the state-of-the-art in **conventional AI**, which is (i) **pretrained**, (ii) **holistic** and (iii) **resource aggressive** AI, we attempt to create a **complementary AI** approach to cope with the specificity of industrial production setting and product functionality features: **Streaming AI**.

**Streaming AI** attempts to align AI technology and methodology with the industrial digital transformation reality, in that it introduces (i) **streaming AI**, i.e. **training models on-the-fly** while in operation, thus avoiding the need for mass data prior to commissioning, (ii) **federated on-device AI**, i.e. an AI that is dispersed and distributed across different types of machinery, appliances, processes and devices, thus avoiding bulky mass storage management and centralized server farms, and (iii) **green AI**, i.e. employing **spiking** deep learning techniques and **neuromorphic** processing principles, thus avoiding exponential training complexity growth induced by increasing model size.

**Streaming AI** is **complementing current trends** in AI research, clearly opposing the main trends of foundational AI and **clearly addressing industrial needs** in AI research:

**Streaming AI instead of Pretrained AI:** **Pretrained AI** refers to models that have already been trained on large datasets and are typically used for specific tasks such as image recognition, speech recognition, translation, or recommendation systems. With **Streaming AI**, on the other hand, we address an approach in which the AI model is **trained on the fly**, i.e., the model learns from the data it encounters while interacting with users or an environment. The model is **continuously improved** by analyzing the results of its decisions and in this way learns to make better decisions. Streaming AI models can be more adaptable and potentially provide better results in unpredictable situations.

**Federated AI instead of Monolithic AI:** **Monolithic AI** refers to a model that runs on a single **central platform or server**. It is a **closed environment** in which all **data is stored centrally**, and all processing and analysis is performed on a single machine or cluster of machines. Typically, a monolithic AI platform is specialized for specific applications and cannot be easily reused for other applications. With **Federated AI**, on the other hand, we attempt for an approach where **multiple distributed devices work together** to solve a **common task** – mainly **found in industrial manufacturing settings**. This enables **decentralized processing** of data and **collaborative training** of models. Unlike monolithic AI, the model does not need to be run on a central server but can be distributed on users' endpoints or in cloud infrastructures. The data remains on the users' endpoints or in local data centers, and only the aggregated results are sent to the central location. The **advantage** of Federated AI is the **decentralized processing** of data and the ability to **customize** models to meet user needs. Distributed processing of data keeps **data secure** and **private**. Federated AI is often **easier to scale**, as more devices can be integrated into the system to achieve higher performance.

**Green AI instead of Red AI:** **Red AI** refers to AI applications that **consume a lot of energy**, resulting in **higher CO<sub>2</sub> emissions**. This can be the case due to the **high energy requirements** of AI models and the **computing power needed** in **data centers** or **cloud infrastructures**. Examples of Red AI applications include **large language models** such as GPT-3.5, GTP-4o or **autonomous vehicles** that require

high computing power. **Green AI**, on the other hand, refers to AI applications that are developed and deployed in an **environmentally friendly** manner. This means that these applications **operate with lower energy consumption** and therefore emit **less CO<sub>2</sub>**. Examples of Green AI include AI models that run on **energy-efficient chips** such as Arm or RISC-V, or applications of AI in the **renewable energy sector**, such as the optimization of wind and solar power plants. There is a growing interest in Green AI, as the energy requirements of AI applications have increased significantly in recent years, and higher energy consumption also leads to higher costs and environmental impact. Some companies have already started to launch Green AI initiatives to reduce the environmental impact of their AI systems.

## Impact

In the **Complex Systems** domain, this research is expected to create **scientific impact** in understanding the fundamental principles of autonomous sensing and reasoning, knowledge based self-organization, and the relation of local individual interaction to collective adaptive behavior in very large scale ( $10^7$  - $10^9$ ) socio-technical systems. Theory driven (ABMs and high performance simulation) and data driven (deployment of prototypes and reality mining) methods will evidence our findings.

In the **Embedded AI** domain, the integration of machine learning techniques with sensing, reasoning and acting mechanisms that implement self-awareness, self-management, goal-oriented behavior and dynamic adaptation will create novel design and operational principles for future, massive scale ICT systems exhibiting collective intelligence.

In the **Pervasive Computing** domain we expect to achieve pioneering models and reference implementations of a planetary scale coordination architecture for globe spanning product eco-systems. **Opportunistic Sensing** combined with **Federated Learning / Streaming AI** based recognition chains may significantly extend the state of the art in machine learning, and advance feature extraction methods and classification algorithms for very resource (compute power) constrained execution platforms.

The potential **industrial** and **commercial** opportunities of a Streaming AI based digital/physical integration –by embracing also the immaterial product life stages– go way beyond the opportunities of contemporary product design, horizontal and vertical integration of manufacturing systems, and traditional supply chain management. It has become very clear over the few years of experience with state of the art tagging technologies (EAS, RFID, NFC, Thin Film Electronics, Visual Markers, Chip Labels, wireless Beacons, etc.), cannot go beyond pure identity management. A new generation of tiny, embedded, always-on, energy efficient, self-managed, connected **on-device AI**, collaboratively creating **intelligence federates** via continuous **intelligence streams** is in quest.

The potential **societal impact** and opportunities of CPPs –which incorporate artificial intelligence (AI) and machine learning (**ML**) to simulate human cognitive processes –are countless, ranging from value sensitive design of **AI operated products**; processing vast amounts of data to provide actionable insights; enable highly personalized user experiences; enable predictive analytics, allowing businesses to forecast trends, customer behavior, and market demands; need driven manufacturing and production line optimization by predicting equipment failures and scheduling maintenance, reducing downtime and costs; self-explaining / attention-aware / supportive products, (emotional) consumer-product engagements, optimization of use of resources / logistics / use-patterns / waste management / recycling strategies, conservation of (natural) resources, etc., - ultimately also fostering a human-centred, flourishing symbiosis of society and technology.





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## Competencies

As a research method we attempt to employ a combination of **theory driven analytics**, computational modeling/simulation, HW/SW platform **prototyping**, together with **hypothesis driven experimental research**. In the past we have exemplified a **synthesis** of **theory driven** and **data driven approach** of research: in the theory driven approach we inherit from established theoretical bodies (information theory, complex systems theory, machine learning theories, behaviour theories, human perception and attention models, collective choice theory, social systems theory, etc.), based on which hypotheses are formulated and data sets are collected (on purpose) to evidence those hypotheses - ultimately, of course, to foster and strengthen the evidence for such (pre-existing) theories. In the data driven approach we deduced insight from mining collected data sets with specific mining techniques (statistical clustering, classification, regression-/factor-analysis, sequence-/pattern-mining), potentially giving raise for new theories.

Our operational research units (JKU Institute of Pervasive Computing – IPC, COMET K1 Centre Pro<sup>2</sup>Future, JKU Research Studio) are well interwoven with international EU funded Pervasive and Ubiquitous Computing projects. The IPC research work is allocated in the domain of **Recognition Architectures** and **Opportunistic Sensing** (FP7 FET projects OPPORTUNITY, SOCIONICAL), Networked Embedded Systems and Energy Efficiency (FFG Projects PowerIT, PowerSaver, ZiT Project Sports Community Token), Human Computer Confluence (FP7 FET project HC2), **Complex Systems and Coordination Architectures** (FP7 FET project SAPERE), **Fundamentals of Collective Adaptive Systems** (FP7 FET Projects PerAda, FoCAS, SAPERE), and **Value Sensitive ICT Design** (FFG Projects Raising Attention, DISPLAYS, 360 Light). Translational research cooperations with industrial partners range from manufacturing, to network operators, consumer electronics vendors and media corporations (Red Bull Media House, Energie AG, Silhouette AG, Google Glass, Sembella, SIEMENS, IBM, Telekom Austria, ONE/Orange, VCM, WRC, etc.). I serve as a permanent consultant for the EU ICT research strategy (EC DG CONNECT, Unit FET, Future and Emerging Technologies), with a strong tradition in identifying and soliciting basic research problems and strategic research fields emerging from the evolution of the global information and knowledge society (see e.g. **FET Whitebook Pervasive Adaptation**, or the **FET Whitebook Human Computer Confluence**).

The **Institute for Pervasive Computing** runs outstanding, state of the art **laboratory equipment** and **experimental infrastructures**, e.g. the **Sensor Lab** (Geolocation Sensors, Accelerometers, Gyroscopes, Position/LocationTrackers, Ultrasonic Sensors, Depth/Thermal Imaging, Pressure Sensors, MEMS, Bio-Signal Sensors, etc.), the **Display Systems Lab** (HDTV DLPs, Wearable Displays, Multiscreen HD LEDs, Tactor/Olfactory Displays, SmartWatches, etc.), the **Human Attention Lab** (head worn eye-trackers (Tobii Pro Glasses 2, Pupil Labs Core and Neon, SMI Glasses 2.0) and **AR** devices (Microsoft Hololens) for attention-, cognitive load-, behavior-, ... analysis, control and interaction as well as Empatica E4 wristbands and Shimmers for **biophysiological sensing** (HR, HRV, BP, GSR, ...), and the **360 Lab** (360 Video Sensors, Capturing, ProcessPipeline Tools, 360 broadcasting technology).

For the purpose of **attention-, cognitive load-, behavior-analysis** as well as **eye-tracking** based research we use systems such as the Tobii Pro Glasses 2, Pupil Labs Binocular Eye Tracker, Pupil Labs Core and Neon, Microsoft Hololens and the SMI Eye Tracking Glasses 2.0. For **biophysiological sensing** (HR, HRV, BP, GSR, ...), we use Empatica E4 wristbands and Shimmers. The IPC's **Cognitive IoT Toolboxes** (powered by Raspberry Pi Models 3B, 4B and Zero, holding various sensors like temperature, humidity, light-intensity, audio, motion, ... and actuators like displays, speakers, motors, ...) allow for wireless, embedded environmental measurements and interaction as well as on-device TinyML. Alongside, TinyML is also enabled via an Nvidia Jetson TX2 and Xavier. Across the research topics we operate a **motion capturing** (MoCap) system with 16ToF at 240FPS cameras (OptiTrack), a collection of **depth sensing** devices, for example the XSens MTx 3-DOF (body worn) and Leap Motion, Intel RealeSense, Microsoft Kinect, various kinds of human body-oriented tracking sensor technologies, such as the MotionJacket and the Intersense IS-900 Precision Motion Tracker.



**Sapere (EU FP7 FET proactive) – Self-Aware Pervasive Service Ecosystems.** Developed self-aware components and a general nature-inspired interaction model and studied and decentralized self-\* algorithms to enforce various forms of spatial self-organization, self-composition, and self-management for data and services, within a self-aware and adaptive framework services for future and emerging pervasive network scenarios. A particular testbed is a social context driven city scale coordination assessment. The expertise in large scale sensing and adaptive systems directly benefit this project.

**FoCAS (EU FP7-ICT, Fundamentals of Collective Adaptive Systems) – Fundamentals of Collective Adaptive Systems.** Coordination action which aimed to integrate, coordinate and help increase visibility to research carried out in the FOCAS FET Proactive Initiative and in research fields related to collective adaptive systems.

**HC2 (EU FP7-ICT) – Human Computer Confluence Research in Action.** Successfully demonstrated new ways for the participatory solicitation of Research Agendas for FET, highlighting research challenges specifically at the confluence of human and computer systems.

**OPPORTUNITY (EU FP7 FET-Open) – Opportunistic activity recognition systems.** Developed methods and system architectures to recognize human activities in “opportunistic” configuration of sensors. We developed the underlying software framework and sensor coordination architecture to allow the discovery, registration and management of nodes, and the execution of opportunistic signal processing and machine learning algorithms. This expertise will be leveraged in this project to design a lifelong learning software framework.

**SOCIONICAL (EU FP7 FET Proactive, N°231288, 2009-2013, as partner) – Complex Socio-Technical System in Ambient Intelligence.** Focusing on the modelling of large scale events with a view towards real-time crowd-behaviour management, we have developed the infrastructure (sensing on mobile devices, server side acquisition, management, storage, query, visualisation) to acquire in real-time the data of large number of wearable devices. This was tested in several city-scale events (Vienna marathon, Linz train station evacuation scenario, etc.).

**Attentive Machines (FFG Pr.N.: 849976):** Multisensory, multimodal sensor framework for modeling attention distribution and quality, activities, workflow processes (eye tracking, depth sensors, accelerometers, galvanic skin response, heart rate variability, etc.).

**Fischer4You (FFG Comet K1: 854184):** Merging ski ability assessment and product features and characteristics for recommendation. Devices and algorithms for recording and analyzing the relevant data. Smartphones and customized devices (e.g.: Shimmer, PIQ - Ski Tracker, Xsense Air Tracker).  
**WorkIT (FFG Comet K1: 854184):** Multi-sensor framework, providing algorithms to recognize work steps and micro-actions using supervised and unsupervised ML; abstract models of workflows that enable appropriate step-by-step guidance of workers.

**GUIDE (FFG Comet K1: 854184):** Functional prototype of a cognitive, head-mounted welding system and associated design and implementation toolchain; digitization of analog factories using 3D reconstruction techniques; implementation of cognitive, (pro)active software modules (e.g. skill detection, cognitive load).

**SeeIT (FFG Comet K1: 854184):** Development of prototypes for subtle stimulation on multimodal channels based on Wickens' Multiple Resource Theory, supporting guidance tailored to the user's behavior, strengths and limitations and the needs of the ongoing process.

**Streaming AI (FFG Comet K1: 854184):** Development of an **AI framework for industrial applications:** In contrast to conventional (i) pre-trained, (ii) holistic and (iii) resource-intensive AI (OpenAI GPT-4o, Bard, LaMDA, Bedrock, etc.), it attempts to harmonize AI technology and methodology with the reality of digital transformation in industry by (i) introducing streaming machine learning methods, i. i.e. training models on the fly, thus avoiding the need for mass training data, with (ii) on-device machine learning methods for AI federations distributed across different manufacturing plants, machines, processes and devices (“Internet of Thinking Things”). This can avoid ex-ante mass data collection and its management in mass storage and centralized server farms.

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# Industrial Artificial Intelligence

Roxana Holom, Evans Doe Ocansey, Paul Heinzleiter, Sandra Wartner

## Vision

Artificial intelligence (AI) surrounds us every day – be it powerful language models in the form of ChatGPT, driverless cars with integrated image recognition or the purchase recommendations in online stores. But AI will also play an essential role in almost all industrial processes and take the topic of “Industry 4.0” to a new level – that of “Industrial AI”. What does this mean for our industry and for Europe as a production location?

### Industrial AI: The logical evolution of Industry 4.0

Machines and robots in large production lines carry out complex but monotonous production steps. In the process, data – for example, sensor data, temperature, throughput times, etc. – is collected. With data-driven AI methods, these manufacturing processes can be made more trouble-free, adaptable and autonomous. The computer science and mathematics methods required for this are subsumed under the term Industrial AI. Industrial AI is thus concerned with solving problems in industry to achieve goals such as creating customer value, improving productivity, reducing costs, optimizing processes, predictive or prescriptive analysis for early fault detection, improved maintenance cycles, and continuous quality improvements.

### People and machine: unbeatable together

These intelligent systems should not be seen as a threat to the human workforce, but as a great opportunity. While AI systems can be used in a supportive manner to optimize workflows and relieve humans or automate repetitive and dangerous

tasks, humans will always remain indispensable as they are better able to react to unexpected events and make decisions. This makes industrial production in Europe not only economically viable, but also more sustainable. Experts from science and industry agree that the future of industry no longer lies exclusively in increasing efficiency and improving production, but rather in the sustainable production of sustainable products.

- **Industrial Artificial Intelligence**
- **Computer Vision**
- **Natural Language Processing**
- **Time Series Analysis**
- **Data Engineering**

### Making photovoltaic production more efficient

One example of this more sustainable production is the manufacture of photovoltaic (PV) products, which are currently in high demand. The latest generation of PV technologies combines high performance with great flexibility for multiple uses. However, their high complexity makes them vulnerable to the occurrence of critical defects with only minor variations in manufacturing, resulting in significant production waste. The EU Platform-Zero project, launched in early 2023, aims to improve the production quality of photovoltaic systems while reducing manufacturing costs through zero-defect manufacturing. This is achieved by applying process monitoring, control and AI strategies. It uses non-destructive inspection methods and

technologies to detect, correct and prevent critical production defects early. Data will be analyzed in real time to optimize the production process and improve product quality.

Digitalization efforts have led to automated data collection, which presents many companies with major challenges in data processing and analysis. RISC Software GmbH relies on smart technologies in the field of data engineering and AI to analyze (real-time) information and collected data pools from texts, images or sensor data and derive suitable optimization measures. Companies are supported in efficiently processing and analyzing their data.

### Data Engineering as a solid basis for the efficient use of Data Science

Before analysis, data from various sources is integrated and made usable efficiently. Data engineering is thus a prerequisite for the efficient use of data science, especially in the Big Data area. Central activities such as data cleansing, data integration, data model transformation, improvement of data usage through fast queries and data preparation using AI are supported.

Artificial Intelligence methods like Machine Learning (ML) require substantial amounts of valid training data of high quality. Other possible applications include preventive maintenance of production machines and in-line feedback loops in production lines to optimize product quality. In this context Data Engineering is applied to collect, integrate, and clean raw data into an integrated database. This database can act as a set of data for training forecasting models or enable a human data analyst to work more effectively with an integrated set of data. To build up such an integrated view of the data is the focus of Data Engineering, which can roughly be split up in these steps: 1) Data cleansing, 2) Data integration and 3) Data transformation.

Data cleansing includes checking the data for completeness and validity, which may also include outlier detection to find wrong sensor values. Data rows with wrong or missing values are then often discarded, especially if sufficient training data is available. Data integration focusses on integrating data from different data streams such as time series data from different sensors. In this case typically the timestamps of the values are used to match up the values from different sensors. Data transformation describes the process of bringing the data into a model,

which supports fast querying of the stored data according to application requirements. Typically, the row keys should be comprised of a data field, which is often used in range queries or equality comparisons. A good example of this could be a location identifier for weather data queries.

### Analysis of structured data and images

Statistical procedures and methods from the fields of visual analytics, data analysis and machine learning enable analyzing (large amounts of) structured data and images (computer vision). Anomalies, connections, correlations and patterns are detected, which can be used for error and root cause analysis in the manufacturing processes. Moreover, the analysis of structured data and images is becoming increasingly important for enhancing quality control, improving production efficiency, and reducing waste. This enables them to make data-driven decisions, optimize their operations, and improve product quality, ultimately leading to greater customer satisfaction and increased profitability.

### Processing unstructured text data

Natural Language Processing (NLP) is a rapidly evolving field that allows computers to understand, interpret, and generate natural language (written and spoken). As an interdisciplinary field of linguistics, computer science, and artificial intelligence (AI), NLP acts as an interface between humans and machines. With higher computing power, advanced algorithms, and access to vast amounts of data, NLP has revolutionized several industries by extracting valuable insights from unstructured data and is constantly expanding the scope of applications. One of them is **information extraction**, which selectively extracts crucial information from text and stores it in a structured manner, using techniques like tagging or Named Entity Recognition (NER). **Text classification** is another valuable application, which automatically sorts text data into predefined categories such as topics or failure classes. Another essential NLP technique is **sentiment analysis**, which recognizes emotions in text and can be used to understand consumer sentiment about products. By analyzing sentiment, businesses can gain insights into customer feedback and preferences on a large scale, improving their products and services to meet customer needs. Overall, NLP offers numerous applications that support a great variety of stakeholders to gain valuable insights from their text data.

## Approach

The industrial sector, like other areas, is going through a digital transformation period, i.e., manufacturing companies are experiencing various digitalization activities [1]. In this context, the industrial data and the way it is processed, visualized and utilized play

an essential role. However, the path from raw data to the integration of data analysis models in the production is in most cases further than expected. For this purpose, RISC Software GmbH is proposing an agile-like approach (highly involving actual actors) for the AI-based data analysis in the industrial sector.

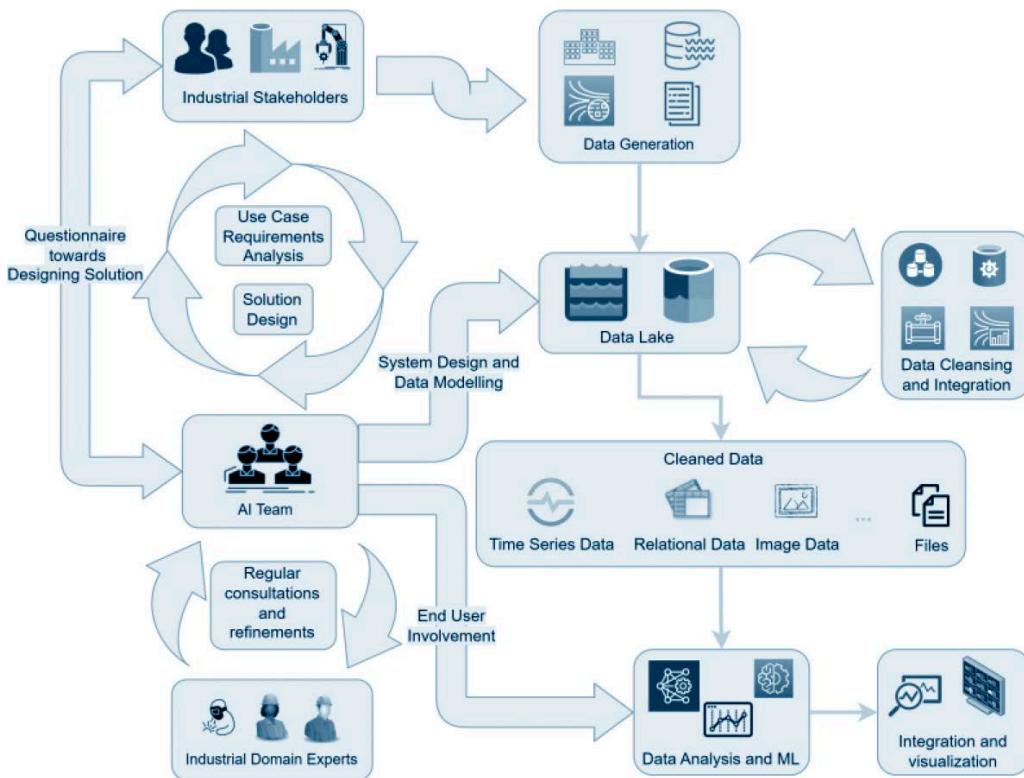


Fig. 1. Agile-like workflow for industrial AI solutions

Figure 1 illustrates a possible agile-like workflow suitable for an industrial AI project. It begins with the stakeholders, which may also be a consortium of industrial companies. However, we do not indicate the internal complexity of the operational structure of such a consortium but rather consider it as a single complex unit. The workflow begins with a continual discourse between the industry stakeholders and the AI Team. After detailed analyses by the parties involved, the use cases and their requirements are established. The AI Team designs solutions suitable for the use cases after further dialogue with the industry stakeholders. Afterwards, the industry stakeholders provide all kinds of data based on the requirements of the use cases collected into a data lake. The data within the data lake is processed, transformed, and loaded into a data warehouse by data engineers within the AI Team. This data engineering process requires inputs from the data scientists within the AI Team, but also from the industry stakeholders,

represented for example by domain experts or process engineers. The final data loaded into the data warehouse is clean and ready to be analyzed by the data scientists within the AI Team. The data scientists perform exploratory data analysis, and per their dialogues with domain experts, the data is further processed. The preprocessed data is then used to train AI models based on the specifications of the use cases. The results of the AI models are then further analyzed together with the domain experts and used to make informed decisions to increase the business objectives suitable to the industry stakeholders. The essential aspect of this approach is the involvement of industry experts in all design and implementation cycles of the AI solution. By conducting regular consultations and refinement meetings, the process of data analysis and ML in the industry becomes more intuitive and comprehensible to all parties involved.

## Data Engineering as a solid basis for the efficient use of Data Science

Data Engineering tasks can be performed using multiple different approaches. A typical classification is the separation into data stream processing and batch processing. Both types represent different methods of coping with substantial amounts of data. In batch processing, massive quantities of data are processed at once, typically in parallel, while stream processing splits the data into small chunks, which are processed immediately as they arrive. Stream processing is especially advantageous if the data is arriving over time and the separate chunks can be processed independently, while data-parallel batch processing is focused on processing large chunks of data at once.

Big data is often stored in a data lake, where raw data can be stored for further processing, like data cleansing, integration and transformation as mentioned above. This approach typically allows us to apply diverse types of transformations onto the data, often using distinct types of processing paradigms as well. This includes for example the execution of a map-reduce algorithm using frameworks like Hadoop or Spark. As an alternative, data streaming approaches like Apache Spark Streaming or Apache NiFi can also be applied to read bulk data and process it as a stream of data records [2].

A good example of such a data lake is the data platform currently being set up within the European project Platform Zero, which focusses on improving the production process of modern 4th generation solar cells to improve their efficiency and power yield. This will be achieved through collecting sensor data from the production process, training of ML models and using these for inline inference for steering the production process towards zero defect manufacturing. The data being collected will be stored and preprocessed using data engineering approaches enabling efficient model training and outlier detection for alerting machine personnel about production deviations. A similar approach is followed within the European project MetaFacturing, where hybrid models of casting and welding processes are being set up, which combine simulation and data-driven approaches to improve the production processes through inline steering and control. Therefore, the collection, preparation and integration of sensor data plays a crucial role in

supporting the modelling effort and thus the improved understanding of the industrial processes.

## Analysis of structured data and images

Clean and well-structured data of different types available in the data warehouse, which are made possible by data engineers, are then utilized by data analysts and data scientists. In this context, these experts, namely, data analysts and data scientists, perform further analysis to extract useful information from the well-structured and clean data essential for the use case specifications. Some of these analyses include correlation analysis among the features and the targets, the probability distributions of the features, data visualization, standardization, and normalization, to mention a few. In the case of time-series data, a sliding window approach may be used to preprocess the data before further analysis. For computer vision models that involve image data, additional features can be introduced using data augmentation techniques to expand the feature range.

The correct choice of training data is a challenging task in the development of practical models. Depending on the field of application, however, models should be able to make valid decisions based on data extracts and must therefore be trained on such extracts. The manner in which these are selected has a strong influence on the practical suitability of the resulting models. On the one hand, the choice has to be made in such a way that no so-called sampling bias arises, that is, the samples adequately reflect the different aspects of the structured data or images. On the other hand, however, the trained models should function correctly, precisely on those events which are of particular interest to the end user. Therefore, it is especially important that domain experts enrich the data with their domain knowledge and thus generate significant value from the data in collaboration with data scientists and engineers.

## Processing unstructured text data

Older systems relied on rule-based or purely statistical approaches, whereas the breakthrough only came with machine learning (especially deep learning) and the availability of large amounts of data. A significant breakthrough in NLP and language model proficiency was achieved with the release of the Transformer architecture in 2017 [3]. To learn language representations, the model



is provided with huge amounts of text data (e.g., books, Wikipedia) in the pre-training phase. At this point, the model does not yet have information about specific tasks such as translating texts or evaluating information and must learn these in the subsequent finetuning phase using an annotated dataset. In this learning process, knowledge from the pre-trained model is transferred to the new model and used as a starting point for training on a specific task (transfer learning).

Open-source models, such as those available on the Huggingface platform (<https://huggingface.co/models>), can serve as a useful starting point for specific use-cases. However, they may not always have the required domain knowledge and vocabulary, particularly in narrow domains or specific applications like

manufacturing. Therefore, fine-tuning is often required to tailor the model to the specific domain. To achieve successful fine-tuning of a pre-trained model, it is crucial to have access to suitable data that meets the required quality standards and is available in sufficient quantities. Manufacturing operations typically generate large volumes of unstructured data from various sources, such as sensor data, product reviews, warranty claims, and customer feedback. To ensure that the models accurately reflect the specific domain, high-quality labels are essential. Generating high-quality labels is often time-consuming and resource-intensive, requiring significant effort and resources. Despite these challenges, the potential benefits of NLP are vast, and organizations that embrace this technology stand to gain a competitive advantage in the marketplace.

## Impact

Applying advanced machine learning algorithms, statistical models, and other data analysis techniques to large volumes of structured and unstructured data enables companies in the industrial sector to harness the power of data and analytics to drive innovation and optimize their operations [4].

### Data Engineering as a solid basis for the efficient use of Data Science

To improve production quality and reduce costs, relevant information needs to be extracted from the collected production data. Through intensive data engineering – often covering multiple steps – process data on the relevant steps becomes usable. Besides supporting the detection of cause-and-effect relationships regarding machine parameters and product quality, Data Engineering can also provide traceability of production and production parameters throughout the entire process.

The impact of Data Engineering in general can be seen in enabling the efficient processing of substantial amounts of data, and thus enabling endeavors such as ML training of larger models or supporting human machine operators by detecting deviations of current machine behavior from historical data. While such results – especially the fully trained models can be integrated in a real-time control loop for automatic machine steering, large sets of well-structured data are also required in explorative data analysis as performed by data scientists. Other examples include the integration of data from various sources and formats, such the integration of time series data from different sensors enabling more accurate predictions of machine behavior and for example enabling predictive maintenance.

In the field of corporate strategy, a large – and valid – database can support data analysts to work more effectively, making more reliable predictions on market development and enabling data-driven C-level decisions. While these capabilities are not specific to the manufacturing and Industry 4.0 fields, they are as valid there as elsewhere.



### **Analysis of structured data and images**

To unleash the full potential of data analysis and machine learning techniques in relevant industrial applications, there is a need to develop specific solutions for relevant use cases. There is a clear gap when it comes to applying the AI solutions for manufacturing industry plants, as most solutions do not meet the needs of the industry (e.g.: integrated analysis of product information with process specific data, results of data analysis are readily comprehensible, simple and clear communication between AI solutions and domain experts). AI solutions addressing these kinds of needs in the industrial sector will generate significant economic and technological impacts in terms of production quality, enhancement of the quality assurance process [5], optimization of material usage and improvement of recycled material usage (with consequent environmental impacts). Furthermore, such AI solutions will have a societal impact aligning with EU policy priorities related to the digital transition and enhancing sustainability in the manufacturing industry and strengthening the integration of AI research and innovation into society.

### **Processing unstructured text data**

In the era of Industry 4.0, it is often no longer sufficient to analyze structured data or image data generated by machines and sensors. Analyzing texts such as free-text error messages taken by machine operators and production staff, machine and maintenance logs of past events, descriptions of problems and solutions often contain meaningful insights for troubleshooting and maintenance decisions. NLP can enable better prediction of machine downtimes [6], help to identify root causes of failures [7], and support quality control and improvement. By analyzing customer feedback, product reviews, and warranty claims, quality issues can be identified quickly, and manufacturers have lower response times to resolve them. NLP can also support machine operators and production staff in making maintenance decisions by analyzing free-text error messages, machine logs, and maintenance logs of past events [8]. Ultimately, the applications of NLP in manufacturing can lead to improved operational efficiency, cost savings, and customer satisfaction.



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## Competencies

The core competencies of the research institution RISC Software GmbH are symbolic computing, mathematics and information technology in the business segments Logistics Informatics, Industrial Software Application, Medical Informatics and Domain-specific Applications. RISC Software GmbH develops individual tools and solutions for its clients - particularly in the area of logistical planning, optimization and ontological process digitalization. With an operating performance of approx. 6.0 million euros and approx. 75 employees, RISC is economically one of the most successful independent research institutions in Austria. This is highly appreciated by international research partners in EU projects (e.g. PLATO-N, PRACE, Boost 4.0), national funding projects (e.g. MEDUSA), as well as clients such as Shell, EADS, RHI, Magna, voestalpine, FILL, WFL, ILL, DS Automotion, Salinen Austria, TRUMPF or ÖBB.

RISC is especially concerned with data collection and processing frameworks, where prognosis calculations and data stream simulation are an important part. The research and application of neural networks, fuzzy algorithms and machine learning methods has been carried out since 1995. Machine learning in combination with visual analytics and big data technologies has become a major focus in recent years, both in international research projects and in industrial research. Further information can be found on the RISC homepage ([www.risc-software.at](http://www.risc-software.at)). Due to RISC's broad range of experience in the fields of data engineering and data science, the main task lies there in particular. With its competencies in explorative data analysis, machine learning algorithms, statistical methods and the combination of data- and model-driven approaches to so-called hybrid models with a focus on domain-specific questions, the research institute is considered the ideal candidate for the planned project within this call.

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Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Commission. Neither the European Union nor the European Commission can be held responsible for them.

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# Active Learning of Autonomous Manufacturing Tasks

Elmar Rückert

## Vision

The automation of industrial manufacturing tasks is characterized by numerous challenges including the complexity of the tasks, the need to safely interact with human co-workers, the complexity of the environmental conditions, and the immense time- and cost-related requirements to fulfill today's customer demands.

At the forefront of these challenges is the automation of single-item production or batch size 1 production scenarios, where classical automation attempts through programmed systems cannot be applied anymore. The research ambitions of the chair of Cyber-Physical-Systems (CPS) are to fill this void through smart teaching and self-learning robotic systems.

In addition to the challenging hardware requirements of manufacturing tasks, safety has to be ensured through compliant robotic actuators, the fusion of visual and tactile sensor information, and through adaptive control systems for monitoring and adapting the autonomous skill execution. Here changing sensor conditions, unforeseen human behavior, sensor failures, or sensor noise have to be considered in the adaptive control strategies.

The learning methods themselves need to be suited for non-robotic experts, and as such require robust interfaces and tools to teach, improve, monitor, execute, or transfer learned skills to novel tasks. Our research vision is to enable non-robotic experts to teach an autonomous robotic system complex skills within a few seconds, to develop tools for seamlessly monitoring quality and safety regulations, and to build cloud-based skill libraries that transfer between tasks, human instructors, and

industrial machines like the ones shown in figure 1.

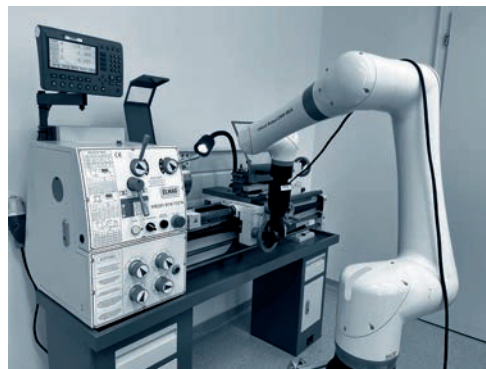


Fig. 1. Illustration of two industrial robotic scenarios where complex tasks have to be executed by autonomous robotic systems. These tasks require fusing visual and tactile information and to adapt the motor torques on-the-fly.

- **Active Learning**
- **Reinforcement Learning**
- **Motor Skill Teaching**
- **Kinesthetic Teaching**
- **Human-Robot Co-Worker Scenarios**

## Approach

Our approach focuses on the joint development of hardware systems and machine learning algorithms. This joint development is essential to develop robust and versatile autonomous robotic systems for interactive co-worker scenarios. For the interaction, CPS develops smart user interfaces based on self-built sensor gloves, augmented reality glasses, and tablets. These interfaces are connected via software and network interfaces, e.g., the robot operating system (ROS2), and enable cloud-based decentralized decision-making and control strategies. Web service interfaces are further developed to correct and adapt the task execution of autonomous systems using mobile devices like smartphones or tablets.

The learning algorithms are based on probabilistic and neural skill



representations [1, 3, 6] that can learn the complex correlation between tactile, visual, and proprioceptive data. These representations are learned through user interactions and through autonomous self-improvement based on sample-efficient deep reinforcement learning methods [2, 5]. A key aspect of our developments is the combination of prior knowledge with the ability to learn new relationships and abstractions from interactions with non-robotic experts and the environment, i.e., through reinforcement learning.

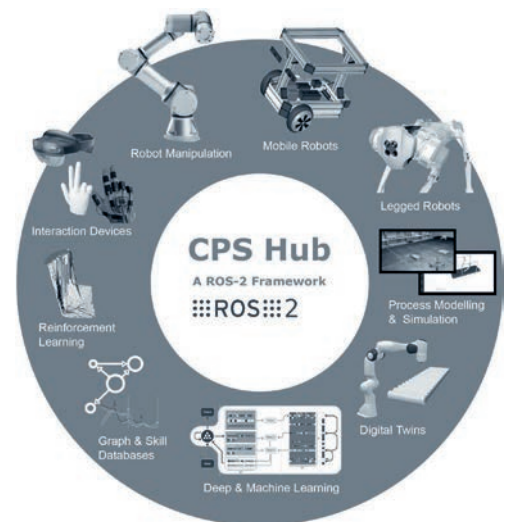


Fig. 2. The approach of the chair of Cyber-Physical-Systems is to build a framework for combining different hardware systems including sensor gloves, augmented reality glasses, compliant robot arms with sophisticated machine learning algorithms for skill teaching, control and monitoring.

## Impact

The research ambitions of CPS have the potential to enable Austrian's small and medium size companies to integrate modern robotic and machine learning systems into their value chain. This integration can improve the competitiveness of our industry, would result in additional industrial collaborations and can provide a sustainable contribution to Austrian's future economy.



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## Competencies

The Chair of Cyber-Physical Systems is dedicated to application-oriented basic research in the areas of artificial intelligence, digitization of industrial processes, and robotics. One focus is on the modeling of intelligent human learning processes with the goal of developing efficient learning methods and prediction models for cyber-physical systems.

CPS is involved in numerous national and international research activities including projects funded by the European commission, the German research foundation (train.ai-lab.science), and the Austrian research promotion agency (FFG Leitprojekt KIRAMET). Further, CPS is cooperating with companies like LUPA-Electronics GmbH, KNAPP AG, Stahl- und Walzwerk Marienhütte GmbH, qoncept dx GmbH, and the voestalpine Böhler Aerospace GmbH & Co KG.



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# Dependable Internet of Future Products

Bernhard Aichernig, Martin Horn, Kay Römer, Klaus Witrals

## Vision

Future factories will have to support lot-size-one production, where every single product instance is tailored to the requirements of a customer. This requires highly dynamic reconfiguration of production lines, where **products and its parts, tools, machines, robots, and humans have to collaborate closely, using the Internet of Things (IoT)** as a substrate for this collaboration. However, in the original Internet of Things vision, IoT devices solely monitor – rather than control – real-world processes using best-effort Internet services that have been adopted to serve Things. Because IoT failures may have disastrous consequences in future production environments, it remains a substantial challenge to **realize safety-critical IoT applications in Smart Factories that automatically control real-world processes in a highly dependable manner**. Here, dependability summarizes extra-functional attributes that allow a user to put trust into and rely on the system. Dependability attributes of particular relevance are reliability (continuity of correct, accurate, and timely service); availability (readiness for correct service); safety (absence of catastrophic consequences on users and environments); confidentiality (absence of unauthorized disclosure of information); and integrity (absence of improper system alteration).

Dependability is challenged, among others, by three threats that make it very difficult to offer these attributes along with quantitative predictions and guarantees on their compliance.

- i. Harsh Environmental Conditions.** The IoT is deeply embedded into

environments with often harsh conditions. In a factory setting, for example, unpredictable wireless signal propagation due to metallic objects, strong interference from other wireless transmitters, and extreme temperature or humidity conditions are common problems. In a scenario with connected robots, mobility has a strong impact on the quality and stability of communication channels.

- **Dependability**
- **Internet of Things**
- **Localization**
- **Verification**
- **Networked Control**
- **Diagnostics**

- ii. Physical and Remote Attacks.**

The smart things forming the IoT are everywhere. Hence, attackers can not only mount attacks remotely via network interfaces, but can get hold of these devices easily to mount so-called physical attacks. There exists a wide range of physical attack techniques that range from permanent tampering and dynamic fault induction techniques to the collection of information through side-channels, e.g., by analyzing a device's power consumption or its electromagnetic field.

- iii. Complexity.** The IoT is a complex system (of systems) where many devices have to cooperate using a dynamically changing communication network. The capabilities and services of these

cooperating devices do not only differ, but they also change over time according to advancing requirements and standards. Apart, some devices may have severely constrained resources (energy, computing power, memory, communication bandwidth). Even worse, the IoT is open in the sense that nodes can join and leave continuously and it is not known in advance how many and which devices will be present to cooperate when required in an often unknown environment. Thus, the IoT has to be scalable to a large number of arbitrarily deployed nodes. Moreover, significant complexity is added by the used AI techniques, like machine learning and cognitive systems, to enhance the Things' capabilities. These properties make it very hard to design and implement IoT applications, rendering them susceptible to design and implementation flaws.

A further challenge is the fact that a system is only as dependable as its weakest part, thus **a truly dependable system requires strong interdisciplinary collaboration to make each component of a system dependable and to ensure the dependable interaction** of all these components among each other. To this end, we have **built up an interdisciplinary team of 11 key and 8 associated researchers at TU Graz** in the framework of an excellence program known as "LEAD projects" [1]. The collaboration focuses on three thematic areas, namely dependable wireless communication and localization; verified dependability by design; and dependable multi-agent systems. Close collaborations among these three areas ensure the dependability of a complete system integrating all these aspects. One of the considered application domains are smart production environments.

## Approach and current Achievements

In times of digitization, dependable wireless communication and localization plays an important role in the Internet of Things. In particular, robust, high-accuracy radio positioning is relevant for many different applications in manufacturing and logistics, where the goals range from positioning and navigation to activity recognition and control and optimization of complex, flexible processes. Ultra-wideband (UWB) and mm-wave radio systems have the capability to provide these

functionalities. The **overall aim of our research is to increase the robustness and scalability of the communication and positioning systems** in order to close the gap towards the development of robust location-aware IoT applications. More specifically, we investigate the scalability of UWB-based systems towards larger areas, more agent nodes, realistic, highly cluttered environments, and higher mobility of agent nodes, as well as increasing the carrier frequency towards mm-wave systems and the impact of man-made radio interference. The development of algorithms and protocols for robust and accurate localization and reliable communication are addressed by these challenges [5]. This requires suitable radio channel models, which may be parameterized to the mm-wave frequency band. To this end, **we developed a wireless sensor network testbed to foster interdisciplinary collaboration** within the consortium and to experimentally verify our research results [4]. **We investigated the impact of interference towards the reliability and accuracy of UWB radio nodes and improved their scalability on a protocol level.** In order to further improve the performance, **we investigated the feasibility of different antenna designs as well as shifting towards higher frequencies with millimeter-wave technology** [6].

A second important research area are verification and design methods, techniques, and tools in order to provide dependability guarantees for IoT devices. More specifically, we focus on the dependability attributes: correctness, robustness, security, and timing. That means an IoT device should meet its specification (correctness) including hard real-time requirements (timing), despite harsh (robustness) and adversarial environments (security). **The goal is to develop design- and run-time verification techniques for these aspects of dependability.** At design time, the aim is to develop abstract formal models with precise semantics such that essential properties, e.g., hard real-time requirements or the absence of side-channel leakage can be verified. At run-time, we aim for the automated learning of finite-state models of IoT devices that provide an insight into their internal design facilitating security analysis and security testing. Finally, run-time enforcement techniques shall provide a fault-tolerant design for dependable cyber-physical systems. The idea is that a verified but simpler controller, called a shield, takes over for a short time-span when safety-critical situations occur. Hence, we take a new holistic approach to verification,

considering design and run-time but also aiming for novel designs where guarantees can be given. To this end, we made significant scientific progress regarding the dependability attributes correctness, robustness, security, and timing. New tools, like Aalpy and Coco [7], support the verification at both, design- and run-time. **We developed verified fallback mechanisms for safety-critical controllers in cyber-physical systems, developed learning-based security testing methods to find bugs in Bluetooth devices [9], verified protection mechanisms against side-channel attacks taking the hardware into account, and finally, investigated real-time verification of software to be scheduled on modern real-time operating systems [8].**

A third important research area are rigorous engineering methods and techniques to support the development and integration of control and diagnosis architectures operating at different levels of abstraction. Core desiderata require the system to perform safely under nominal and anomalous conditions. The underlying research objectives can be classified into the four major research topics: networked control and communication, probabilistic inference, model-based diagnosis and execution monitoring and dependable cognitive architectures. Multi-agent systems rely on communication and control across networks. It is hence vital to further develop the analysis and design strategies for robust networked communication and control from the first project phase. **The objectives include the development of controller design techniques and the required analysis and simulation tools for control systems with network-induced uncertainties** like time delays or data packet losses. Fusing information from various sources is essential for the integration of control and diagnosis algorithms in multi-agent systems. In order to deal with uncertainties, probabilistic inference is the method of choice for information fusion. For large systems, however, it is often only feasible to use approximate probabilistic inference methods. **One objective hence is to clarify the relationship between probabilistic inference and state estimation, elaborate on the benefits of utilizing probabilistic graphical models, and hone our understanding regarding the failure of traditional approximation methods. The timely and reliable detection of faults or malfunctions and the adequate reaction to them is another key for dependability.** In multi-agent

systems, this has to be achieved on different hierarchical layers, i.e., the fast and reactive layer (e.g., servo position control) as well as a slower and deliberative control layer (e.g., mission planning and execution). One research **objective is the development of model-based diagnosis strategies for those layers.** In the multi-agent scenario, diagnosis information has to be exchanged between the agents via a communication network and the agents have to agree on a common belief of the overall health state of the system. For dependable cognitive architectures, a **primary aim of the research is to formalize the specification of dependable autonomous robots.** Formal methods allow for disambiguation, reproducibility of solutions and they facilitate the automatic verification of safety and fairness properties by means of model-checking. However, there is currently a need for theoretical grounds for making the right architectural decisions of autonomous systems. To this end, new stability criteria for networked control systems allow a holistic design of dependable control systems even in the case of communication failures like packet losses or significant time-delays. In order to evaluate the proposed criteria, **a probabilistic communication network model was developed** with a focus on real-world network traffic scenarios. The model was verified with realistic network traffic obtained from a wireless sensor network testbed. Moreover, a step towards bridging the gap between probabilistic reasoning and model-based diagnosis methods was made, resulting from the fruitful collaboration of the participating institutes. This **allows to design dependable diagnosis solutions for complex and networked dynamical systems.** The diagnosis techniques are a key ingredient of a dependable cognitive architecture for multi-agent systems. For this architecture, dependability guarantees are provided via system theoretic methods and formal verification tools.





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## Competencies

As part of the **research excellence program “Dependable Internet of Things in Harsh Environments”**, we have built up a critical mass of experienced **researchers at Graz University of Technology**, who are not only excellent in their individual fields of expertise, but who have established a close collaboration network among each other and understand the scientific languages of their collaboration partners. The areas of expertise include **wireless systems** (Jasmin Grosinger, Reinhard Teschl, Wolfgang Bösch), **wireless signal processing** (Erik Leitinger, Klaus Witrisal), **wireless networking** (Carlo Boano, Kay Römer), **security** (Daniel Gruss, Maria Eichlseder, Stefan Mangard), **formal methods and testing** (Bernhard Aichernig, Roderick Bloem), **embedded machine learning** (Franz Pernkopf, Olga Saukh), **networked control** (Martin Steinberger, Martin Horn), **real-time systems** (Marcel Baunach), **information theory** (Gernot Kubin), **robotics** (Gerald Steinbauer-Wagner).



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# The Digital Thread as a Success Factor in Mechanical Engineering

Elmar Paireder

In cooperation with representatives of the Mechatronics Cluster Advisory Board and partners of the "TraceMe" lead project.

## Vision

In Upper Austria in particular, mechanical and plant engineering is considered as THE backbone of the economy, which is strongly characterized by small and medium-sized enterprises and a high capacity for innovation. Today, product innovations in mechanical and plant engineering are increasingly based on the close **interaction of the classic mechatronic sub-disciplines of mechanics, electronics and information technology**. Mechatronics makes indispensable contributions to the inexorably advancing digital transformation of engineering and business processes and their artefacts. The aim is to utilize and industrialize the potential that arises from these highly dynamic interactions profitably and to apply them in development, production/manufacturing, commissioning, use, maintenance, service and even reuse or recycling in the sense of a sustainable circular economy successfully.

The challenges are various and are found in the **horizontal and vertical integration** in increasingly network-like value creation systems. On the one hand, the digital transformation is reflected in concrete, visible products and services that are provided for implementation in small and medium-sized enterprises or industry. On the other hand, supporting software systems (assistance systems), which as "invisible" elements significantly support the digital transformation along the value creation networks, are becoming more and more important. Technologies that are still part of scientific research are also to be understood as medium-term

enablers. New basic knowledge, new methods and technologies will support and accelerate the digital transformation, therefore the future, open overall picture will have to be supplemented again and again. From a technological perspective, approaches and technologies such as IoT (Internet of Things), AI (artificial intelligence) / ML (machine learning), data analytics, cyber physical systems or virtual reality, simulation or digital twins and much more are increasingly being integrated into products.

However, the **digital transformation** in companies also requires changes in workflows and a technologizing of processes across entire value creation networks. The basis for the increasing automation of production

- **Digital Thread**
- **Digital Transformation**
- **Requirements-Engineering**
- **Model-based-Systems-Engineering**
- **Machinery- & Plant-Building**

and development processes can be the development of a description language adapted to the problem, known as a Domain Specific Language (DSL), which enables domain-specific modelling of the underlying processes and products. Semantic technologies (ontologies, logic, rule-based systems) can in turn be used to digitize business processes along the value creation paths. The use of ontologies attempts to map significant parts/modules (data interfaces, data plausibility rules (logic),

user interface data elements and many more) in a digital process twin [1]. The use of graph databases also seems to make sense. They provide a solid basis for analysis, especially when the focus is on the connections between different entities.

Reality still shows too often that a performance increase takes too long to be justified by a simple cost-benefit calculation. Solutions are sometimes not “sellable” to the customer or the added value is not seen. The necessary trust in new technologies is also lacking or fails due to basic requirements such as a correspondingly good data quality or data connection, which are not or only insufficiently available. In addition, legally compliant and DSGVO-compliant data processing often represents an uncertainty factor that acts as an innovation inhibitor for many companies. In some cases, companies in the mechanical and plant engineering sector are not yet ready to use the possibilities of digitalization in new, attractive business models without leaving their core business. The focus is often too much on external digitalization (products, services, CRM, SCM, etc.), which means that the necessary internal digitalization (technologies, mindset, processes, their structures, models, tools, etc.) and thus also their scaling are neglected.

The technologies and their use are also significantly influenced by framework conditions such as agile and shorter development cycles or also by the human factor and its technical and methodological competence. In addition, standards and norms and other legal framework conditions pose a challenge when implementing new technologies [2]. All these factors are of great importance for the digital transformation in mechanical and plant engineering and must definitely be taken into consideration.

## Approach

One key to success lies in the best possible design of a **continuous, digitalized engineering and management of technical requirements**. In [3], requirements engineering is understood as the elicitation, specification, analysis and structuring of requirements. However, this requirements basis is by no means static, but is subject to constant analysis, prioritization, further development, refinement, verification and validation in the further course of the product development process [4]. According to [3], the

process-accompanying work with the requirements basis in the product development process, here also referred to as requirements management, comprises both the process design and the operative requirements management throughout the entire product development process [5].

In contrast to highly regulated industries such as aerospace or medical technology, continuous, digitalized requirements engineering and management is sometimes only used to a very limited extent in mechanical and plant engineering companies. There are many reasons for this. Particularly in the case of highly customized parts (engineer-to-order) in conjunction with often comparatively short project durations, it is difficult to justify expenditure in requirements modelling without the benefits resulting from continuous further use in process chains. Often, requirements at system level are not “distributed” enough across disciplines and trades, are mostly still document-based and scattered across different IT systems such as CAx systems and databases, which are not or insufficiently digitally linked with each other. The challenge lies in the currently largely unstructured processing of requirements. In principle, digital requirements engineering is divided into requirements in internal product development, customer/market requirements in a product development cycle and the specific requirements of (external and internal) stakeholders in a project implementation. Depending on the purpose and origin of the requirements, the methods and use of tools for processing (engineering) and managing (management) the requirements differ. The structure of requirements ranges from classic prose formulations (e.g.: text in an e-mail for a request for proposal) to formal models (e.g.: concrete system and construction plans in CAD format). Data in this understanding can be models, parameters, measured values, bits & bytes, etc. In order to ensure complete data consistency in value creation networks, digital engineering and management of requirements is necessary, which includes the modelling of technical requirements as well as the development of data models and the associated IT system landscape and enables the use of requirements models in internal processes [5, 6, 7, 8]. This is always under the premise of a DSGVO-compliant processing of the required data. For the coming evolutionary steps in the digital transformation, a continuous, digital and semantically processable requirements management is therefore

a basic prerequisite. Only through digital interaction with customers and the digital processing and management of their needs and wishes can digitalization, automation and also software-based decisions in value creation be made possible.

errors in manual/analogue technical specifications throughout the entire product value chain. This enables shorter development times, lower engineering costs (e.g. also through the use of cloud services) and lower change costs.

What is important here is a corresponding consistency across all relevant company areas in the sense of a **digital thread** [5, 9]. A digital thread describes a framework that connects data flows and enables a holistic view of the data of a machine, plant or process throughout the entire product life cycle. The digital thread creates homogeneity and enables different views of objects through targeted, universal access to data (models, parameters, documents, measured values, etc.). It runs along interlinked data sets, weaving its way through engineering and business processes as well as functions, thus creating continuity: a key objective of digital threads is to bring the right information to the right people (users) at the right time and in the required form. The benefits of Digital Threads are speed, agility and efficiency in product development, order processing and operational processes, as well as in all the individual tasks that are linked to them.

Continuity in the sense of the Digital Thread is also a basic prerequisite for the use of **Digital Twins** [1, 5], which enables the representation of products or systems, machines, controls or workflows in a virtual environment. The Digital Thread is in turn the digital strand (the digital backbone) through which all digital representations of products, systems or processes can be interconnected and integrated throughout the entire life cycle [5, 9]. It links all the functions of digital twins such as designs, performance data, product data, supply chain data and software that play a role in the development and creation of a machine, plant or service.

The introduction of a Digital Thread concept with a framework strategy for manufacturing processes is therefore desirable, as it enables controlled analysis and use of data throughout the lifecycle of a product, which can be processed into valuable new information. Digital threads can thus improve engineering and manufacturing processes in many ways [5]. On the one hand, it can improve communication and transparency between the disciplines involved. On the other hand, the quality of products, sub-assemblies and projects can be improved by making changes more controllable and reducing

## Impact

The great challenge lies in the development of concepts that make the high **interdisciplinarity and complexity of products and engineering processes** more manageable. Machines and plants can no longer be viewed only from the perspective of the individual disciplines, but must be understood as a complete system [3, 5, 6, 10, 11], since established discipline-specific development methods no longer meet the challenges of interdisciplinary product development, even in medium-sized mechanical engineering. Although the VDI2206 "Development Methodology for Mechatronic Systems" [11] provides an approach from mechatronics - the interdisciplinary system design should create a uniform system understanding in the sense of an interdisciplinary system description at an early stage - there is a gap between the rapidly increasing product complexity of advanced mechatronic systems and their mastery - this requirement will continue to increase in the future [5, 6, 8, 11]. Companies are challenged to shape interdisciplinary cooperation.

One approach that is considered to play a promising role in this context is **systems engineering or model-based systems engineering** [7, 12]. This is understood to mean the consistent and interdisciplinary description of the system to be developed in system models, which, in conjunction with appropriate methods and tools, provide the developers with means of expression that each discipline understands equally. The differences in the thinking and conceptual worlds of the individual disciplines can thus be overcome and misunderstandings prevented. However, this also requires changes in the role, understanding and task profiles of the individual experts.

Such systems are well established in highly standardized economic sectors such as the aviation or automotive industry and primarily deal with the early phases of the product life cycle - starting with the collection of customer or system requirements up to the development/simulation/testing of very complex products (e.g. aircraft) or of very variant-rich but comprehensively described series (e.g. automobiles).

In the meantime, these concepts are also becoming increasingly important in the development, production or construction of individual machines and systems. Model-based system development and the associated interdisciplinary exchange via CAx models, system models, etc., as well as new description languages and tools to support the exchange of data (models, parameters, etc.) across company divisions are promising starting points [5].

These approaches must be simplified for the high customer-specific (engineer-to-order) share in mechanical and plant engineering on the one hand (quick applicability without high training costs), but also expanded with regard to later phases in the product life cycle (production/assembly, operation, service). In addition, redundancies can be avoided in the sense of a single source of truth. This is intended to create a framework for action that makes "engineering of the future" possible in the sense of "production of the future".

One aspect that must be taken into consideration from the outset in the development of digital thread concepts and their implementation in practice is the **legal framework**. These must be identified and examined for their specific relevance to the project in order to be able to implement a Digital Thread concept not only in a value-creating and technical way, but also in a legally sound way and thus in a way that achieves the overall goal. Interdisciplinary cooperation in the form of a technical-legal co-creation process is therefore necessary. Selected legal areas with project-specific relevance are, for example, antitrust and competition law, data protection law or aspects of civil and also criminal liability.

In summary - the development and implementation of advanced, yet practical **digital thread concepts is THE competitive deciding factor for mechanical and plant engineering**, enabling customized and flexible development, production and installation of highly complex machines, plants and systems. The realization requires new methodological approaches and the use of new technologies, especially to ensure the consistency and automation of the processes.



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## **Competencies**

This article is based on a discussion in the advisory board of the Mechatronics Cluster, in which challenges for the mechatronics location - and thus for mechanical engineering - Upper Austria were discussed from November 2020 and detailed in further workshops and personal discussions with representatives and intermediaries of the Upper Austrian innovation network. In terms of content, the main focus was on the role of mechatronics as an enabler of the digital transformation in mechanical and plant engineering. Findings from this were subsequently used for a project submission in the #uppervision2030 “Digital Transformation” call for proposals from the province of Upper Austria. Under the title “TraceMe - Requirements-driven Digital Transformation Competences in Mechanical and Plant Engineering”, eight companies and six research institutions have been working since September 2022 on the development of a technological framework in the sense of the digital thread to ensure digital continuity across all value creation networks and to handle the increasing complexity in mechanical and plant engineering.



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# Batteryless wireless Sensor Nodes

Thomas Ußmüller

## Vision

Modern society and peoples everyday lives are heavily influenced by various electronic devices. These devices cover a wide range of different branches, including consumer and industrial electronics and can be used for communication and entertainment, provide safety functions in cars or collect environmental data, to name a few examples. A lot of these electronic are nowadays connected to the internet and are part of the Internet-of-Things (IoT). The IoT comprises the network of physical objects, such as machines, devices, and sensors, interconnected via embedded, digital communication interfaces. This allows quick and decentralized information processing, execution, sharing and broadcasting. Hereby, data transmission uses either private point-to-point structures or the world wide web. As IoT technology is beneficial for organizing and handling processes, it is assumed that it's importance will continue to rise. A study by IOT Analytics [1] highlighting the importance of IoT estimated a total of 41.2 Billion connected devices in 2025. 75% of these devices (30.9 Billion) are expected to be IoT devices.

Modern industrial manufacturing, often referred to as Industry 4.0, is characterized by the integration of smart technologies and the digitization of traditional manufacturing processes. The goal is to create a more efficient, flexible, and responsive manufacturing system that can adapt to changing market demands and customer needs. The IoT is one of the key technologies that is driving this transformation. It enables manufacturers to connect machines, devices, and sensors throughout the production process, from the raw materials stage to the finished product. This connectivity

enables manufacturers to collect vast amounts of data that can be used to optimize and automate the production process. For example, sensors can monitor the temperature, humidity, and other environmental factors that affect the quality of the raw materials. This data can be used to adjust the production process in real-time to ensure consistent quality.

In addition to improving quality, connected IoT devices can also increase efficiency and reduce costs. By connecting machines and systems throughout the production process, manufacturers can identify bottlenecks and inefficiencies that are slowing down production. This data can be used to optimize the production process, reducing waste and increasing throughput. Potential use cases include for instance the detection of machines running at less than optimal efficiency and the in time refill of production materials. Other benefits include a more flexible and adaptable production with respect to changing market demands. By connecting machines and systems throughout the production process, manufacturers can quickly

- **Wireless Sensor Networks**
- **Energy Harvesting**
- **Internet of Things**
- **RFID**

reconfigure their production lines to produce different products or respond to changes in customer demand. Another huge potential of IoT systems for industrial manufacturing is the implementation of predictive maintenance. Predictive maintenance is a proactive maintenance strategy

that utilizes data analysis and machine learning algorithms to identify equipment problems before they occur. The primary goal of predictive maintenance is to prevent unplanned downtime, increase asset availability, and reduce maintenance costs. For this various types of sensors and data collection methods are required in order to monitor the performance and condition of the equipment. The collected data is then analyzed to identify patterns and trends that indicate potential equipment failures. Machine learning algorithms are used to build predictive models based on historical data, which are used to forecast future equipment performance and identify potential problems. One of the primary benefits of predictive maintenance is that it allows maintenance teams to plan and schedule maintenance activities based on actual equipment conditions rather than on pre-determined schedules. This means that maintenance is performed when it is needed, reducing unnecessary maintenance and associated costs. Related to the manufacturing process the IoT also has the potential to revolutionize supply chain management. By connecting suppliers, manufacturers, and customers, the IoT can enable real-time tracking of inventory and shipments. This connectivity can reduce the risk of stockouts and delays, improving customer satisfaction and reducing costs.

Another important aspect for the future of industrial manufacturing is the implementation of digital twins. These are virtual models of physical machines and systems. Digital twins can be used to simulate the behavior of machines, systems and even complete factories, enabling manufacturers to test and optimize their production processes without disturbing the actual production. Digital twins can also be used to monitor and control machines and systems in real-time, improving efficiency and reducing downtime. A crucial aspect for digital twins is the link between the physical and the virtual world. Physical assets must be identified in the virtual world and vice versa. This link can easily be established with the help of IoT devices.

The benefits of IoT in the industrial environment are enormous, but unfortunately, to date, their full potential has not been realized. There is still a vast room for improvement in this area. One critical aspect that needs to be addressed is the need for wireless sensor systems. These sensors will allow for the maximum benefit

of IoT in the industrial environment. Wireless sensor nodes however intrinsically require energy for their operation as they are electrical devices. In 2014 the International Energy Agency commented: "To participate in networks, devices and equipment must remain 'on' all the time; thus their increased functionality comes at an energy cost" [2]. Taking today's technology, these components are likely to operate on batteries. Envisioning billions of manufactured devices in the future, technology must evolve and address the energy challenge in order to reduce the impact on the environment. Besides the environmental impact, the regular battery changes cause significant maintenance costs. The total cost of ownership of these devices makes them often prohibitively expensive for lots of applications.

This problem can be solved with batteryless systems. Batteryless electronic devices obtain their energy required for operation either the energy harvesting or through wireless power transfer from another component. In most cases this component is the reading device of the wireless sensor node. Hence this technology will be a key enabler for IoT application in industrial environments.

Future IoT devices for industrial applications are envisioned to be:

- **Connected:** The wireless sensor node used for machine monitoring is highly connected. The sensor node gathers data from the machine and can communicate with different backend systems, such as Manufacturing Execution Systems (MES). The data collected by the sensor is then saved in time series databases, which can be used for further information processing. Advanced technologies such as Artificial Intelligence (A.I.) algorithms can be applied to the data to gain deeper insights into the machine's performance and identify potential areas for improvement. With its advanced connectivity, the wireless sensor node provides businesses with the tools they need to make data-driven decisions, optimize their processes, and ultimately increase their profitability.
- **Data provider for machine learning:** Wireless sensor nodes are an indispensable data provider for machine learning in various industries. These sensors gather data from machines, tools and materials, which can then be

used to train machine learning models. One possible application of this technology is in predictive maintenance, where machine learning algorithms are used to detect patterns in the data that indicate potential failures or issues before they occur. By leveraging data from wireless sensor nodes, businesses can improve the accuracy of their predictive maintenance systems and reduce downtime. The wealth of data that these sensors can provide is also useful for other machine learning applications, such as anomaly detection, optimization, and quality control.

- **Flexible:** Introducing a flexible sensor node that can be used for a variety of applications. This sensor node is versatile enough to be mounted on moving or rotating parts, making it an ideal solution for monitoring and analyzing various machines or devices. Additionally, the sensor node can be installed in hard-to-reach areas, providing an efficient way to capture data without the need for complicated wiring or infrastructure.
- **Maintenance-free:** The wireless sensor node used for machine monitoring is designed to be maintenance-free, which means that once it's mounted, no further attention is needed. The sensor can operate for the full lifetime of the machine without requiring any additional maintenance or battery changes. This feature is particularly useful in industries where machines operate continuously and any downtime for maintenance can result in significant losses.
- **Low TCO:** Novel IoT devices for industrial applications will feature a lower Total Cost of Ownership (TCO) compared to traditional monitoring systems. One reason for this is the low cost per sensor node, which is made possible by advances in wireless communication technology and integrated circuit design. Additionally, wireless sensor nodes are designed to be maintenance-free, meaning there are no ongoing costs for maintenance, repair, or replacement. Finally, these sensors are easy to connect with existing systems, making it simple to integrate them into a business's operations.
- **Long lifetime:** Novel sensor nodes are designed to have a long lifetime, exceeding the lifetime

of the machine. These sensors can stay in place for an extended period, with no need for removal or replacement. The maintenance-free design means that no further attention is needed, and there is no need for battery changes, which can be a significant cost and hassle with traditional monitoring systems.

- **Small in size:** Wireless sensor nodes are becoming increasingly small in size, making them ideal for monitoring hard-to-reach areas and integrating them into workpieces. These sensors are miniaturized, allowing them to be mounted in tight spaces where traditional monitoring equipment cannot be used. The small size of wireless sensor nodes also makes them easily integrable into workpieces, providing real-time data on their performance and usage.
- **Easy retrofitting:** Wireless sensor nodes offer a valuable solution for retrofitting existing equipment without the need for significant modifications. This enables businesses to protect their investments by extending the lifespan of their existing machinery, allowing them to stay in use for a longer period. The retrofitting process is feasible, as wireless sensors are small and easy to install, without requiring major alterations to the machines.

## Approach

The potential for IoT in industrial production is vast, with many possibilities yet to be fully exploited. However, further research is necessary to ensure that the technology can meet the requirements of the manufacturing sector. One significant challenge in this area is the need for low maintenance requirements and a low total cost of ownership (TCO), which can only be achieved if **battery-free wireless sensor nodes** are used. In this setup, one or more battery-free sensor nodes communicate with a central interrogating device, commonly referred to as reader. This device is responsible both for communication and power transmission to the wireless sensor node.

Typical wireless communication is based on the transmission of electromagnetic waves. The majority of systems on the market, such as cellular phones, WiFi and Bluetooth use active transmission of a modulated

radio frequency (RF) signal in order to transmit information. Active wireless data transmission requires 10 mW or more in the transmitter circuit. In addition, the receiver has to stay constantly on in order to listen to incoming data signals from other devices. This also adds significantly to the overall power consumption of the system.

An **immense reduction** of the **required energy** in the order of several magnitudes is possible with backscatter communication. The first publication describing the principle dates back to 1948 [3]. The operation principle of such a backscatter system is similar to primary radar systems, which consist of two parts: A transceiver (transmitter and receiver) and the object to be detected. Backscatter radios also use a transceiver typically called reader or interrogator. The object in case of a radar system is replaced with an electronic circuit typically referred to as tag or transponder. Hereby the data signal is not sent actively but instead the tag modulates the reflection coefficient. Therefore, the incoming wave from a reader device is simply reflected. At the same time, energy is transmitted from the interrogating device through wireless power transfer. This means that **no battery in the transponder** is needed.

Hence, it makes this principle a perfect candidate for future IoT systems.

In order to achieve a batteryless operation in combination with sufficient functionality of the wireless sensor nodes the whole system has to be **optimized for lowest power consumption**. The lower the achievable power consumption, the greater the achievable communication distance between reader and sensor node. Besides the optimization of system aspects with wireless power transmission and backscatter communications also the various components of the sensor node itself have to be optimized. This includes components such as the antenna, the rectifier for power supply and additional sensor circuitry to name a few.

As of now, backscatter systems are commonly used for **identification** and simple **localization** of certain objects. However, in the last years research was conducted on **sensing** and **actuating** possibilities within passive backscatter systems. Possible applications include the measurement of environmental parameters, such as temperature [4] or chloride ions in concrete [5]. Other use cases include the precise localization of objects [4,6] or the control of actuators with zero power standby [7].



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## Competencies

The group of Prof. Ussmueller has extensive knowledge in the design of circuits and systems for ultra low power wireless sensor networks. Recent projects by the group include BaKoSens 4.0, which has been running from September 2017 until August 2022 and focuses on the implementation of a batteryless wireless communication and sensor platform for Industry 4.0. Further work includes the project CryptoZE funded by the Tyrolean Innovation Program, focusing on the development of ultra-low power circuits for encryption in battery-free systems. Another project is SensorBIM, where UHF RFID sensors are advancing digitization in the construction industry.

The group for Microelectronics and Implantable Systems at the University of Innsbruck is well equipped with the necessary measurement capabilities required for the topic. This includes a state-of-the-art RF measurement laboratory (network analyzer, spectrum analyzer, software defined radios, logic analyzer, etc.) for developing and measuring circuits up to 40 GHz. Also available are commercial RFID readers and tags as well as a wafer prober for measuring single ICs up to complete wafers. Furthermore, an EMC/antenna measurement chamber is available. This can be used to measure and characterize the developed systems without external influence, which is especially important for ultra-low power circuits. In addition to that a design environment for chip development from Cadence including the required PDKs (Process Design Kit) from Globalfoundries and TSMC is also already available.



## Impact

From a **scientific perspective** research progress in the field of batteryless wireless sensor networks is expected to have an impact on numerous disciplines. In the field of integrated circuit design novel circuit topologies with reduced power consumption will influence fields such as mobile communications and analog integrated circuits. Other aspects include novel antenna structures for wireless communication and sensing systems as well as innovations for increased communication range in wireless systems. Probably the biggest impact is the feasibility of investigations which are to date not yet possible. Batteryless wireless sensor networks allow for instance the in-situ monitoring of data in medical implants and the data acquisition inside the building envelope.

From a **commercial perspective** batteryless sensor networks offer a range of commercial benefits to businesses of all sizes. They offer simplified use, making it easier for companies to collect data on a range of metrics, from temperature to machine performance. In addition they deliver enhanced real-time data for predictive maintenance, which identifies potential equipment failures before they occur. Overall they increase efficiency and reduce cost by optimizing operations and increasing efficiency. Additional benefits include new business models and new revenue stream based on the collected data.

The biggest **societal impact** of batteryless wireless sensor networks in an industrial environment is probably the increased efficiency of the manufacturing processes and hence a reduced requirement for workers at the production line. Finding enough qualified personal is a significant burden for the industry today. This problem is expected to even increase over the next couple of years. Batteryless wireless sensor networks help increasing the efficiency of manufacturing equipment and hence help to increase the output without the need of additional workers on the production line.

Besides the impact on the field of industrial manufacturing batteryless systems are expected to have a significant impact also for lots of other application scenarios. This includes an increased energy efficiency of buildings with the help of digital model of the buildings (building information modeling, BIM). Other use cases include enhanced traffic control, smart city scenarios, consumer electronics and improved medical care.

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# Process-integrated Quality Control through Photonic Sensing

Peter Burgholzer

The **Research Center for Non Destructive Testing GmbH (RECENDT)** is a member of the **UAR Innovation Network**, which consists of a total of 18 highly specialized R&D centers (as per 2023). Research on cutting-edge technologies for efficient production is one of the major fields of strength of the UAR Innovation Network. Within the research fields Smart Systems, Digital technologies and Sustainable materials, the involved R&D centers conduct research in a variety of topics like process engineering and optimization, software engineering and modelling, high-tech materials and components, energy efficiency and many more. In addition, the available expertise is also successfully implemented in medical technologies.

## Vision

**RECENDT** is known for its **research into new methods of non-destructive materials testing**, predominantly with **(infrared) light and light generated (ultra) sound**. These methods for material characterization can be used not only for classical materials and composites, but also for biomedical “materials” such as human tissue. For example, carbon fibers in an epoxy matrix can be characterized with exactly the same photoacoustic sensor technology as blood vessels in human tissue. One and the same sensor technology, including the corresponding signal processing, often **covers many different applications in a wide range of industries**.

New sensor technology and signal processing for non-destructive material characterization is often **non-contact and in-line capable, i.e. it can be integrated into a production process**. The view below the surface or the non-

contact measurement of the chemical composition is not an end in itself, but enables as in-line sensor technology a sustainable and efficient high-tech production. The ongoing paradigm shift from classical quality control at the end of the production process to process-integrated quality control enables a continuous adjustment of the process parameters. The concrete implementation of **process-integrated quality control** for specific production processes takes place in the production facilities of the industrial partners.

Existing photonic sensor systems and the new photonic sensor technology together with corresponding signal processing can be used for numerous applications. By combining them with concrete application fields, the benefit of this non-contact sensor technology becomes obvious in comparison with

- **Infrared Sensing**
- **Terahertz Sensing**
- **Laser Ultrasound**
- **Photoacoustics**
- **Ill-posed Inverse Problems**
- **Regularization**
- **Reconstruction**
- **Zero Defect Manufacturing**

destructive quality control. It enables process-integrated quality control by adding process know-how through continuous adjustment of process parameters. The research question is: How can the process parameters be adjusted on the basis of the information captured by the photonic sensors in order to ensure optimal process control of the production?

The high demand from companies for research to **move from classical quality control at the end of the production process to process-integrated quality control** shows its necessity. In quality assurance, this is a paradigm shift that has been known for some time in ecology, for example. Originally, environmental protection mainly meant filtering out pollutants, e.g. harmful gases through air filters or through wastewater purification in sewage treatment plants. These “end-of-the-pipe” solutions were added as “add-ons” to known production processes and were a significant advance at the beginning. From the company’s point of view, however, environmental protection was often regarded as a “necessary evil” that caused additional costs as an “add-on”. It was only later that the efficiency of material and energy flows was considered and the entire product life cycle from the “cradle” (raw material) to the “grave” (disposal) or even better in the circular economy from the “cradle to cradle” was included. In further respects, it was then not a specific product but the benefit created by a product or service that was considered as the reference for the material and energy balance. In any case, this development turned environmental protection from an original cost factor into an efficiency driver in many areas. For quality assurance, this is an essential step that makes new products possible in a quality that has not been possible before. However, this development, brings with it some new requirements:

- In-line sensor technology in the production line must be “real-time” and as contactless as possible. Acoustic (ultrasound, but also audible sound) and optical (including infrared, terahertz) methods and possibly even eddy current or magnetic sensors are particularly suitable for this.
- Additional sensors for the acquisition and control of the essential process parameters over the entire process chain from the raw materials used through numerous intermediate products to the final product provide a large amount of measurement data.
- Process know-how (from the production plant, possibly supplemented by modeling and simulation) must be implemented for quality control
- Automated adjustment of process parameters to control product quality

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## Approach

Up to now, the main focus has been on **classical quality control at the end of the production process as an “add-on”**: finished products are inspected with two possible results: OK meets specifications and is shipped, not OK is called scrap and does not meet an essential specification and is disposed of or can be repaired or is disassembled again and fed into the production process as raw material. This procedure does not require any change in the production process - the quality control is added at the end of the existing production process. For safety-relevant products (e.g. aircraft components), 100% quality control is required. For other products, random samples are sufficient for quality control and statistical methods can be used to guarantee freedom from defects with a certain significance. This also allows the use of destructive methods of quality control - for 100% quality control, clearly only non-destructive testing methods can be used. Only if the reject rate increases significantly, the production process or the quality of the required raw and auxiliary materials will be considered more closely or adapted. Due to the delay between the production process and the quality control at the end, a lot of rejects can be produced in such a case before quality improving measures take effect.

Many production companies still work very successfully with this classic procedure, whereby the classic quality control is sometimes supplemented by an incoming inspection of the raw materials used or by a quality control of the intermediate products. The disadvantage of this classical quality control is that with the rejects, expensively produced products

and expensively purchased raw materials end up in the waste and the sometimes high energy expenditure during production is lost. **Classical quality control works well if the raw materials and auxiliaries used vary very little and the production process can be kept very constant.** This will become increasingly rare in the future, as the **use of recyclates instead of new raw materials** as input in the production process means that these **can vary greatly in composition and consistency.** The same applies to renewable raw materials. This requires **constant adaptation of the production process** to such variations in order to be able to continue **to guarantee optimum product quality.**

The **process-integrated quality control** propagated here **requires corresponding measurements** not only at the end of the process, but **over the entire process chain and in-line, i.e. in the production line.** Additional process know-how is also necessary in order to change the process parameters so that the production process runs optimally again. In this way, not only can rejects be avoided as far as possible (“zero defect manufacturing”), but in addition, faults are detected and corrected at an early stage. By adjusting the production parameters to the raw materials actually used, products and processes can be optimized and “safety” tolerances, e.g. in the component thickness due to the variation of the starting materials, can be reduced. As a result, process-integrated quality control enables even better product quality, higher resource and energy efficiency, and thus an overall reduction in costs. Classical quality control as an “add-on” is associated with additional effort and thus with additional costs during operation and, since the rejects are visible there at the end, often also with a negative image among the production employees.

The large amount of measurement data thus generated should be processed in real time in a model (e.g. Digital Twin) of the production process in order to determine the required manipulated variables in the process parameters for controlling the production process. In order to guarantee the short response times often required for controlling the production process, **artificial intelligence (AI) methods, e.g. deep neural networks,** are increasingly being used for this purpose. Such new methods, e.g. **Compressed Sensing,** allow to use additional pre-existing knowledge in the measurement (e.g. “sparsity” in a certain mathematical basis or data for training neural

networks). As a result, these methods can achieve better results for the same amount of measurement data than using conventional methods, such as least-square minimization. However, such new methods often require a different way of collecting measurement data, e.g. random selection of measurement points. The **classical separation between sensor technology and signal processing dissolves** and a close interlocking occurs. The additional process know-how required for process-integrated quality control is usually available in the production plant or can be supplemented by modeling and simulations with various production parameters. If these simulations are performed sufficiently close to reality, their results can also be used as training data for neural networks.

## Impact

Using **photonic sensors to characterize materials and processes** has many advantages. First, light-matter interaction is very rich on information, i.e. it allows to characterize the sample under test very well. Second, photonic sensing is contact less, thus it is non-destructive and in-line capable, i.e. it can be integrated into a production process.

The reconstruction of the process parameters, e.g. chemical composition or internal structure, can be done from photonic measurements, but it is not an end in itself: it enables energy- and resource-efficient production and products. This is exactly what the paradigm shift from the classic production process with precisely defined input materials and process control to the adaptive process with varying input materials through in-line sensor technology, predominantly through contactless photonic sensors, makes possible. We **enable continuous adaptation of the process parameters for individual applications** via the process expertise contributed by the industrial partners and **thus enable energy- and resource-efficient production.**



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## Competencies

To obtain information (e.g. to reconstruct the location and size of defects or other internal structures, or the chemical composition of a sample with spectroscopy) with photonic sensing, an **inverse problem usually has to be solved mathematically in addition to the actual measurement**. In order to solve the ill-posed inverse problem to be able to infer the chemical composition or internal structures in materials from the data measured with photonic sensors, we have gained a lot of experience in the past. In addition to the deep learning methods (see e.g. IEEE Signal Processing Magazine [1]), we could exploit the “**sparsity**” of signals to gain additional information with **compressed sensing** or **super resolution imaging** methods [2]. Properties characteristic for photonic signal generation, such as the “sparsity”, are to be used to obtain better images with fewer artefacts, and this in a much shorter time. With so-called **L1 minimization**, this additional information enables the reconstruction of images with less measurement effort and thus a much faster measurement (Compressed Sensing, see [3] and [4]). The **basic idea of compressed sensing** is inspired by image compression methods such as JPEG. Here, an image is not stored pixel by pixel, however an (almost) equally good image impression can be stored and transmitted with considerably less information and thus less effort. With compressed sensing, the data compression is already carried out during acquisition in order not to first measure all pixels with a lot of measuring effort and then “throw away” the majority of them during the subsequent image compression. In an Austrian Science Fund (FWF) project “Compressed Sensing in Photoacoustic Tomography” we have investigated these methods for photoacoustic tomography together with Prof. Markus Haltmeier from the Institute of Mathematics at the University of Innsbruck. Through this and other collaborations on **machine learning / deep learning and other reconstruction methods** (e.g. with the Institute of Signal Processing at JKU or Silicon Austria Labs), we are actively involved in the scientific community and continuously at the cutting edge of science. This ensures that we are always involved in current scientific developments and thus not only go beyond the current state-of-the-art in the proposed PSEEE project, but also stay informed about progress in other research groups and can react to it.

The same applies to the area of **photonic sensing**. At RECENDT we are very well integrated into the respective scientific communities and are constantly reviewing manuscripts for peer reviewed journals or research projects. As a principal investigator and executive director of RECENDT, I have been active for many years on the **international scientific committee that organizes the International Conference on Photoacoustic and Photothermal Phenomena** [5], which takes place every 2 years, and the **International Symposium on Laser Ultrasonics and Advanced Sensing. At Photonics West/BIOS in San Francisco**, I am co-organizer and member of the program committee of the conference “Photons plus Ultrasound” and member of the editorial board of the Elsevier **journal Photoacoustics** [6] (Impact Factor 9.656).

In a very basic work, we combined the different scientific fields of information theory, thermodynamics, regularization theory, and non-destructive imaging, for photonic sensing. The goal was to get a **better understanding of how information gaining for subsurface imaging works and how the spatial resolution limit can be overcome** by using additional information [7]. The resolution limit was derived from irreversible processes during the propagation of the signals from the imaged subsurface structures to the sample surface. The reason for the resolution limit is the information loss during signal propagation to the sample surface, which turned out to be equal to the entropy production. Incorporating sparsity and non-negativity in iterative regularization methods gives a significant resolution enhancement, which we could experimentally demonstrate by one-dimensional imaging of thin layers with varying depth and by three-dimensional imaging, either from a single detector or from three perpendicular detectors on the surface of a sample cube [7]. Such “additional information” can be supplied in a general way by the information contained in the training data for a neural network, which showed the best results [1]. The information retrieved by these methods and algorithms allows the **in-line control of adaptive industrial production processes to address improving energy efficiency**.



**Photonic sensing and these mathematical reconstruction methods for solving the inverse problem are strongly linked.** For example, for compressed sensing in particular, it is necessary to realise a “random” excitation, i.e. through a random pattern (random spatial excitation), or temporal or spectral random components. As a result, these mathematical methods are also well suited to being integrated with sensor technology to form an **“intelligent” sensor**. New photonic sensors are also researched, such as **quantum sensors, high frequency laser ultrasound, or optical computing in chemometrics.**

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# 6G for Production

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## Vision

Wireless communication technology has radically transformed our society over the last decades. The two most important technology pillars for this transformation are **microfabrication technology** and **information theory**. Since the early 1970's when the first integrated circuits appeared, the number of transistors on integrated circuits followed Moore's law and doubled approximately every 18 months, which today enables both, the processing of an enormous amount of data at very high speed and the storage of data in miniaturized devices at lowest cost. Making optimum use of this tremendous processing power and storage capability is the main topic of information theory, which was founded in by C.E. Shannon in the 1940's. The continuously growing research community in information theory laid not only the theoretical foundations of all modern information and communication technologies (ICT) but also developed methods to reach fundamental boundaries within close limits. With the standardization of GSM (Global System for Mobile Communications), the first digital pan-European cellular communication system, and its successful commercial start in 1991, wireless communications started to become an almost ubiquitous commodity within less than two decades. The billionth GSM subscriber was connected in Q1/2004 (GSM Association) and in 2012 GSM subscription reached its maximum with almost 4 billion subscribers (Ovum, June 2016). The first generations of digital cellular systems like GSM, UMTS (Universal Mobile Telecommunications System) and its data-centric evolution HSPA (High Speed Packet Access) as well as LTE (Long Term Evolution) have been mainly designed toward

increased spectral efficiency to enable bandwidth-hungry applications for human users. This changed with fifth-generation (5G) cellular systems, for which new application areas beyond the classical mobile phone/tablet/notebook usage were envisaged already before standardization started. Thus, 5G is not only an evolution of mobile broadband networks. It brings new unique network and service capabilities. Firstly, it ensures user experience continuity in challenging situations such as high mobility (e.g. in trains), and very densely or sparsely populated areas. In addition,

- **5G, 6G**
- **Wireless Networks**
- **Wireless Sensor Networks**
- **Internet of Things**

5G is a key enabler for the **Internet of Things** (IoT) by providing a platform to connect a massive number of sensors, devices, and actuators with stringent energy and transmission constraints. Furthermore, mission-critical services requiring very high reliability, global coverage and/or very low latency, which are up to now handled by specific networks, are natively supported by the 5G infrastructure. However, one has to state that this vision for 5G has by far not yet arrived. Especially the support for ultra-reliable and low-latency communications (URLLC) is not yet fully provided by network operators, hardware providers and protocol stacks. Nevertheless, 5G is already on the way to becoming a key enabler for **factories of the future**. In fact, 5G is not only seen as an evolution of mobile broadband networks but also as an "ecosystem" able (i) to provide the unified

communication platform needed to disrupt new business models and (ii) to overcome the shortcomings of past and current communication technologies. Along these lines, we expect that 5G technology has the potential to enable a new family of services and applications in factory scenarios and, at the same time to unlock new business opportunities for manufacturing for the vast community of industries, SME, and academic bodies.

While 5G is currently deployed worldwide and the sketched new network and service capabilities are applied to various verticals, research on 6G, the next generation cellular communication system is already underway. Here topics like THz communications, integrated communications and sensing (ICAS), reconfigurable intelligent Surfaces (RIS) and their extension to holographic RIS, etc. are actively researched. These technologies target the physical level of the wireless communication network and are important enablers for more reliable and deterministic communication links. In addition, 6G is about to integrate right from start machine learning (ML), artificial intelligence (AI) and edge computing for improved communication performance. Specifically, deterministic end-to-end communication has to integrate new software technologies to solve problems resulting from complexity and real time demands.

With those topics and their application potential in mind, we envision 6G (i) as technology being integrated in production processes and plants, (ii) providing not only a trustworthy communication framework for production but also integrating various sensing capabilities to improve the production process in terms of quality, speed and resource efficiency and (iii) as key enabler to realize real-time capable digital twins in production. Future production systems will rely on wireless communication networks as they introduce flexibility into the planning, operation and control of industrial processes. In addition, digital twins combined with real-time communication allow integrating also the online simulation of production plants and processes, thus reaching a new level of cyber-physical systems (CPSs).

Of great value for productive industry is that 6G networks will be characterized by pervasive ML and closed-loop autonomy across all layers of the network management infrastructure. This will lead to extensive knowledge that includes Radio

Resource Management (RRM) and slicing, dynamic resource allocation for the access domain, or to optimize offloading decisions for Mobile Edge Computing (MEC) applications. Many recent results are also focusing on deep learning-based management and orchestration for the Network Function Virtualization (NFV) ecosystem, focusing on Virtual Network functions (VNF) service chaining. Applications of ML are only recently emerging, aiming for global optimization and automation. One unsolved challenge with network automation and network in production is that often no single solution exists to simultaneously optimize each individual objective. Several methods have been proposed for solving multi-objective problems, such as Pareto dominance, swarm optimization mechanisms, or multi-objective Deep Reinforcement Learning (RL). However, existing efforts focus almost exclusively on the network management automation via traffic prediction in relatively large time windows (typically minutes), usually ignoring their high variability. 6G in production enables a holistic view and objective to solve many of the complex problems in achieving sustainability and efficient production.

## Approach

The use of wireless communications in the industry in general and specifically in production is lagging far behind its use for personal communication. Obviously, this is due to the stochastic nature of the wireless communication channel, which results in lower communication reliability as compared to wireline communication. Another reason is that research and development for a long time was focused very much on increasing data rates for human users, as here market size and user demand were and still are huge. In industry the market for wireless communication is largely fragmented and the requirements for communication technologies are extremely diverse.

Starting with 5G and even more so for 6G we have a worldwide applicable wireless communication standard, which on the one hand provides a huge market opportunity for the communications industry (semiconductor manufacturer, equipment manufacturer, network operator, etc.). On the other hand, the available and emerging technological pillars of 5G and 6G will allow us to effectively tackle the reliability issues of wireless communications for industry and on top bring added value to the

production process itself.

In the standardization process for 5G two new “modes” – **URLLC** (ultra-reliable low latency communications) and **mMTC** (massive machine-type communications) were natively included, which will have a significant impact on future production facilities and production processes. While these two “modes” will make cellular communication better applicable to industrial requirements, significant further research and development is required to better deal with the stochastic nature of the wireless channel and make use of 5G and even more so of 6G beyond its basic function as a flexible communication network to improve production.

Our research approach targets two directions. First, using the sensing capabilities – from already well-established channel estimation and interference detection to using communication waveforms, usually OFDM (orthogonal frequency division multiplexing)-based, for active and passive radar sensing – to realize **ICAS** capabilities, will allow achieving awareness about the local environment and its current and future influence on the communication performance. In combination with classical signal processing and ML/AI algorithms and methods both embedded in the devices and on the edge as well as operated in the cloud, this will allow us to predict the communication conditions of the wireless network into the short-term future and thus take proper actions to ensure a trustworthy, dependable, and safe operation of the communication network even in difficult channel conditions.

Our second line of research targets the integration of various sensing capabilities – both by the cellular network itself (e.g. with radar-based sensing and wireless localization of mobile network nodes) and by wirelessly integrating conventional sensors like cameras – to improve the production process in terms of quality, speed and resource efficiency. As can be easily seen, the methods used for both lines of research are basically the same. However, in the first case, the overarching target is to provide a wireless communication network with a quality of service (QoS) level similar to a wireline-based network. While in the second case, the capabilities of the wireless communication network are used to significantly enhance future production facilities and production processes beyond the flexibility one has gained by switching from static wireline networks to flexible wireless networks. One of the most prominent

enhancements in this respect will be the implementation of real-time capable **digital twins** of production processes, enabled by wireless communication.

## Impact

The Communications Engineering Group at the Institute for Communications Engineering and RF-Systems and the Wireless Communication Research Group of Silicon Austria Labs contribute with activities and results of research projects related to information technology, operational technology, and industrial production. More specifically, depending on the partners' category of projects, outcome will target national and international manufacturing industry. Industrial end-users will benefit directly by the advanced communication services at their manufacturing sites embracing digitization and automation through communication. We also influence other industries through knowledge transfer and demonstration of the system. Publications along the technology value-chain of 5G and 6G communication will promote wide-spread distribution of knowledge into industrial production process.

Some of these specific research foci target the manufacturing industry which is undergoing a profound change through digitization and automation under the industry 4.0 vision. 5G with its advanced capabilities promises reliable and efficient communications and brings new operating models to design products and services for smart factories. These aspects of the 5G communication technology have not yet been adopted by the industrial users so far. An important aspect is the availability of 5G test and trial facilities that can help in demonstrating the potential of the technology for industrial scenarios. The collaboration of SAL and NTHFS aims to showcase 5G capabilities for industrial use cases and strengthen the position for 6G research. 5G/6G technology brings in several key benefits for the manufacturing processes. In addition to digitization and automation, 5G/6G communication supports minimizing production line downtime using reliable and scalable networks, enables manufacturing flexibility through wireless connectivity, allows monitoring and control of critical manufacturing applications, supports real-time decision making using locally deployed edge processing, and increases production yield through efficient use of resources.

In terms of sustainability, wireless communications support more flexibility towards production design for industrial manufacturing, collaborative robots, AR/VR, healthcare, and applications for the automotive industry. The benefit is not only in provisioning wireless interfaces but in improving operational effectiveness, improving control operations to increase production yield, digitization, and improving manufacturing processes. Automation and control can also be an enabler to reduce resource consumption, as improvements, like timely data transmission, increase the efficiency of industrial processes resulting in reduced energy consumption. In addition, automation of industrial processes through advanced communication technologies can be cost-effective, flexible to changes, and efficient, thus supporting responsible and sustainable production.

The activities and outcomes create high impact towards the use and deployment of 5G/6G campus networks and related technologies required for automation and digitization of manufacturing processes [6]. The requirements analysis of the use cases and service provisioning for localization and tracking, teleoperations, as well as high-quality video streaming will attract local and regional industries. This is because many industries are interested in these services, however, negligible attention is given to demonstrate and highlight the capabilities of 5G/6G.

Towards the economic impact, it is of particular importance to promote the transfer of technologies developed to industrial end-users. These concepts go hand in hand with economic sustainability, as more efficient use of resources leads to equal or better results in production.



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## Competencies

The Communications Engineering Group at the Institute for Communications Engineering and RF-Systems performs research focused on dependable, real-time capable wireless sensor networks for industrial applications, trust in wireless communication networks, real-time wireless localization systems based on UWB and 5G/6G, and architectures and signal processing methods for wireless transceivers. This research is largely carried out together with Silicon Austria Labs in the course of cooperative research projects funded by industry, national funding agencies and EU (H2020-ECSEL GA:876038-Intelligent Secure Connected Trustable Things (InSecTT); H2020- ECSEL; GA: 737422-Secure Connected Trustable Things (SCOTT); H2020- ECSEL GA: 737422: Dependable Embedded Wireless Infrastructure (DEWI); HORIZON-JU-SNS-2022-STREAM-C-01-01 Deterministic end-to-end communication with 6G (Deterministic-6G); 5GEARING 5G-DEPLOYMENT FOR SMART INDUSTRY USAGE GA FO999899772 Breitband Austria 2030: GigaApp FFG; Industry financed Projects: Concealed Condition Sensing (Con2Sens); 5G Communication for Factories(5G Cofact); Wireless Security & Safety CLASSifier Environment (WS2CARE) )

All these projects are/were supporting and making use of the lab facilities including micro- and millimeter wave measurement equipment up to 170 GHz, wave prober up to several hundred GHz, antenna measurement chamber, and software radio prototyping equipment. We have local computational power with a GPU array, versatile local computational and storage facilities. Additionally, a research and deployment testbed is built up at the campus of JKU in the LIT Factory where we operate a 5G testbed with of the shelf and research devices. Industry collaborative robots are installed to demonstrate the effectiveness of the application of wireless communication in production.



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# Production System Optimization

Sophie N. Parragh

## Vision

Data is considered the new oil. However, like oil, data needs to be processed to be turned into something valuable, and this something valuable is first information and then insights. Data can be used to find unknown patterns, to make predictions about the future, and to provide input for prescriptive analytics which in turn is able to provide decision support. Companies are now able to collect and store large amounts of data. These data can be generated by production processes, like sensor data or energy consumption profiles, by the observation of customer behavior, e.g., how much and when they order, and by the products themselves, during their useful lives, if quipped with the right technology (thinking of cyber-physical products). All these data are raw as is the oil before it is processed. As such, organizations do not only need the capacity to collect and store data but also to use these data for improved decision making, which can be framed as data-driven management. **Data-driven management** is in turn based on analytic capabilities. Davenport and Harris [1] define **analytics** as “The extensive use of data, statistical and quantitative analysis, explanatory and predictive models, and fact-based management to drive decisions and actions.” They distinguish between descriptive analytics, predictive analytics, prescriptive analytics, and autonomous analytics. Each type being more advanced than the other. Prescriptive analytics is concerned with quantitative techniques and technologies to identify the best action. While here modeling is usually still done by a human, in autonomous analytics, advanced machine learning based techniques may replace (some of) the human modeling. Our vision are production systems that

seamlessly integrate the data collected in production contexts with analytic models and advanced optimization algorithms so as to produce long-, medium-, and short-term production plans which exploit the full potential of the wealth of data available today and that are also able to integrate the production plans into their larger logistics contexts.

This vision translates into a demand for modeling and solution approaches that are able to make use of the now available data. While so far, many approaches still rely on the assumption that all data about the future is deterministic or known with certainty, much of the planning relies on **predictions about the future** which involve some uncertainty that should be accounted for. Predictions about the future may be provided, e.g., in

- **Operations Research**
- **Mixed Integer Programming**
- **Optimization under Uncertainty**
- **Data-Driven Management**
- **Prescriptive Analytics**

the form of possible future scenarios, continuous or discrete probability distributions or in the form of possible ranges. Uncertainty may concern, e.g., future demand, costs or processing times. While there is a large body of research on theoretical concepts how to deal with these **different forms of information concerning the uncertain future**, their use in the context of practical **production and logistics system optimization** is still under development and may require different,

more data-driven approaches as well as the integration of simulation and optimization, especially to address settings where the system's uncertainty becomes difficult to account for.

## Approach

In order to incorporate parameter predictions based on the available data into production system optimization, accounting for the inherent uncertainty of predictions, there exist two well-established approaches. The first is to rely on modeling paradigms that approximate the underlying probability distributions learned from the data by scenarios, where, in general, the more scenarios there are sampled the better the approximation is, and the other approach relies on either scenario information without probabilities or possible parameter ranges.

The first approach is usually used in a (two-stage or multi-stage) **stochastic programming** expected value setting, meaning that the average performance across all potential future scenarios is optimized. The second approach resides in the robust optimization domain that, in its base setting, tries to hedge against the worst case. However, over the years also intermediate approaches have been conceived by various researchers in this domain.

One of them is known as budget uncertainty **robust optimization**. This approach allows to, instead of hedging against the worst case, assume some limit on the maximum number of parameters which will take their worst-case values at the same time, a more realistic assumption in many cases and resulting in a much less conservative view. Depending on the considered setting, one or the other approach may appear more appropriate. If the uncertainties of the systems become very complex, a combination of **simulation and optimization** in rolling horizon frameworks is a possible alternative. Here the optimization's results are directly evaluated in a simulation and allow feedback and re-optimization in a loop.

As in many other contexts, business and data understanding is important, but **key** is problem understanding and **modeling**. From a modeling perspective, we rely on **operations research techniques**, especially **mixed integer linear programming (MIP)** as the main paradigm. It allows to mathematically frame the considered optimization problem and to clearly define the considered objectives and constraints and to include parameter

uncertainty in well-defined settings. While a model is the starting point and can be used as input for advanced out-of-the-box MIP-solver software, with increasing problem size and complexity, they reach their limits. Since parameter uncertainty tends to increase the developed mathematical representations of the considered production system considerably, potentially resulting in millions of decision variables that need to be considered at the same time, decomposition-based approaches are a natural choice. They allow the solution of master and subproblems in such a way that global optimality of the obtained results is not sacrificed. Run-times may, however, still be prohibitive in **practical** and especially **large-scale settings** [2]. To obtain good solutions, but not necessarily optimal solutions in acceptable run times, **metaheuristics**, as, e.g., employed in [3], and **matheuristics** have proven of value. Metaheuristics rely on different top-level paradigms to guide simple heuristics in the search-space towards better solutions. Matheuristics combine heuristic (i.e., approximate techniques that rely on often simple rules) and mathematical programming such that they are still able to exploit the power of available MIP-solvers. In large scale production scheduling, also advanced **constraint programming** frameworks are valuable tools [4].

In production system optimization, usually there is not only one objective that should be optimized but several. A classic approach is the combination of these objectives by means of weights, known as weighted-sum scalarization. If the weights that should be assigned to the different objectives are not known, e.g., because the decision maker's preferences are not clear, **multi-objective optimization** in a Pareto setting can be used. Generic exact methods [5,6] compute all (or a subset of all) available **trade-off solutions**. To appropriately deal with parameter uncertainty and the complexity of production systems, our methodologies need to become more data-driven, both in single objective and multi-objective settings. They need to **integrate predictive and prescriptive analytics approaches**. This boils down to modeling the available information in such a way that the optimization engines of the prescriptive analytics field can best use this information and provide optimal or close to optimal decisions in large scale systems under uncertainty. Learning from past data as well as decisions is key. In our research, we develop new and enhance existing optimization algorithms for production system optimization under uncertainty.

We evaluate the **integration of heuristic and exact optimization algorithms with machine learning techniques** to best understand where this integration is most fruitful. We expect that the best performing methodologies will integrate the two worlds and not rely on one or the other paradigm. We also expect that only the integration of predictive and prescriptive analytics will allow to tap the full potential of the available data.

## Impact

Advanced data-driven approaches, **integrating predictive and prescriptive approaches**, especially decomposition-based methodologies, for production system optimization are expected to advance the **scientific state-of-the-art** in optimization for production planning under uncertainty. The resulting methodologies are also expected to contribute towards providing the theoretical and algorithmic basis for **data-driven organizations**, specifically data-driven manufacturing companies. The results obtained during simulation studies will also contribute towards better understanding how much (past) data is needed, when integrating prediction and prescription (or optimization) and how, in general, the available (or in the future available) data can be exploited in the most beneficial way.

Depending on the objective that is optimized and the data that is deployed, the developed data-driven optimization approaches will also be able to compute not only the most cost-efficient solutions but also, e.g., the most energy-efficient ones. Approaches able to consider multiple objectives simultaneously will allow the **analysis of their trade-off relationships** and further advance their understanding, leading to **improved, better informed decisions** in a data-driven setting.



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## Competencies

My research unit (JKU Institute of Production and Logistics Management) focuses on the development of optimization algorithms for prescriptive analytics in production and logistics contexts. Recent research work addresses production planning under uncertainty, intertwining optimization and simulation (FWF project HybridMRP), large scale production planning and scheduling (FFG project OMES), shop floor optimized production scheduling [3] and generic exact solvers for optimizing with multiple objectives (FWF project MOMIP) [5,6]. In a wider logistics context, we work, e.g., on the optimization of electric fleet composition and vehicle routing (research project HUGO), shared mobility systems, facility location under uncertainty, and personnel task selection and scheduling. My institute participates in the European Digital Innovation Hub “AI5production”, funded by the European Commission, and I serve on the strategic advisory board of the Center of Excellence for Smart Production.



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# Geo-Energy Production

Keita Yoshioka

## Vision

The world population has exceeded 8 billion on November 15, 2022 for the first time (worldometers.info) and it is more than 10 folds increase since the industrial revolution began in 18th century. With the increase in population, **not only the total energy consumption but also the energy demand per population increased.** For example, in 1971, the worldwide energy demand was 231 EJ with the population of 3.7 billion (62 GJ per head) and in 2021 it was 592 EJ with the population of 7.7 billion (76 GJ per head). The worldwide energy demand will continue to increase considering that 1 billion people currently live without access to electricity. Out of the total energy demand, fossil fuels (Coal, Oil, and Natural Gas) accounted for 87% (199 EJ) in 1971 while its share was 82% (490 EJ) in 2021.

**Although the fossil fuel demand decreased in terms of percentage, the total amount of its consumption increased significantly.** For this reason, our society is expected to rely on fossil fuel for decades to come. However, at the same time, adverse impacts of climate change are no longer disasters happening in distant places. They are literally happening in our backyard. We must act now and I believe our Petroleum/Geo-energy Engineering program at Montanuniversität Leoben can and should have a bigger role in this fight against climate crisis through our knowledge and skills in dealing with subsurface. Specifically, we need to dispose gigatons of CO<sub>2</sub> per year underground to achieve net zero emission (IPCC, 2022). In any scenarios projected by IPCC, **we will not achieve net-zero carbon emission without massive scale up of CO<sub>2</sub> underground sequestration**, and any technical or

societal obstacles should be addressed as soon as possible. We also need to drastically increase production and enhance transport systems of hydrogen which would not be economical without abundant storage spaces that subsurface can offer (e.g. depleted oil and gas reservoirs and salt caverns). Hydrogen must be stored in subsurface economically leaving as little hydrogen as possible in rock's pore spaces and safely without impairing the mechanical integrity of geological sealing capacity. We also need geothermal energy not only for power generation but also for heating homes and industrial use to reduce the reliance on natural gas.

Historically, the discipline of petroleum engineering concerns hydrocarbon (oil and gas) production through subsurface system. We study mass and heat transport, chemical reaction,

- **Computational Geomechanics**
- **Fracture Mechanics**
- **Geothermal Energy System**

and mechanical deformation in geological formations. We design and evaluate how to access subsurface formation through a well often drilled several kilometers deep penetrating through various geological formations such as rock salt or igneous rock. We operate production systems through various pumps installed at surface or subsurface and intervene them as necessary. All these skills are necessary to meet the increasing demand for hydrocarbon, but they are also **essential for the energy transition in the aforementioned areas where subsurface is relevant.** While there

exist quite a bit of synergies between conventional petroleum production and energy/waste storage and geothermal production, we also need to adapt and advance both in the teaching and the researches.

Our specific research focus areas are: 1) **subsurface integrity** during energy (e.g. hydrogen) storage and waste (e.g. CO<sub>2</sub>) disposal, 2) **supercritical geothermal system**, and 3) production/injection **well stimulation**.

## Approach

**1) Subsurface integrity** of energy/waste storage is studied through numerical simulations, laboratory experiments and field observations. Our particular focus is on **numerical simulations** where we model the behavior of the subsurface environment under different operational scenarios. This involves developing computer models that simulate the geomechanical response of the host rock and the surrounding geological formations to changes in pressure, temperature, and stresses. These simulations can help to **forecast the risk of subsurface failure**, and can be used to **assess the design of subsurface energy/waste storage systems**. We mainly use an open source code, OpenGeoSys (www.opengeosys.org), for method development. With the implementation being publicly available, simulation procedures, underlying assumptions, input parameters etc. are transparent to all the parties involved for reviews. The computer models need to be validated against laboratory experiments where the system's conditions are under controlled, and need to explain field observations (e.g. geophysical data) when applied in field scale.

**2) Supercritical geothermal resources** where the water is at or above the supercritical condition (373.95 Co and 22.064 MPa) are considered to be **2 to 5 times more productive** in terms of power generation because of their high enthalpy (Friðleifsson et al., 2014). Practical challenges to exploit such supercritical geothermal resources are two holds. One is its depth that meets the supercritical condition for water and associated drilling difficulties in both technical and economical points. The other challenge is its perceived low permeability in rocks below the brittle ductile transition. However, the study conducted by Watanabe et al. (2017) challenges this notion of low permeability below the brittle ductile condition. Their experimental study under high temperature and

high pressure demonstrated that the morphology of hydraulically induced fractures changes from planar to dendritic in supercritical conditions. Their study indicates that supercritical geothermal reservoirs can be hydraulically stimulated to form a dendritic fracture network, which may be suitable for economical development of supercritical geothermal resources. Our main objective of this topic is to understand and formulate the hydraulic fracture behaviors in supercritical geothermal conditions from experimental and numerical standpoints. Under such conditions, both fluid and rock rheologies change and we do not fully understand know how the fracture morphology is impacted by these changes. To separate the effects of fluid rheology from those of rock rheology, we conduct hydraulic fracturing experiments on non-porous and porous materials that have different brittle to ductile transition conditions so that working fluid (e.g. water) can be either above or below the supercritical condition. From these experiments and numerical simulations, we study interplay of rock rheology with that of fluid, and assess the implications of the findings regarding rheology of fractured rock and fluid flow on magmatic hydrothermal processes.

**3) Well stimulation** is not only required for conventional oil and gas production, but also for CO<sub>2</sub> injection to maintain the injectivity of geothermal wells where chemical treatment known as acidizing is commonly performed (Pasikki et al., 2010). Furthermore, for a system called, Enhanced Geothermal System, **the creation of a geothermal reservoir involves stimulating the rock formation** with water injections. Therein, we need to understand the subsurface geology, including rock properties, fracture network, and fluid flow pathways in order to design well stimulation. As fluid is injected, rock and fluid interaction can induce mineral dissolution and precipitation, permeability enhancement, and stress changes. Numerical modeling and simulation tools can provide valuable insights into these behaviors and uncertainty quantification. Also, continuous monitoring is essential to ensure safe Enhanced Geothermal System operation (e.g. induced seismicity).

## Impact

Our **scientific impacts** are two-folds. The first is in the area of computational science through our method development. Our particular computational technique is novel concerning failure initiation as it is based on the successive energy minimization (Yoshioka et al., 2021), and coupling techniques in multi-physical processes in subsurface. The second scientific impact is through its application. As subsurface process cannot be easily replicated in laboratory scale, numerical simulations bring new insights on our understanding of subsurface such as supercritical geothermal systems such as fluid re-injection impacts in Enhanced Geothermal System (Parisio and Yoshioka, 2020).

The **economical impact** of subsurface **energy storage** is realized through cost reduction by enabling more efficient use of renewable energy sources, such as wind and solar, which can be intermittent in nature. By storing excess energy during times of high production and using it during times of high demand, energy costs can be stabilized and grid reliability can be improved. **Supercritical geothermal energy production** has a potential to scale up geothermal production by 2 to 5 folds, and opens up new prospective in the areas already exploited for conventional geothermal resources. EU is actively funding in this subject through field scale research projects in Iceland, Italy, Mexico and New Zealand.

Another impact of our research is **energy security**. Underground energy storage can enhance energy security by providing a reliable and flexible source of energy and it is of great importance given recent geopolitical situations in Europe. Impacts associated with CO<sub>2</sub> sequestration cannot be understated. IPCC estimates gigatons of CO<sub>2</sub> per year need to be sequestered to reach zero emissions and we are currently storing around 40 megatons per year, which needs to be scaled up drastically.





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## Competencies

Though my research group has been just formed in late 2022, I am bringing my past experiences in Japan, US, and Germany to my group. My most recent project on supercritical geothermal energy was funded by Deutsche Forschungsgemeinschaft – DFG and Japan Society for the Promotion of Science – JSPS, partnering with the Helmholtz Centre for Environmental Research – UFZ (Germany), Technische Universität Bergakademie Freiberg (Germany), The National Institute of Advanced Industrial Science and Technology (Japan), Kyoto University (Japan), and Tohoku University (Japan). An ongoing project on development of crack simulation tool in rock is currently funded by Japan Organization for Metals and Energy Security - JOGMEC, which funds another project on numerical modeling of wormhole partnering with Waseda University (Japan). Another project on chemo-mechanical aging of cementitious materials is funded by European Joint Program on Radioactive Waste Management – EURAD and is partnered with Belgian Nuclear Research Centre (Belgium), the Helmholtz Centre for Environmental Research – UFZ (Germany), and the Spanish National Research Council (Spain).

Furthermore, I have been part of the development team for an open source project, OpenGeoSys (opengeosys.org), which is maintained at the Helmholtz Centre for Environmental Research - UFZ in Germany and is led by an international consortium of academic and research institutions.



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# Industrial Scalability of Production in Vertical Farms

Markus G. Tauber, Stefan Gindl, Yasin Ghafourian, Martin Wögerbauer

## Vision

In the context of contemporary challenges such as climate change, population growth, urbanization, soil sealing, and economic instability, which are adversely affecting global food production and distribution systems, addressing the increasing demand for food necessitates the exploration of innovative approaches. One promising avenue to address the pressing demand for food availability is vertical farming which is increasingly driven by biologists seeking to understand plant growth in controlled environments. Additionally, digitalization of food production in vertical farming allows for industrial scale food production to match the growing food demand through greater productivity and less environmental impact as a result of integrating digital technologies [1,2]. Furthermore, the progress of vertical farming, primarily driven by biologists, goes beyond just food production. While vertical farming is often associated with leafy greens such as salads, it includes various plant species with diverse applications. Plants are not limited to culinary purposes alone but are also used for medicinal products and dietary supplements. As such, vertical farming extends beyond food production, encompassing a wider range of plant-based products beyond traditional food crops.

The production of essential ingredients for our lives, including food and medicinal products, can be made more sustainable and automated through paradigms such as Industry 4.0 and Industry 5.0. The integration of the Industrial Internet of Things (IIoT) can play a crucial role in this transformation.

However, to address challenges such as supply shortages and overcome the limitations of traditional industrial production systems, unconventional features may need to be considered in the context of vertical farming. This emerging field requires a keen focus on scalability and flexibility, as it is of utmost importance to meet the unique demands of plant-based production systems. Scalability enables vertical farming systems to be expanded to larger scales, allowing for increased production capacity, efficiency, and commercial viability. It also allows for adaptability and responsiveness to changing demands, making these

- **Digital Industries**
- **AgriFood and Natural Resources**
- **System of Systems**
- **Self-Adaptability**
- **NLP**
- **Industrial Internet of Things**

systems more effective in meeting the growing global need for sustainable food and medicinal production. Individual aspects of plant-based production systems are often mentioned in various application domains, such as “digital industries” as well as “agrifood and natural resources”, as documented in the Strategic Research and Innovation Agenda (SRIA)<sup>1</sup> for Electronic Components and Systems, providing further evidence of the growing importance of scalable and sustainable production methods.

<sup>1</sup> [ecssria.eu/ECS-SRIA%202023.pdf](https://ecssria.eu/ECS-SRIA%202023.pdf)

## Approach

One approach to enhance the scalability and sustainability in vertical farming is adopting self-adaptable systems. Through optimizing resource allocation, energy efficiency, pest management, and continuous improvement, self-adaptability leads to more efficient and sustainable agricultural practices. Self-adaptability is achieved by using methods like MAPE-K (Monitor, Analyze, Plan, Execute, and Knowledge) [3] which is a mature framework [4], serving as a guideline for building compute systems with properties like self-organizing, self-healing, self-adaptable. We see it being applied to cyber-physical systems, where this approach has also found application in various domains, including the emerging field of the Industrial Internet of Things (IIoT). The IIoT enables the collection of information and real-time adjustments of settings in industrial facilities, leading to greater automation and optimization of processes. Additionally, technological trends such as Natural Language Processing (NLP) [5], edge computing [6], and edge AI [7] have the potential to further influence the landscape of self-adaptable systems. These advancements have expanded the capabilities of the MAPE-K approach, allowing for more sophisticated and dynamic adaptations in complex industrial environments.

The integration of technological trends such as Natural Language Processing (NLP), edge computing, and edge AI with the MAPE-K approach can offer potential solutions to address scalability challenges in vertical farming. Practitioners in the field of vertical farming have identified that achieving homogeneous production conditions are crucial for mass production of plants.

One effective approach involves using sizeable boxes to emulate specific conditions rather than large industrial production halls. However, to achieve higher yields, practitioners need to implement AI-based systems within larger cyber-physical systems to ensure homogeneity. Different architectural approaches, such as cloud, edge, far edge, fog, IIoT, and embedded AI, are available, but their optimal combination needs to be investigated for effective implementation in vertical farming systems. This strategic integration of technology and innovative approaches can enable vertical farming to achieve scalability, adaptability, and commercial viability, addressing the unique demands of plant-based production systems and contributing to more



sustainable food and medicinal ingredients production.

Another aspect of scale and flexibility in vertical farming is the ability to quickly change the type of product being grown. While traditional digital industries can be easily modeled and modified, it is more challenging to modify a plant production system due to the nature of plant growth. However, there are many documented observations on how to produce or grow plants that can be leveraged. Therefore, utilizing standardized autonomous control loops like MAPE-K can help ensure that the control process is well understood. Additionally, the extraction of information through Natural Language Processing (NLP) can further enhance the adaptability and responsiveness of vertical farming systems.

By leveraging NLP techniques, valuable insights and data can be extracted from diverse sources, shortening the time required to create appropriate control systems e.g., MAPE-K cycles. This integration of standardized control loops and NLP-based information extraction can contribute to the efficient and effective management of vertical farming systems, enhancing their scalability, flexibility, and ability to quickly adapt to changing product requirements.

In addition to addressing scalability and flexibility, autonomous control loops in vertical farming also need to achieve homogeneous conditions. An individual control loop is relatively simple, but the plethora of parameters to achieve homogeneous environmental conditions are substantial. Furthermore, the operation of multiple control loops in parallel requires appropriate conflict resolution strategies. Further topics which will improve the scalability of the approach on an organizational level will be the capability of conducting remote support via e.g., using AR technologies to compensate for the potential scarcity of experts in the area.

## Impact

Advanced technologies such as NLP, edge computing, and edge AI with standardized autonomous control loops like MAPE-K in vertical farming systems are a significant step towards Industry 4.0 and Industry 5.0. By leveraging IIoT technologies, these systems can create scalable and flexible production systems that can adapt to new situations and compensate for supply chain issues.

This strategic integration of technology and innovative approaches can result in systems where plants for medicinal or food purposes can be easily produced, and appliances can work autonomously without human intervention. These systems will adapt to new situations and compensate for supply chain issues, making them highly flexible and resilient.

The use of NLP techniques further enhances the adaptability and responsiveness of these systems by extracting valuable insights and data from diverse sources. This allows for informed decision-making and precise adjustments in the production process. Overall, the integration of standardized control loops and NLP-based information extraction in vertical farming systems hold the potential to create efficient, autonomous, and adaptable systems that can address the unique demands of plant-based production and contribute to more sustainable food and medicinal production.



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## Competencies

In my past and present research units we have conducted several projects in related topics. This includes AgriTec4.0 (IWB/EFRE) [8], in which we have been conducting investigations into the IT/OT infrastructure required for successful implementation of advanced aeroponic systems.

In **AIMS5.0** (KDT JU) we are launching a new research initiative focused on policy creation for the automation of vertical farming and food production, with an emphasis on leveraging methodologies like MAPE-K.

In **AGRARSENSE** (KDT JU) we are investigating ways to enhance the infrastructural scalability of medicinal plant production systems.

In **Eden** (FFG), we focus on exploring the impact of scaling aquaponic systems through community engagement on their circularity.

In **Arrowhead tools** (ECSEL JU)[9], we have conducted comprehensive investigations into various aspects of the Industrial Internet of Things, with a particular focus on security.

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# Numerical Design

Stefanie Elgeti

## Vision

In recent decades, the two classical pillars of scientific and engineering knowledge acquisition, namely theoretical reasoning and experimentation, have been complemented by computational knowledge acquisition. One area where computational approaches have gained significant traction in recent years is the numerical design of both engineering components and their manufacturing processes. Numerical design refers to approaches in which design solutions are recommended to the designer by computer-based assistance systems with varying degrees of autonomy.

A distinction can be made between **design optimization**, where manually generated initial designs are optimized by a design algorithm with respect to specific criteria, and **generative design**, where the entire design layout is generated from scratch. The former is generally associated with shape optimization methods, while the latter can be addressed by topology optimization approaches. In both cases, numerical design touches on a number of research areas as prerequisites: modeling of physical systems, numerical simulation, (geometry) parameterization, and optimization techniques.

Overall, numerical assistance systems have the potential to make the design process more explorative. In the interaction with the assistance system, the human creativity can be enhanced while at the same time improving the efficiency of the design process.

## Approach

The engineering design process can be divided into (1) system design, (2) conceptual design, and (3a) individual component design and (3b) catalog component selection. Numerical design is primarily concerned with the design of individual components. A typical numerical design process involves four main components: (1) geometry parameterization, (2) forward simulation, (3) objective function, and (4) optimization algorithm. The following is a discussion of state-of-the-art methods for each of these components.

- **Numerical Design**
- **Finite Element Methods**
- **Isogeometric Analysis**
- **Machine Learning in Design**

**(1) Geometry parameterization:** This component ensures that the geometric layout is described in such a way that it can be understood and manipulated by a computer. The gold standard here, especially in computer-aided design (CAD) software, are spline-based representations [1]; most commonly non-uniform rational B-splines (NURBS), but also T-splines or subdivision surfaces. Splines are a common choice in design optimization [2]–[4], but they can also serve as a means for analysis [5]. In terms of design optimization, parameter-free design approaches are a viable alternative [6], [7]. Since the computational mesh also represents the geometry, this approach offers high flexibility, but requires advanced optimization algorithms. A variation of this approach would be the use of

a signed distance function or point clouds. In recent years, machine learning approaches have also been used to represent geometry. The most prominent example is variational autoencoders (VAE) [8]. A VAE is a deep neural network that learns the underlying structure of a 3D shape in an unsupervised manner. In topology optimization, two general approaches can be distinguished [9]. The first category relies on some kind of marker function on a background grid. This category includes density-based approaches, homogenization approaches, or the level-set method. The second category uses the computational grid to represent geometry by activating or deactivating certain elements to add or subtract material from the part.

**(2) Forward simulation:** As the name implies, the output of a forward simulation is the state of a physical system given a specific parameter configuration. Important aspects to consider in a forward simulation are the accuracy of both the underlying physical model and the numerical scheme, as well as the flexibility and efficiency of the method. Numerous numerical schemes have been developed in the past, such as the finite difference, finite volume, and finite element methods at the continuum level and the discrete element or material point method at the particle level. All of these methods are suitable for design optimization in principle, but it is the specific application that determines which method is the most appropriate.

Given the importance of efficient simulations in the many-query context of optimization, there has been an increased interest in surrogate and reduced-order models. These methods have the same input-output behavior as high-fidelity forward simulation, but can be evaluated very efficiently after some training. Examples of such methods are proper orthogonal decomposition [10], reduced basis methods [11], Gaussian process regression [12], and others.

**(3) Objective function:** The objective function quantifies the quality of a given configuration with a single number. A well-chosen objective function is the key to successful optimization. Objective functions are usually cumulative quantities such as drag, lift, compliance, or mass. The objective function is usually formulated to be minimized, not maximized. It is also possible to include multiple objectives in a single objective function in a weighted sum. When identifying a possible objective function, it is

recommended to first test the behavior of the function outside the optimization environment. One should verify that over the full range of parameters, the objective function actually measures what is intended and that it is sufficiently sensitive to changes in the parameters.

**(4) Optimization algorithm:** Design optimization in the form of shape and topology optimization belongs to the category of continuous optimization. Moreover, it is an example of a PDE-constrained optimization problem, i.e., besides the objective function to be minimized, there is an equality constraint consisting of a partial differential equation (PDE), in our case the forward simulation. One can always try to find a global optimum of the objective function, i.e., a point where the objective function is smaller than at all other feasible points in its vicinity. In particular, since there is no more concrete definition of a global optimum than the one just given, finding a global optimum will require a significant amount of exploration of the optimization space. Given that each forward simulation can be computationally intensive, this may be prohibitively expensive. Instead, one can choose to find a local optimum starting from a user-defined initial design. In this case, for smooth and twice continuously differentiable objective functions, clear criteria for a minimizer can be formulated based on the gradient and the Hessian of the objective function [13]. These values not only allow to identify a local optimum, but also provide criteria for an appropriate search direction. This leads to the idea of gradient-based optimization algorithms, where the search direction is determined based on the gradient and (an approximation of) the Hessian matrix. If analytical gradients are not available, they can be computed using finite differences. However, if the number of optimization parameters is very large, this leads to a significant computational burden. Instead, algorithmic differentiation or adjoint methods should be used. If gradients cannot be computed, trust-region methods are a viable alternative. These methods locally approximate the objective function using a surrogate function whose minimum can be easily determined. This point provides the next iteration where another surrogate function is computed.

## Impact

For many decades, numerical analysis was a tool for the, maybe somewhat quirky, pioneers among the engineers. An option one could resort to when there were no other options. Partially, this can be attributed to the fact that numerical analysis is a costly process; in early days, spatially-resolved analysis was unthinkable. Analysis had to be performed on very crude meshes, often times missing important effects — an example could be turbulence modelling, where the observation of turbulent effects require a sufficiently high mesh resolution. Consequently, the development of reduced physical models became imperative. However, forming a reduced model required great insight into the physics — that sometimes simply was not available.

While science has traditionally rested on the principle that insight could only be gained from either theoretical deductions or experimental evidence, this view has radically changed in recent times with the birth of computational science. This has transformed forever the way that scientific discoveries are made, and how engineering and medicine is done. Its impacts encompass virtually all aspects of our daily lives.

Computational science is rapidly gaining ground among application engineers and establishing itself as a fundamental investigative tool among practitioners. Major milestones along this path have been the tremendous increase in computational power, allowing for increasingly accurate and detailed models, and the growing emphasis on validating numerical results against available experimental data. An immediate consequence has been a paradigm shift in engineering design: Experimental testing was increasingly replaced by numerical simulation. Although the world of design and the world of analysis have traditionally been separate, this dichotomy is being reconciled. One element is CAD-compliant analysis methods, most notably isogeometric analysis (IGA) [5]. But other developments have also contributed to a close intertwining of CAD and numerical analysis, allowing CAD systems to increasingly become the design engineer's sparring partner in the creative process of engineering design.





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## **Competencies**

Stefanie Elgeti's research is centered around engineering design and design optimization [4], [14]. Her contributions encompass both inverse formulations [15] and iterative procedures using optimization frameworks. One of her key competences are spline-based geometry representations [4], [16]–[18]. In shape optimization, spline representations allow to obtain smooth shapes that can be drawn from a vast and flexible design space. At the same time, expert experience or manufacturing conditions can be included as a shape constraint. As such, splines provide an ideal balance between design flexibility and consideration of previous knowledge. A further advantage is the direct compatibility with the CAD/CAM manufacturing process and the direct connection to isogeometric methods [17], [19], [20]. The recent work on splines in the group of Elgeti has been enhanced with the development SplineLib [21], an open-source library facilitating design and analysis using splines. Another important aspect of Elgeti's work is the development of objective functions [4], [14], [22], [23]. On the simulation side, Elgeti is not only involved with developing application-specific finite element methods [24]–[26], but also with obtaining reduced order models [27]. In recent times, the group of Elgeti has gained experiences with machine learning approaches. These include surrogate models [10], variational autoEncoders for shape representation [28] as well as reinforcement learning in profile extrusion [29], [30].

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# Structural Mechanics and Digital Twins

Yury Vetyukov

## The Role of Structural Mechanics

Manufacturing engineering has strong overlaps with mechanical engineering. Virtual prototyping and CAE, automation and model-based controller design, cyber-physical systems and digital twins require accurate and efficient (possibly real-time) predictions of the behavior of mechanical components. In the recent decades progress has been achieved in the basic understanding of structural mechanics, its ability to handle complicated elastic and inelastic structural behavior at different size scales as well as to serve as a basis for analyzing multi-physical systems featuring electromagnetic components or fluids with possible melting or solidification. This progress, however, stands in the shadow of the rapid development of numerical methods of analysis and growing computer power. The synthesis of the basic theory and advanced computational techniques requires proficiency in both fields, but can potentially result into successful treatment of outstanding and challenging problems, which were previously rendered as inaccessible or computationally too costly.

Various analytical techniques contributed to the advances in the field of structural mechanics over the recent decades [1]. Thus, the direct approach in the framework of Lagrangian mechanics along with the direct tensor calculus allows treating nonlinear structural theories of dimensionally reduced continua. Large deformations and stability of shells with initial curvature or rod structures are described not only by partial differential equations, but also in the weak form by variational equations with clear physical meaning, which allow direct transition to computational schemes. Additional

advantage of the variational form is that it may be transformed to the mixed Eulerian-Lagrangian kinematic description, which is particularly relevant for axially moving structures, see below. The constitutive behavior of the possibly inhomogeneous cross-section of a rod or of a through-the-thickness element of a shell is revealed by means of the asymptotic treatment of the respective three-dimensional problem of continuum mechanics. Altogether, these techniques often allow for an elegant simulation technique with little or moderate computational effort, where otherwise just a brute force numerical approach with high computational cost would have been possible.

- **Thin-walled Structures**
- **Numerical Simulations**
- **Inelasticity**
- **Axially Moving Structures**
- **Arbitrary Lagrangian-Eulerian Description**

## Axially Moving Structures<sup>1</sup>

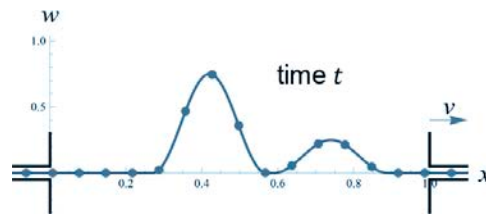
Deformable structures, continuously moving across a given control domain appear in numerous technical applications, to name a few: transport belts and belt drives, hot metal rolling and sheet metal forming, rotating wheels and brake discs, laying of offshore pipelines, wire coiling, paper production, casting of polymer films, etc. In operation these processes are prone to perturbations, have a tendency to diverge from the desired regime of motion and may display complicated and sometimes even counter-intuitive mechanical behavior. Such flexible



axially moving structures [2] are not only difficult to run and control reliably. Moreover, they are inherently difficult to model, analyze and simulate. Clearly, this mix of practical relevance – also in the field of manufacturing engineering – and scientific challenge is responsible for the vivid research activity.

Owing to the underlying gross motion, the traditional material (Lagrangian) kinematic description of structural mechanics becomes inefficient for axially moving structures as material particles enter and leave the control domain. Growing attention of researchers is devoted to various kinds of non-material modelling based on different problem-specific variants of the Arbitrary Lagrangian-Eulerian (ALE) approach, both in the analytical studies as well as in the numerical analysis. Issues related to geometric nonlinearities, proper imposition of boundary conditions, moving frictional contacts, dynamic stability and inelastic material behavior require thorough analytical studies and sophisticated numerical techniques.

Belonging to the broad class of ALE formulations, the Mixed Eulerian-Lagrangian kinematic description (MEL) features the transformation of the equations of structural mechanics



with the wave speed  $c$  applies in the geometrically linear range, as long as the small deflection  $w(s,t)$  is considered a function of the material (Lagrangian) coordinate  $s$  and time  $t$ , such that a dot has the meaning of a total time derivative computed in a given material particle. The boundary conditions, however, are to be imposed in time-varying points because new particles

$$x = s + vt, \quad w = w(x,t), \quad \dot{w} = \partial_t w + v \partial_x w, \quad \partial_t w = \frac{\partial w}{\partial t} \Big|_{x=\text{const}}$$

The total time derivative is decomposed into a local time derivative  $\partial_t w$  in a given point in space plus a convective term; note, that  $\partial_x w = w'$  owing to the

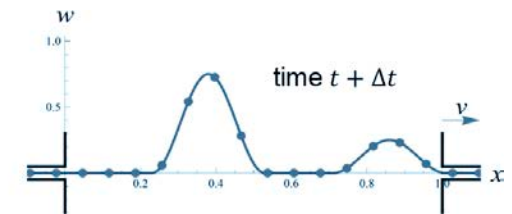
$$\partial_t^2 w + 2v \partial_t \partial_x w = (c^2 - v^2) \partial_x^2 w, \quad w|_{x=0,L} = 0$$

(mostly written in terms of the variational equation of the principle of virtual work) to a new set of independent coordinates. This problem-specific coordinate transformation helps matching the boundaries of the control domain, across which the material is moving, with the discretization domain of the numerical scheme, to the advantage of the latter.

The basic idea is well illustrated by the example of waves traveling in a string, which is transported across a control domain of the length  $L$  with the velocity  $v$  to the right. The figure below demonstrates configurations of the string at two subsequent time instances. The waves are running upstream (to the left) slower than downstream, compare the displacements of the crests of the two waves over the time period  $\Delta t$ . The wave equation

$$\ddot{w} = c^2 w'', \quad \dot{w} = \frac{\partial w}{\partial t} \Big|_{s=\text{const}}, \quad w' = \frac{\partial w}{\partial s}$$

Also known as traveling structures, they perform steady gross motion across a given spatial domain in a direction, which is called axial. Analysis of deviations from this nominal motion, either intentional or undesired, is of importance for the design and control of various machines.



are located at the entry and at the exit of the control domain at each time instant. Boundary value problems (BVP) with time-varying boundaries are generally difficult to solve. A conventional workaround is to consider the deflection as a function of the spatial (Eulerian) coordinate  $x$ , which, in this simple case, can be easily related to the Lagrangian coordinate:

geometric linearity, and  $x=v$ . Using the transformation (2) twice in the wave equation (1), we obtain the BVP

This seemingly more complicated Eulerian form of the wave equation (1) is actually easier to solve both analytically and numerically, since the boundary conditions are now imposed at fixed points in space. Moreover, the employed transformation effectively uncovers an important physical property, namely: as soon as the transport velocity grows above the wave speed,  $v > c$ , the type of the partial differential equation

$$s = s(x, t), \quad w = w(x, t).$$

The material coordinate  $s$ , which is the arc length in the undeformed reference state, and the finite transverse deflection  $w$ , are considered in dependence on the Eulerian coordinate  $x$ , which expresses

changes. The solution starts growing in time, which is known as dynamic instability.

At large vibrations, the geometric nonlinearity essentially couples the transverse deflections and the axial motion of the continuum. It is then efficient to define the deformed shape of an axially moving string or beam in terms of two functions:

the *basic idea* of the *MEL description*: In each spatial point in the axial direction  $x=const$  relations (4) identify a material particle and its transverse deflection; see [3] for a numerical implementation.

## Applications

The simple idea of the MEL description was put into practice in various applied projects.

- **“Modelling of the Sheet Run and Control for Hot Roll Mills“**, project partner: Primetals Technologies GmbH (former Siemens VAI Metals Technologies), Erlangen, Germany. The motion of hot elastic-plastic sheet metal from one roll stand to the subsequent one on a roller table was efficiently modeled using a finite element mesh, which is not moving in the axial direction [4]. This was crucial to achieve the necessary continuity of the simulation results in response to control variables such, that a coupled model with the controller would work reliably and provide results in real time.
- **“Modelling and simulation of lateral dynamics for an endless metal process belt“**, funded by Austrian Research Promotion Agency (FFG), project partner: Berndorf Band GmbH, Berndorf, Austria. Process steel belts moving between rotating drums find use in production of wood and laminates, chemical products, rubber and plastics, optical films, paper, etc. The lateral run-off of the process belt is usually suppressed by a controller. However, currently available controller designs require high belt tension, which is sometimes not beneficial for the production process and increases the wear of the belt. The project focussed on developing the software simulation tool for modelling a steel belt with imperfect geometry, running on two rotating drums, and its experimental validation. Expertise in geometrically nonlinear theories of shells and rods, contact mechanics and MEL description as well as numerical methods determined the success of the project [5].
- **Roll forming** is a highly efficient continuous production process for steel profiles of various cross-sectional shapes. An initially flat, thin metal sheet receives incremental bends at subsequent roll stands as it travels through the rolling line. An efficient simulation tool featuring a geometrically nonlinear elastic-plastic shell model of the metal sheet, moving axially in contact with roll stands was implemented in the framework of MEL kinematic description and validated experimentally [6].



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# Data as an Asset in Data Spaces

Günther Tschabuschnig

## Vision

In the manufacturing industry, data is becoming increasingly important to optimize processes, improve quality, and reduce costs. The concept of data spaces has emerged as a way to manage and organize this data. A data space is a virtual space that contains all the relevant data for a specific manufacturing process or system. This data can come from various sources, such as sensors, machines, and human input. By organizing data in a data space, it becomes easier to access, analyze, and utilize.

Data spaces enable manufacturers to gain a better understanding of their operations and identify areas for improvement. For example, by analyzing data from sensors on a production line, a manufacturer can identify bottlenecks and optimize the process to increase efficiency. Data spaces can also be used to monitor product quality by analyzing data from sensors and cameras throughout the manufacturing process. In addition to improving operations and quality, data spaces can also facilitate collaboration between different teams and departments or even organisations. By providing a decentralized location for data, teams can easily share information and work together to solve problems. Data spaces also enable manufacturers to incorporate new technologies, such as artificial intelligence and machine learning, into their operations. Businesses strive to be in control of their data. Control is important when managing data internally, but even more important when sharing data with others. The core function of a data space is to instill trust between participants and negotiate available

data contracts. They enable control over the sharing of data and create value for all parties involved.

A data space is both an inter-organizational arrangement and a supporting technical infrastructure for sharing data. Participants may already have a level of trust: some may have a prior relationship and trust each other, while others may be unrelated and untrustworthy. Data rooms even enable data to be exchanged between direct competitors. Data space connectors facilitate and coordinate the sharing of data assets while enforcing the requirements set by the data provider. A connector includes policies,

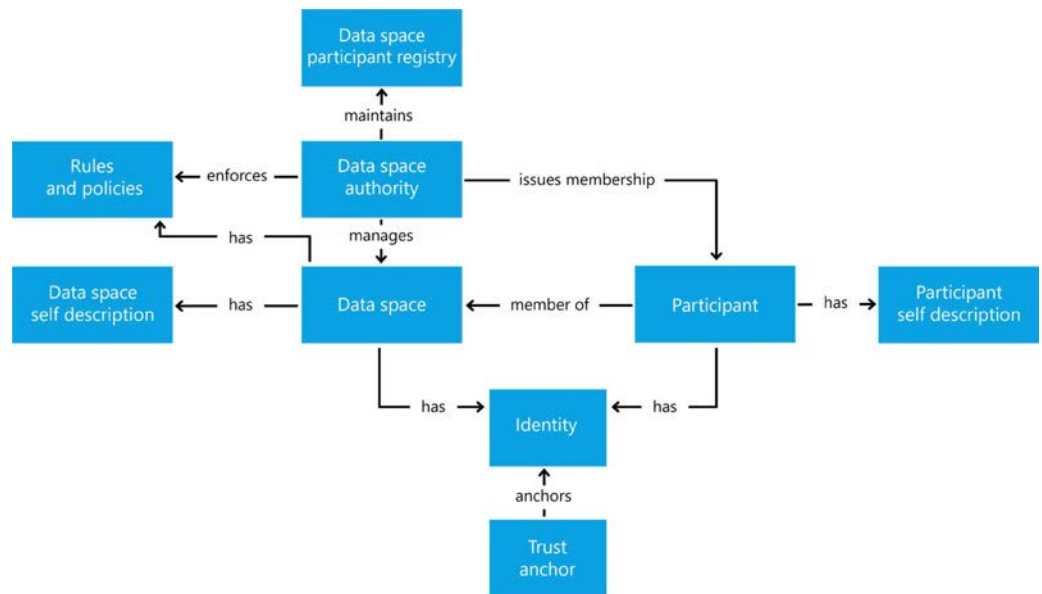
- **Data Space**
- **Data Economy**
- **Gaia-X**
- **Data-driven Business**
- **Data Assets**

configuration, and other metadata artifacts that can run on any cloud infrastructure, on-premises, or on an edge device.

Sharing data in a data space is not limited to sending data from one participant to another, but can also be more complex. Basically, all data sharing consists of peer-to-peer interactions. All multi-actor scenarios are based on peer-to-peer data contracts between two participants. A data space offers added value that goes beyond individual data transmission by enabling collective data services and applications. These additional

capabilities require certain functional requirements to be incorporated into the design of a data room.

Different business, regulatory, legal or technical requirements require different architectures and approaches. Some data spaces may



Source: IDSA Dataspace Rulebook - Overview of Data Space entities

require centralized components with centralized control, while others are designed to give their participants maximum autonomy and control over how they share their data.

be negotiated.

A very similar process is used to establish trust in a data space. It is necessary to assess the attributes of the participants and to compare them with the requirements, guidelines and rules of the data room, the participants and the individual data contracts.

## Approach

The foundational concepts of a data space:

- Establishing trust
- Data discoverability
- Data contract negotiation
- Data sharing & usage
- Observability
- Vocabularies and semantic models

Building trust is fundamental to a data space. To create value from data, it must interact with other data and then support decision making. The different entities must trust each other - without trust, the data is not shared. Data spaces can create context-specific trust where trust previously did not exist or where it is difficult to establish - for example between competitors. As people build trust with one another, they evaluate attributes of the other person: attributes that are immediately verifiable or attributes that require an external authority to verify (e.g., a passport). In order to build trust, these attributes are compared with guidelines. When a sufficient number of policies are met, trust is established. Based on the evaluated attributes, different levels of trust can

The sharing of data among participants requires the provision of. The information about the data must be published with an agreed vocabulary for queries and controls governing access to the catalog items.

Two participants can share data directly with each other by communicating offline or online without the need for a catalog. With more participants, however, a catalog function increases the findability of databases and services considerably. If there is more than one catalog due to a federated or decentralized design, the catalog must allow federated search of records in catalogs in multiple locations. Catalogs do not provide the data itself, but they do offer data contract offers.

Once a subscriber has joined a data space and discovered available data offerings, the data sharing mechanism is set in motion. Data sharing is the core activity that enables further data processing and value creation through the use of data.

Data sharing ranges from transferring a file once, accessing an API, registering



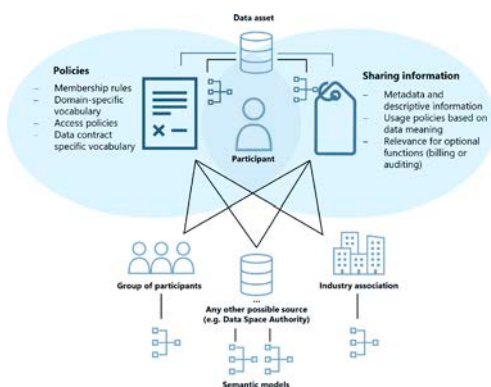
for an eventing service, subscribing to a data stream, to data-sharing methods where the data stays at the source and algorithms and processing code do the processing be copied in place. Data sharing does not require physical movement of data assets, although often it will.

However, before data can be shared, a data contract offering must be negotiated to reach a Data Contract Agreement (DCA) that lays out all the guidelines and details of the data sharing process.

Vocabularies are used to ensure that everyone means the same thing when using a specific term. The vocabularies for each level can be easily referenced by the metadata publishing mechanism at the respective level. A data space can reference the required policy vocabulary through its self-description. A participant can also leverage its self-description to publish additional vocabulary requirements. And at the data contract level, this information can be easily stored in the metadata associated with the contract at the catalog level.

The sharing of data always takes place in a peer-to-peer data space, with data discovery taking place via catalogues. This basic functionality does not cover any form of business model. Since many data spaces require not only the search for available data but also platforms for trading, buying and selling data, it is to be expected that many different models of data marketplaces will emerge within data rooms.

Again, these can be centralized marketplaces, federated marketplaces, or individual decentralized business platforms. Similar to how resources can be bought and sold on exchanges, functions can be created for data contracts. A marketplace can also provide a catalog that enables data to be found and a business platform for buying and selling data. Or it can simply act as a broker, facilitating the negotiation of data contracts for a fee.



Source: IDSA Rulebook: Vocabularies and their relationship to data assets

## Impact

The lack of a general legal status (access regime) for data, partial application of intellectual property rights and trade secret protection and the restrictions of personal data protection result in a fragmented and incomplete regulatory framework. To address these shortcomings in data sharing and reuse, the EU Commission presented the “European strategy for data” in February 2020 describing the vision of a common European data space. The Commission has proposed different regulations (Digital Markets Act (DMA), Digital Services Act (DSA), AI Act ) on harmonized rules for data governance, data access and use as part of the EU’s digital strategy.

Beside other regulations the Data Governance Act (DGA) entered into force on 23 June 2022 and will be applicable from September 2023 after a 15-months grace period. On 23 February 2022, the Commission proposed a regulation on harmonized rules for fair access and use of data, the Data Act Proposal (DA-E). With both acts the Commission aims to make more data available for use, by setting up rules on who can use and access what data for which purposes across all economic sectors in the EU.

The DGA aims to make more data available by regulating the reuse of publicly/held, protected data, by promoting data sharing through the regulation of novel data intermediaries and by encouraging the sharing of data for altruistic purposes. It aims to make public sector data more widely available for local businesses, researchers and communities for the development of innovative data-driven services. A specific focus is on the public sector data which is subject to legal restrictions and thus out of the scope of the Open Data Directive. Therefore, the proposal covers public sector data which is legally protected on the grounds of: (a) commercial confidentiality including the trade secrets; (b) statistical confidentiality; (c) intellectual property rights of third parties; (d) protection of personal data. This objective of providing access to data that is not accessible as open data may be seen as indicative of the emergence of a distinct regime for the data held by public bodies. The public sector bodies enabling the use of such protected data are required to be technically equipped to ensure that data privacy and confidentiality are fully preserved. The proposal does not interfere with the substantive rights on data as it refrains from prescribing a right of access or reuse but lays out certain harmonized rules and conditions guiding member states for establishing mechanisms for the reuse of publicly held data.



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## Competenties

Key resource for the success of companies is data. The volume of data generated grows from year to year, but is often not used for relevant decisions. Reasons for this include the high level of distribution and fragmentation of data, lack of resources, lack of interconnectivity of already established data infrastructures or simply inexperience or great respect for this important topic.

This is where DIO (dataintelligence.at) steps in. It strives to establish a data space in which a secure cross-departmental, cross-organisational and/or cross-sectoral data exchange takes place and the combination of relevant data along the value chain is efficiently enabled. The DIO network is made up of large companies, SMEs, EPU, start-ups and natural persons. It is precisely this diversity that is a great strength of the cooperation platform. All participants have one thing in common: they have recognised the need for a functioning data ecosystem in Austria.

Working groups, data spaces and use cases help to look at data challenges in a concrete and domain-specific way. Data spaces focus on superordinate domains (economic areas, industrial sectors or other specialised fields of application), with a decentralised data infrastructure on which data circles can build. In a data space, data is made available for potential innovative services while maintaining data sovereignty.

dataintelligence.at

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# Data-Driven Production and Business

Herbert Jodlbauer, Stefan Wagner, Roman Froschauer, Manuel Brunner

## Vision

The manufacturing industry is poised to undergo a transformation powered by data. Collaborating in highly connected value networks, companies are leveraging **data and analytics applications to boost productivity, create novel customer experiences, and enhance their societal and environmental footprint.** Such a value network can be defined as a dynamic structure consisting of an interconnected population of organizations, including small businesses, large corporations, intermediaries, universities, research centres, public sector organizations, and other parties that influence the system.

In order to achieve the vision of hyperconnected value networks, manufacturers need to utilize a diverse range of data and analytics applications, such as prescriptive maintenance, advanced robotics, and supply network tracking and tracing. These applications rely on the crucial **data assets** that are the foundation of their operations. This data can be used to extract actionable insights through analysis of reports and dashboards, **forecast future outcomes** through advanced analytics of historical data, and enable self-optimizing systems through autonomous action powered by self-learning algorithms using both historical and real-time data.

Despite the fact that most manufacturers have embarked on their journey towards data excellence in manufacturing, many are still **struggling to fully capitalize** on its potential value. According to a 2021 survey of over 1300 manufacturing executives (World Economic Forum Whitepaper, 14.01.2021), only 39% have

been able to successfully scale data-driven use cases beyond the production process of a single product, thus achieving a clearly positive business outcome.

However, data generated from various internal and external sources pave the way for various **data-driven approaches** for **value-added businesses, manufacturing, and customers.** Data-driven approaches help to redesign and improve customer channels (platforms, on-demand solutions, on-demand service platforms, analytical engines for customers, digital components) and customer relationships (transactionally optimised, personalised with mass cost structure, etc.). To effectively use big data and data from multiple sources in manufacturing, the focus should be on **extending current analytics** to include all three types of data-driven methods and analytics: Descriptive, predictive,

- **Business Analytics**
- **Prescriptive Analytics**
- **Value Network**
- **Optimization**
- **Resource Efficiency**

and prescriptive. Furthermore, cross-organisational processes, the connection to the end-customer, and value networks have great potential to be optimised through data-driven methods and business analytics [1]. Our organization envisions a future where data is utilized to its fullest potential in both production and business environments. Specifically, the implementation of data mining, data analytics, and business analytics

methods should be emphasized to achieve this goal. To accomplish this, it is essential to (i) identify and understand potential use cases, (ii) analyse these cases, (iii) tailor and apply data-driven analytics methods, (iv) evaluate their effectiveness, and (v) disseminate the results in the sense of applied research, making them accessible to the broader community. Various use cases exist in production, ranging from production planning and control, predictive maintenance, optimization of parameter settings, visualization of complex issues, decision support, process simulation, and resource reduction [2]. Similarly, in value-added networks, ranging from optimization of orders, traceability of goods, networking of partners, monitoring of pollutant emissions (CO<sub>2</sub> footprint), intensification of **on-demand solutions, and ad-hoc networking** and organization all present potential use cases. Furthermore, consistent and comprehensive use of data has the potential to facilitate early recognition of customer needs, optimization of the product life cycle, development of circular economy models, identification of influencing factors in the value network, and fundamental optimization of sustainability.

## Approach

There are research gaps in the design of data-driven business models regarding the relationship between these partners. Arising questions are: How should data users utilise supply chain partners for data collection, generation, or analysis? According to which criteria should purchasing decisions be made on the basis of external data? For whom and in what way is data-driven value creation and capture carried out along the supply chain?

Consequently, traditional industry chains potentially lose relative importance since business can be carried out faster and often with more new opportunities. The developments have shown that consumers profit from an increased access to a vast selection of goods, which in turn will cause a restructuring and redistribution of profits among the stakeholders along the **virtual value chain**. Over time, more and more companies make use of **internet platforms** that allow them to integrate external customers and other stakeholders from a value network to boost the innovation of their business. However, the IT tools used on these internet platforms are not able to merge the content of multiple users in an adequate way, so

that the resulting business models suffer from a low level of quality. One approach is to ensure the improvement of these IT tools by learning from the existing data and identify unaddressed needs and create value for the users.

**Servitisation** is another forward-looking approach where manufacturers leverage their digital platforms for servitisation in an Industry 4.0 context. They call for further research on specific capabilities (e.g., digital analysis, network orchestration, value co-creation skills) that manufacturers need to manage platform-based service innovation systems and thereby improve the understanding of the **strategic dynamics of platform-based servitisation**.

Current literature suggests an active flexi-directional interlinkage between various physical items, parts, processes, and their software-based digital counterparts to foster the value network approach. In detail, we propose establishing **holistic real-time interoperability**, adapting processes actively, and building capable and secure IT and data infrastructures. Those interlinkages are the basis for swiftly reacting to changing environmental conditions and realising emerging opportunities, whether digital or physical.

By combining machine learning, optimization algorithms, and simulation, we push research in the area of **prescriptive analytics** in order to create software solutions to solve complex planning problems and to **support human decision makers**. As complex and multi-layered production systems are inherently highly dynamic, decision processes must deal with changing conditions reflected in stochastic and uncertain data. New **open-ended evolutionary optimization algorithms** that also include automatic learning enable the development of robust and adaptive optimization systems, which continuously learn by observing data from enterprise information and machine execution systems and recommend optimal actions [1]. Thereby, white-box machine learning techniques, such as symbolic regression, also enhance the interpretability of models and make them understandable to humans increasing the trust and acceptance of such systems [2].

## Impact

### Scientific Impact

The scientific impact for research is, that new methods are developed to better analyse the organisation, the structure and the interaction of value networks, and to optimise business decisions on the operational, tactical and strategic level. Due to the fact that value networks are multi-level and multi-layered, interpretable models and efficient algorithms are needed to analyse and optimise these networks in their complexity and to obtain trustworthy, applicable and robust results. The **newly developed models expand the methodological toolbox** of research and lay the foundation for further research in this area.

### Commercial impact

Companies are faced with the challenge of having to react to **customer needs** with the shortest possible response times (on demand). The economic impact of the models to be developed results from the fact that companies should be able to **predict** customer needs as far as possible. Furthermore, the models to be developed should support them in being able to **react ad-hoc** to changes in production. With data-driven models, companies should also benefit from optimising their production processes and making them **more sustainable** c. f. resource-efficient [5]. Consistent data models make it possible, with the corresponding domain knowledge available, to understand the past, shape the present and predict the future.

### Social impact

The greatest social impact is achieved by meeting **customer requirements** on demand and **reducing waste** in the sense of overproduction or unnecessary warehousing. The reduction of waste and the data-driven optimization of the production process enables a positive impact on society in terms of **sustainability**.







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## Competencies

The Center of Excellence for Smart Production (**CoE-SP**) is a distinguished network embedded within the **Upper Austria University of Applied Sciences**. Its primary objective is to undertake research and development initiatives in the field of smart production. Through collaboration and interdepartmental networking, CoE-SP promotes the exchange of information between the faculties of Hagenberg, Steyr, and Wels for both teaching and **research** and **development** (R&D) purposes. Pilot projects that focus on “**Innovative applications for the digitalization of production**” are carried out jointly with Upper Austrian companies. CoE-SP comprises eight **thematic fields**, namely, the Internet of Things, Business Analytics and Prescriptive Analytics, Human-Centered Technologies, Assistance Systems, Operations Management, Product Development, Additive Manufacturing, and Business Models. These thematic fields are seamlessly integrated into projects, forming a common **competence node**, which is essential for tackling the topic of smart production.

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# Data Quality

Johanna Schmidt, Krešimir Matković

## Vision

Data builds the basis for any informed decision in data-driven applications, ranging from statistical analysis, predictive analytics, forecasts, artificial intelligence (AI) model development, and cyber-physical systems. As such, data-driven approaches rely on a broad selection and collection of data to cover as many aspects of a studied phenomenon as possible. When collecting a large amount of data, techniques for efficiently storing and accessing these data become more and more important. However, in focus on collecting as much and as wide a range of data as possible, ensuring high data quality is often treated as a low priority or even completely neglected [1]. Yet, **high data quality** is a key requirement for accurate decisions and the development of digital tools supporting data-driven decision-making. Poor data quality today remains one of the main obstacles to deploying and carrying out data-driven operations like AI model development [2]. Even the most sophisticated AI algorithms can lead to unsatisfactory results and cause poor performance and failure when based on bad-quality data. For decisions to be accurate, data must also be accurate. Ensuring data quality is, therefore, essential for understanding and addressing biases present in the data to avoid perpetuating and amplifying these biases in automatically generated outputs. A diverse and representative dataset enhances a model's ability to generalize well across different situations and inputs, ensuring its performance and relevance across various contexts and user groups.

As one illustrative example, one may think of time-dependent data (e.g., time series data). Time-dependent data is an essential source of information for

computing forecasts and predictions. A common issue when dealing with forecasting data is the presence of missing values. Time series data might contain missing values for several reasons, including measurement failures, formatting problems, human errors, or a lack of information to record [3]. If prevalent, missing values can significantly impact a forecasting or prediction model's accuracy. Imagine a forecasting model to predict material demand in a manufacturing environment where certain materials are sold out or unavailable. There would be no production and usage data to record while the material is out of stock. As another example, AI-assisted predictive maintenance

- **Data Competence**
- **Data Science**
- **Data Quality**
- **Visual Computing**
- **Visual Analytics**
- **Data Visualization**

solutions depend on a large data pool representing different situations and possibilities (e.g., default operation, faulty production cycles, different environment conditions) to work effectively. Unfortunately, such a broad range of labeled data is hardly available nowadays [4], and small sample sizes and lack of diversity hinder the generalizability and accuracy of developed solutions.

Ultimately, maintaining data quality is critical to realizing the full potential of data-driven applications in delivering value and driving innovation. Being aware of this issue, analysts expend

excessive time and effort manipulating data and assessing data quality issues. The initial process of data preparation, whereby data undergoes manipulation of raw data into usable and workable formats, is currently the most work-intensive part of developing data-driven applications. It is fairly well known and an accepted fact that data preparation for modeling and analysis takes up to 80% of the total project time [5]. To quote Andrew Ng, Professor of AI at Stanford University and founder of deeplearning.ai, it can be said that *“if 80 percent of our work is data preparation, then **ensuring data quality is the important work of a machine learning team.**”*

Ensuring data quality requires human interaction. Many aspects of data quality, including correctness and completeness, can only be thoroughly evaluated by including domain knowledge in the process. Data visualization [6] and Visual Analytics [7] (summarized as Visual Computing) are established methods to allow humans to understand and interact with data. In this white paper, we propose research towards more closely including **Visual Computing** techniques in the **data quality evaluation and data preparation lifecycle** for data-driven decisions in production. This includes research on (i) Visual Computing methods for Big Data analysis, (ii) visual representations for data quality issues in large datasets, (iii) close coupling between input data and outcomes of data-driven approaches to understanding the influence of input data, and (iv) new measures for evaluating the value of data.

We aim at a close interplay between Visual Computing in the data-driven applications development process. Visual Computing builds a bridge between data and humans. It enables human users to interact with data, understand patterns and connections, and include their knowledge and insights into the development process. Visual Computing is crucial when working with data-driven applications, as visual means allow human designers to gain insights into the applications' behavior, performance, and operation.

The need for improved data quality in conjunction with improved visual interfaces is also stressed by the EU European Big Data Value Strategic Research and Innovation Agenda (2017):

- *“Data cleaning, integration, curation tools and services are required for data users to be able to differentiate noise from valuable data and to be able to integrate them and make*

*them ready for analysis processes. Methods for improving and assessing the data quality have to be agreed and curation framework and workflows delivered.*

- *In the data visualization domain, the tools that are currently used to communicate information need to be improved due to the significant changes brought about with the volume and variety of Big Data. Advanced visualisation techniques must consider this variety (i.e. graphs, geospatial, sensor, mobile, etc) of data available from diverse domains. Tools need to support capabilities for the exploration of unknown and unpredictable data.*

## Approach

Research about data quality has already started in the 1980s [8]. Since then, data quality is often associated with the **fitness for use** principle [9], which refers to the subjectivity and context-dependency of this topic. Several approaches tried to overcome the context-dependency and tried to develop unique, agnostic standards and measures for data quality.

Standards for data quality have been defined by the ISO/IEC JTC 1 (“Information technology”) subcommittee 7 (SC 7) on software and systems and engineering. SC 7’s working group 06 published several ISO standards for data quality from 2008 to 2015. These standards provide concrete data quality measures as well as an explanation of how to apply them (ISO/IEC 25012:2008). The standard defines the measurement of data quality as a set of operations having the object of determining a value of a measure and defines a set of normalized quality measures (between 0 and 1). In parallel, subcommittee SC 4 (“Industrial data”) of the technical committee ISO/TC 184 (“Industrial automation systems and integration”) published a data quality standard in 2015. Their standard defines prerequisites for the measurement and reporting of information and data quality (ISO 8000-8:2015(E)).

The *Data Management Association (DAMA)* defines data quality management as data quality analysis, improvement, and assurance [10]. Over the years, several different data quality management methodologies (often declared as frameworks or methods) have been proposed [11]. Existing methodologies generally follow different characteristics and emphases. However, four necessary

core tasks can be extracted from these methodologies: (1) state reconstruction, (2) data quality measurement, (3) data cleansing, and (4) the establishment of continuous data quality monitoring. Some methodologies include additional activities like monitoring data integration. State reconstruction describes the collection of contextual information on the observed data. Data quality measurement refers to automatic methods for data quality assessment. Data cleansing describes correcting erroneous data, including data standardization, de-duplication, and matching. Data quality monitoring describes the ongoing measurement of data quality and the permanent assurance of sufficient data quality. Data quality measurement is considered to be the most challenging step in the whole management process. One important question for data quality concerns metrics and measurements for (automatically) evaluating the quality of a dataset. Over the years, researchers proposed various classifications and evaluation mechanisms for data quality. As currently largely accepted concept is to refer to data quality as dealing with a multi-dimensional problem (i.e., having to consider multiple quality dimensions) [12]. Over time, the following four main dimensions [13] of data quality have emerged:

- **Accuracy:** Accuracy describes the closeness between data and the real-world phenomenon they are supposed to model. From the natural sciences perspective, accuracy is usually defined as the magnitude of an error.
- **Completeness:** Completeness defines the breadth, depth, and scope of information contained in the data.
- **Consistency:** Consistency captures the violation of semantic rules defined over data items.
- **Timeliness:** Timeliness describes how current the data are for the task at hand. Timeliness also refers to data update frequency and volatility (i.e., how fast the data becomes irrelevant).

A common metric to evaluate accuracy is dividing the data items considered to be “correct” by the number of data items that have been tested. Similarly, researchers define completeness by dividing data items that are considered “complete” by the total number of data items. Unfortunately, domain-agnostic methods for automatically calculating data item accuracy and correctness

are hard to find. In both cases, domain knowledge and knowledge about the context are required to formulate measurements for data items being “correct” and/or “complete.” The need for domain knowledge also applies to consistency, where domain knowledge needs to be encoded into rules to evaluate whether data items violate these rules. Timeliness can, in many cases, be evaluated based on the temporal domain.

Despite the existence of standards and metrics, the **evaluation of data quality** is still considered to be a highly manual task [14]. Since data quality dimensions require context and domain knowledge to be included in the evaluation, the question of combining this with automatic data quality assessment still needs to be sufficiently answered. The fact that data quality assessment is **still done manually** confirms the subjectivity and context-dependency of data quality mentioned at the beginning. As such, data quality assessment requires the inclusion of domain knowledge in the process, which requires keeping human users in the loop. Visual Analytics [7] uses data visualization approaches to allow human users to interact with data and develop and test data-driven models built from the data exploration process. As such, we propose **Visual Analytics** as the proper technology to **improve and ensure data quality** in the development process of data-driven applications [15]. Although Visual Analytics has already proven helpful for assessing data quality [16], for example, when working with time-dependent data [17] and for decision-making [18], the broad usage of visual tools for data quality assessment has yet to be achieved. Existing approaches are targeted towards concrete use cases and datasets or only cover some dimensions of data quality (e.g., only concentrate on accuracy), which neglects the multi-dimensional nature of data quality assessment [13].

We aim to develop Visual Analytics frameworks to empower humans to evaluate and assess data quality by incorporating their domain knowledge and experience. This includes (i) researching means for working with large amounts of data, as scalability is still considered a major issue in data analysis, (ii) researching visual techniques for analyzing the multiple dimensions of data quality, (iii) researching methods for visualizing and quantifying uncertainty from pre-processing operations, (iv) enhancing data quality understanding by researching new data quality metrics for heterogeneous data, and (iv)

improving system's interactivity (e.g., with natural language methods) to support humans in interacting with the data. We believe that, as such, Visual Analytics will serve as a key technology for data quality assessment in the future.

## Impact

Improving means for measuring, evaluating, and editing data quality have a direct and essential influence on data-driven applications. Data quality improvement supports effective manufacturing processes, enables **more accurate decisions** about the production process, empowers fraud detection, and improves the users' experience with data-driven applications. Despite the inherent challenges, the upside of improved data quality is enormous. Even minor improvements can yield substantial payoffs.

Visual Computing tools for evaluating data quality are increasingly necessary for **industry and commercial opportunities** since data are growing more extensive and complex. Poor data quality is considered responsible for costing organizations an average of \$15 million annually [19]. Production processes require reliable data to function optimally. When based on complete and accurate data, data analysis or predictive analytics are less risky for misinterpretation and poor decision-making, and analysis results can more reliably be trusted. With modern techniques that ensure high data quality, of collected data, analysts will spend less time searching for error correction information and manual correction steps. Companies are more likely to profit from the significant advantages of data-driven decisions, including an **improved understanding** of trends, new insights, and product improvements.

The potential **societal impact and opportunities** of better tools for data quality assessment and management are extensive and range from a better understanding of the importance of accurate data to a **better understanding of analytic results** and data literacy. Poor data quality in many cases comes from manual data editing tasks (e.g., text fields) where users have to manually curate data, where it can easily happen that mistakes are made. With easy-to-access Visual Analytics techniques for data quality curation, users would have the chance to quickly check data entries and better understand how edits influence the quality of the whole dataset. Visual Computing, applied to involve humans in the process, is a technique to bring knowledge about data and data quality to **all levels of the data curation workflow** in production processes.





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**Johanna Schmidt** leads the research group Visual Analytics at VRVis Zentrum fuer Virtual Reality und Visualisierung GmbH and coordinates the corresponding research area. Her main research focus is on information visualization and visual analytics of large time-series data. She works with interactive visual systems that can support tasks like data quality assessment, decision making, and predictive modelling.

**Krešimir Matković** is a senior researcher at VRVis who heads the research group Interactive Visualization and coordinates the research area Complex Systems. He is interested in extending visual analysis technology to challenging heterogeneous data, in particular to a combination of multi-variate data and more complex data types. Krešimir further focuses on developing a structured model for interactive visual analysis supporting a synergetic combination of user interaction and computational analysis.

Founded in 2000, the **VRVis Zentrum fuer Virtual Reality und Visualisierung GmbH** with locations in Vienna and Graz is today Austria's leading institute in the field of visual computing. This key enabling technology specializes in combining human capabilities with computers' strengths through innovative visualization methods for making large amounts of data accessible for effective workflows and complex decision-making processes. As a competence center funded within the COMET program, VRVis and its about 70 employees work in close collaboration with national and international partners from science, industry, and business. In the course of more than 50 successful research cooperations, a large number of customized technology solutions have already been developed, among others in the fields of visual data analytics, artificial intelligence, XR, digital twins, and simulation.

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# Secure Prescriptive Analytics – Combining Data- and Simulation-based Models

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## Vision

In the wake of the current digital transformation, today’s cooperations produce a considerable and growing amount of data in various ways. Leveraging these data sets is becoming increasingly important for companies to gain a competitive advantage [1]. Business analytics is an efficient process to derive insights from data and drive proper decisions and actions to stakeholders [2]. To derive human-understandable insights, business analytics utilizes machine learning, statistical analysis, predictive analytics, and explainable AI techniques to analyze and transform data into better interpretable models. These models are capable not only of identifying outcomes and anticipating trends, but also providing meaningful insights and supporting decisions. Prescriptive analytics as an interdisciplinary method deals with the determination of decisions and is consequently referred to as the engine of digitization. This involves looking from the past (“What happened? Why did it happen?”) and present to the future (“What will happen?”): Building on the first three stages of analytics (descriptive, diagnostic, predictive), the established analytics techniques are coupled with simulation and optimization to support decision making which is recently considered as the fourth stage - prescriptive analytics, see Figure 1. Recently, research on PA is increasing [3].

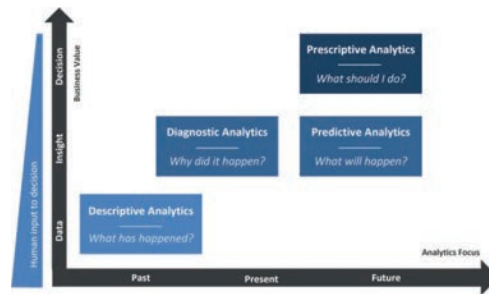


Fig. 1. Four stages of business analytics. Prescriptive analytics is focused on the future and has the highest business value.

- **Prescriptive Analytics**
- **Privacy Preserving Machine Learning**
- **Symbolic Regression**
- **Interpretable Deep Learning**

Our goal is to develop a comprehensive framework that makes the methods broadly applicable while reducing the process time and achieving better results. A central aspect of the concept is the modeling of real systems. In this context, variable and hierarchical mappings are developed that enable an accurate, yet fast analysis of data. The modeling concept allows the integration of new or additional data sources to further increase prediction accuracy. To promote trust in this technology, the employed methods must be adapted to preserve the confidentiality of the data and to promote technological trust. By this means, we label our approach Secure Prescriptive Analytics.

Another aspect is the interpretability of the generated models. These must be

understandable and comprehensible to humans to create the possibility of deriving new domain knowledge, leading to a feedback loop. For example, incorporating new knowledge of how systems work leads to improvements of predictive accuracy. Overall, Secure Prescriptive Analytics is a promising vision that has the potential to improve decisions and confidence in those decisions in various areas, e.g., industry, commerce, banking, etc.

## Approach

In the analytics domain prescriptive analytics builds upon the descriptive, diagnostic, and predictive stages which are coupled mainly with modeling and optimization in order to support prescription. Modeling, for example in the form of a simulation, is used to digitize processes and workflows, while machine learning in the predictive phase maps facts captured in data from the past and present into the future. Optimization processes calculate the best possible decisions for the future under the given framework conditions and assumptions. However, a serious and comprehensive treatment of prescriptive analytics is only possible if it builds on the descriptive, diagnostic and predictive phases. This means that only the interaction of the wealth of methodological competencies as well as the associated methodological research with simulation and optimization components allows the topic of prescriptive analytics to be dealt with in the required breadth and depth. This methodological breadth includes, among others, the research field of simulation ("Digital Twin"), optimization (respectively operations research), process mining, machine learning (white-box modeling, interpretable deep learning), simulation-based optimization and surrogate models.

Data-based methods pose a particular challenge when dealing with corporate data, as they require a large amount of data, special hardware and tend to be computationally intensive. This hardware is usually not available locally to every user (e.g., a manufacturing company), which is why company-internal data is transmitted to data centers. To ensure the trustworthiness of the data, privacy preserving methods are necessary. They ensure, during data processing, that no conclusions can be drawn about its owner. An additional aspect is that some machine learning approaches can be reverse engineered to reconstruct data. On the one hand this poses a threat to the underlying business model and on

the other hand, it poses a threat to any information worth protecting that may be contained in the data. In practice, users also want or need to understand how the results of data-based models come about, e.g., what relationships in the inputs (e.g., temperature, pressure) can be determined and what effect they have (e.g., quality of the product). Only through this understanding can confidence in the processes be established. Machine learning approaches, such as white-box or interpretable deep learning, fundamentally enable the necessary interpretability of models, however they still leave room for improvement. On the technical level, for example in the transmission and storage of data, it must be ensured that no data can be recorded by unauthorized third parties. These aspects are summarized in the context of this application under the term "secure".

As the recent work of [4, 5] underpins, only the amalgamation and integration of those methods will lead to Secure Prescriptive Analytics. Hybrid modeling is intended to achieve a closer coupling between the generation of classical simulation models and data-based, machine-learned models. In particular, the resulting methods allow for more efficient, trustworthy and confidence-building modeling. Hybrid modeling can deal with the system models with the following variants (Figure 2):

- Variant 1 (V1): Development of a classical simulation model by analyzing existing data and mapping processes e.g., as discrete-event simulation by experts (e.g., software engineer or domain expert).
- Variant 2 (V2): Development of a data-based model by applying machine learning techniques on the available, consolidated and pre-processed real-world data (e.g., material, sensor, process data).
- Variant 3 (V3): Development of a surrogate model, i.e., a representative of the simulation model, based on the input and output data of many experiments with the simulation model using machine learning techniques.
- Variant 4 (V4): Generation of additional, synthetic data (e.g., for rare events) using simulation experiments (see variant 3) to fill in missing aspects of an existing real-world data set. Subsequently apply machine learning techniques for model development.

- Variant 5 (V5): Mapping of one or more system components as a process model using process mining methods. The automated derivation of a simulation model based on the created process model.
- Variant 6 (V6): Integration of domain knowledge using process mining. To generate machine learning models, data and the collected processes are used as a basis.

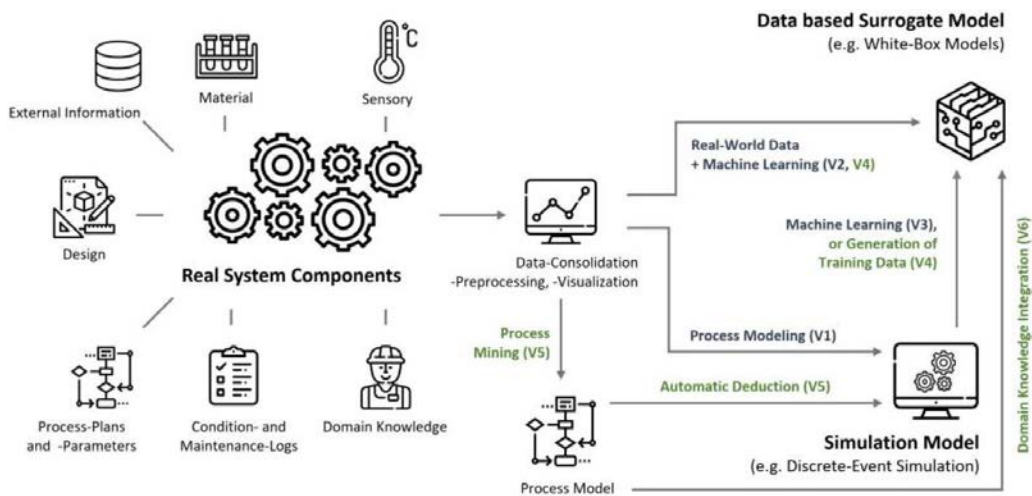


Fig. 2. Variants for modeling real system components.

Like an organizational chart that hierarchically structures a company, Secure Prescriptive Analytics pursues the idea of first breaking down complex systems (e.g., technical production facilities, supply chains, etc.) into smaller system components and then modeling them. The developed models are connected and summarized over several levels to ever more extensive subsystems and ultimately result in the overall system being represented. In this hierarchy, the modeling variants (V1-V6) are applied. To allow fast evaluation of complex simulation models, surrogate/representative models are trained and used whenever appropriate (speed versus accuracy).

## Impact

Systems are modeled using the concepts presented above using different modeling methods. This phase results in a hierarchically structured system model with several, possibly different, complex model variants per component. Finally, this system model is integrated into an optimization process as a fitness function in the prescriptive analytics concept. Figure 3 shows an example of SPA in a production planning use case. Here, the SPA platform optimizes the production plan according to the actual state of the real-world and predictive models, which provide information about different aspects in the system, e.g., wear and tear.

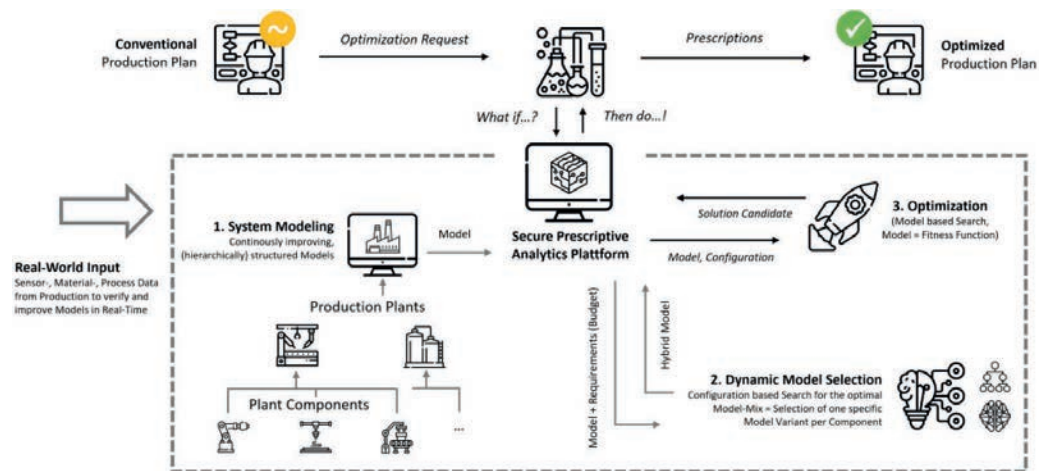


Fig. 3. An example of SPA for production plan optimization; the dashed rectangle represents the SPA environment.

Due to the constantly increasing amount of data which accumulates over time, better representative models can be developed over time. Suppose the surrogate models meet the accuracy requirements during the optimization request. In that case, they can replace more complex simulation models, saving time. Consequently, it is also possible that better or simpler proxy models will replace the current proxy models as the process progresses. Furthermore, due to the comparatively short time required to evaluate a simplified proxy model, the optimization can be accelerated, resulting in new potentials:

- More powerful optimization methods can be used.
- A better-quality result can be achieved for existing tasks.
- More complex tasks (e.g., optimization of overall company processes: production, logistics) can be tackled and solved.



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## Competencies

A software prototype currently being developed implements a Secure Prescriptive Analytics platform. This platform is made freely available in the form of open source. The Upper Austria University of Applied Sciences Campus Hagenberg (FH Hagenberg), Software Competence Center Hagenberg (SCCH), and RISC Software GmbH (RISC) bundle their research competences privacy preserving machine learning, explainable machine learning, simulation, as well as optimization within this project.

Further information is available at <https://www.secureprescriptiveanalytics.at/>.

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# Securing Supply Chains with Blockchain Technology

Alexander Eisl, Stefan Craß

## Vision

**Blockchain technology** has been making waves in various industries, and the production sector is no exception. A blockchain is a special form of distributed database ("**distributed ledger**") that can securely and transparently record transactions and data (Nakamoto 2008). In production processes, Blockchain-based solutions enable all parties involved to track and trace goods and materials from the point of origin to the final destination. This **transparency** helps to prevent fraud, counterfeiting, and other forms of malpractice. Additionally, blockchain technology can help to reduce paperwork, streamline processes, and increase efficiency. Overall, blockchains are a very useful technology for securing process data in supply chains.

From a more technical perspective, each computer node in a blockchain network contains a copy of the ledger. The participating nodes communicate without a central server in the form of a "**peer-to-peer**" network. By using **cryptographic processes** based on digital signatures and hash functions, blockchains allow the creation of a trustworthy decentralized database in which data can be transparently stored in a way that is immutable for potential attackers. A **consensus mechanism** is used to ensure that all nodes have the same view of the data and that a consistent state is achieved.

One key advantage of this network approach is **decentralization**, which not only enables software architectures **without a central server** or a "**trusted third party**" but also ensures **automatic data replication**. This guarantees the resilience of the system, so that even if individual nodes fail, the blockchain as a whole continues to function (**no**

**single point of failure**). Furthermore, it creates a maximum in transparency and **traceability of transactions**. Originators, timestamps, and contents of all transactions as well as their sequence are clearly visible and verifiable for all involved parties. Additionally, the cryptographic protection mechanisms of the blockchain guarantee the **immutability** and **forgery protection** of the data. Trust in the distributed database is thus greatly increased compared to central databases which are controlled by individual companies and can be vulnerable to hacker attacks,

- **Blockchain**
- **Distributed Ledger**
- **Supply Chain Management**
- **Internet of Things**

among other things.

The addition of "**smart contracts**" [4], which are decentralized computer programs that can automatically enter data into the blockchain in response to certain events, enables **business process automation**. For example, payments can be released as soon as the receipt of a delivery is confirmed. This automation can reduce transaction costs, speed up the production process, and improve accuracy. Smart contracts execute the actions according to their clearly defined set of rules based on the data stored in the blockchain, enabling the coordination of partners even without mutual trust and without a neutral authority acting as a trusted third party. Blockchains are also characterized by their high **flexibility**. They form a generic basic infrastructure that can store any transaction data and can be adapted to specific requirements

at any time using smart contracts.

Despite the novelty of this technology, these benefits are already being recognized by the industry, as demonstrated by a recent analysis of the World Economic Forum: “The emergence of blockchain technology holds great promise for supply-chain organisations, perhaps as much as any new development in the industry’s infrastructure since it switched to standardised containers decades ago. The case for blockchain is stronger as the COVID-19 pandemic underscores the need for more resilient global supply chains, trusted data and an economic recovery enabled through trade digitization. At the same time, blockchain may engender a fair share of puzzlement and anxiety among supply-chain leaders unfamiliar with it as a new and unfamiliar digitisation tool.” [10]

Our vision is **to investigate potential applications of blockchain technology in industrial applications**. One major focus point of our research is the **design, prototypical implementation, and evaluation of blockchain-based solutions** that have the potential to increase transparency and efficiency within supply chains by enabling the secure tracking of goods and process steps. A second focus point is the investigation of the **secure integration of blockchain technologies with the Internet of Things (IoT)** by means of trustworthy and reliable sensors (e.g., for plant monitoring or cargo transport). This next logical step of the Industry 4.0 concept benefits not only the companies involved, but also regulators and authorities, for instance when checking whether raw materials come from legitimate suppliers. Additionally, we plan to address and solve problems related to shortcomings of current blockchain-based solutions with regard to **scalability, efficiency, sustainability, usability, security, privacy, and data protection**.

As an **interdisciplinary research center**, we are not only interested in **technical challenges**, but also in the analysis of **economic and legal perspectives** of production use cases. We analyze how supply chains can be improved by integrating the three value streams (physical goods, information, and money) using blockchain concepts. In addition, we are also researching relevant **business models, incentive schemes, and regulatory frameworks**.

## Approach

Fifteen years after the seminal white-paper on Bitcoin [9], blockchains are still an evolving technology. There are currently well over 1,000 different blockchains, as well as related technologies, generally referred to by the term **“distributed ledger technology” (DLT)**. The underlying protocols of these systems can vary widely. While the first generation of blockchain technologies (e.g., Bitcoin) was mainly focused on decentralized currencies, second-generation blockchains like Ethereum added decentralized computation via smart contracts [4]. The newest group of blockchain protocols (sometimes termed **“Blockchain 3.0”**) aims at providing practical feasibility for diverse use cases by means of increased scalability, sustainability, cost-effectiveness, privacy, and security.

Current research challenges for blockchain technologies include the efficiency of consensus mechanisms, limitations regarding performance and scalability, privacy concerns, re-centralization aspects, interoperability, attacks on blockchain integrity, and smart contract security [3,6,8]. Important design decisions for specific blockchains may, however, suffer from technological bias of the respective developer teams and other project stakeholders involved. **Independent scientific research**, as provided by our research center, can **help to identify potential challenges and suggest innovative solution approaches**.

For example, one important challenge with blockchains is the **inefficiency** of the used consensus protocols, which are sometimes based on the so-called **“proof of work”** method. This approach generally requires a lot of computing time of the nodes involved (and thus energy). This is normally also associated with high transaction fees and long waiting times until a transaction is confirmed. In contrast, many modern blockchain technologies now rely on alternative consensus protocols (e.g., **“proof of stake”**) that are not affected by these problems. Another alternative to the efficiency challenge are so-called **“permissioned blockchains”** (or **consortium blockchains**) like Hyperledger Fabric [5], which define access restrictions to the ledger. In this case, reading and/or writing is only possible by certain, clearly defined persons or systems. In contrast to “public” blockchains, in which participants can only be identified by their public key and thus remain (mostly) anonymous, all participants are

known in permissioned blockchains. This restriction allows more efficient consensus algorithms to be used. In addition, it is also possible to selectively share data only with certain partners. In our research, we try to identify the **best blockchain for particular use cases**, while incorporating also economic and legal perspectives.

In the past few years, blockchain technologies have been evaluated for use in several application domains outside of the classical finance use cases for which they were originally designed. This includes applications for tracking goods and processes within a supply chain [10] or for secure data storage in industrial IoT scenarios [7]. In such use cases, privacy and data protection requirements are often critical, but are also in conflict with the transparency and immutability properties of blockchain-based systems. In our current research, we are investigating different application scenarios specifically related to the production sector:

- **Due diligence in supply chains** [1]: Suppliers can document compliance with human rights and environmental regulations by securing process data on a tamper-proof blockchain, which can then be validated by other companies along the value chain as well as auditors and public authorities.
- **Circular supply chains** [2]: Using a smartphone app for consumers and unique QR codes, recyclable plastic bottles can be tracked and traced on a blockchain to monitor their lifecycle. As an incentive for their participation in the recycling process, consumers are rewarded with a special token, which can be seen as an application-specific cryptocurrency that can be redeemed for useful rewards (e.g., the chance to win non-cash prizes).
- **Data integrity for sensor networks:** To prevent retroactive tampering with sensor measurements in industrial settings (e.g., to obfuscate incorrect handling of a consignment in a food supply chain), sensor data can be secured using a blockchain. For increased efficiency and data protection, only hash values (i.e., “digital fingerprints”) of the sensor data are actually stored on-chain.

Open research challenges related to these topics include the definition of **secure interfaces between the physical world and its digital representation** and the analysis of **tradeoffs between data transparency**

**and privacy**, as well as the design of **highly scalable** blockchain-based solutions, suitable **incentive schemes**, **interoperability** mechanisms, and fair **governance** frameworks.

Regarding research methods, we typically start projects with a systematic analysis of the economic, legal, and technical context. During the requirements analysis phase, our methods include literature and market research, stakeholder workshops, data analysis, threat modeling, simulation, and process modeling. Based on the identified requirements, we use established software engineering methods to develop a **prototypical implementation**, which is subsequently evaluated from a qualitative and quantitative perspective (e.g., validation by stakeholders and benchmarking).

## Impact

The **scientific impact** of our ongoing research lies in the continuous improvement of blockchain-based protocols for supply chain applications with regard to key factors like efficiency, interoperability, security, and privacy. Blockchain technology enables end-to-end traceability and transparency of products in a trustless environment, while facilitating secure and efficient transactions via smart contracts. We will continue to look for additional use cases that may benefit from this decentralized approach.

**Benefits for industry** may include efficiency gains, reduced costs, increased trust in received data, transparent access to data across the entire value chain, simplified audits by third parties, and independence from central service providers. Additionally, blockchain-based token systems may provide new financing options for companies and reward programs for customers. New business models enabled by the technology provide chances for innovative startups as well as established companies.

Regarding the **societal impact**, the transparency provided by blockchain (e.g., in the form of origin and quality certificates) can increase the trust of customers in the involved companies and their products. This may also raise awareness and thus indirectly improve sustainability and working conditions within some supply chains. Due to their democratic governance approach, decentralized blockchain architectures can also help to avoid a concentration of power in the hand of individual companies or governments, which could otherwise lead to problems like censorship.



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## Competencies

ABC Research GmbH is an **application-oriented research organization** operating the Austrian Blockchain Center in the **COMET program** since 2019. It forms a **network of national and international scientific institutions, companies, and associated partners**. The center has expertise in all areas relevant to the application of blockchain and distributed ledger technology: computer science, mathematics and cryptography, management and economics, engineering, data science, and law. The Center's mission is to be the **one-stop-shop Austrian Research Center for Blockchain (and related) technologies** to be applied in industrial applications like industry 4.0 / IoT as well as financial, energy, logistics, government, and administrative applications.

Within the COMET program as well as nationally funded research grants, we are currently researching several topics related to supply chain management, IoT, and circular economy. We are also part of the **European Digital Innovation Hub (EDIH) “Applied Cyber Physical Systems”**, where we provide blockchain-based support services for small and medium enterprises.

Additional information can be found on our website: [abc-research.at](http://abc-research.at)

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## Keywords Index

## 1-9

**3D Printing** 21, 28, 37, 42, 59, 60, 70-72, 74, 102-104, 115, 119, 134, 147, 153-154, 158, 163-164, 186-189, 222, 236, 238

**5G** 294-296, 297-298

**6G** 5, 7, 9-10, 12, 294-298

## A

**Accounting, Ledger** 18, 86, 354-355, 358

**Actuator** 54, 158, 166, 186, 188-189, 251-253, 256, 266, 285, 294

**Additive Manufacturing** 36-37, 39, 58-60, 62, 70-75, 102-104, 134-135, 139, 158, 162-164, 168, 208, 211, 229-230, 232-233, 235, 340

**Agriculture** 10, 12, 92, 237, 317

**AI** > Artificial Intelligence

**Alloy** 11, 13-14, 71, 74, 123, 162-165, 165-166, 1169, 180-185, 211, 235-237, 241

**Architecture, Building** 59, 71, 76, 112, 124, 126, 144, 158, 200, 212, 276, 287

**Artificial Intelligence (AI)** 5, 7-8, 10, 12, 19, 28-29, 31, 33, 42, 46, 57-59, 64-69, 77, 93, 95, 138, 152-154, 156, 163, 166, 202-206, 235-236, 244-245, 247, 249, 250-255, 257-260, 263-265, 268, 271, 276, 283, 290, 295-296, 304, 313, 315, 317, 330, 333, 335, 342-343, 346-348

> Green AI, Deep Learning, Machine Learning, Neural Network

**Auction** 36, 38

**Augmentation** 85, 245-246

**Authentication, Identification** 28, 85, 129, 176, 253, 285, 337

**Automation** 9, 13, 20, 25-26, 28-29, 31-32, 51, 59, 64-65, 67, 98-99, 118, 152-153, 155, 157, 163, 215, 245, 265-266, 269, 276, 278, 280, 295, 297, 299, 313, 316-317, 324, 343, 354

## B

**Banking** 349

**Batch Size, Lot Size** 52, 156, 207, 250, 266

**Battery** 92-93, 95, 191, 195, 205, 283-287

**Biocatalysis** 112, 116, 128-129, 132-133

**Bioeconomy** 116, 133, 146

**Biopolymer** 112, 114, 147-148

**Biorefinery** 146-147

**Biotechnology** 112-113, 115-117, 131-132

**Blockchain** 134, 136, 139, 354-359

**Building, Architecture** 59, 71, 76, 112, 124, 126, 144, 158, 200, 212, 276, 287

**Business** 5-6, 9, 11, 14, 18-19, 25-26, 29, 35, 49-51, 59, 64, 73, 84, 88, 90-91, 98, 134-135, 138, 141, 152-153, 155, 157, 159, 166, 168, 196, 205-206, 251, 260, 264, 276-278, 280, 284, 287, 295, 301, 305, 330-332, 336-338, 340, 346-349, 353-355, 357

## C

**Catalyst** 86, 94, 113, 118-119, 121-123, 133

**Chemistry, chemical** 10-11, 13-14, 72, 77, 84-86, 88-97, 92, 96, 104, 106-110, 112-113, 116-118, 122-123, 128-131, 132-133, 146-147, 154, 158, 162-165, 168, 170-175, 180, 187, 189, 200, 207-208, 215, 218-220, 222-223, 229, 235-237, 240-241, 291-292, 306-307, 327

**Circularity, circular** 5-6, 18, 29, 41, 43, 77, 89, 91, 98, 107, 119, 128, 135, 141-142, 146, 154, 158, 202-203, 205, 218, 220, 276, 316

**Climate** 33, 56, 59, 68, 69, 82, 85, 98, 99, 101, 120, 123, 127, 135, 141, 144, 146, 147, 149, 150, 155, 182, 194, 298, 304, 307

**Cloud** 35-37, 39, 42, 154, 159, 253-254, 266-267, 278, 296, 313, 317, 330

**CO<sub>2</sub>** 5-6, 10-11, 13, 20, 31, 37, 68, 70, 76-78, 92, 94, 97, 106-112, 114-115, 117, 128-129, 131-132, 140, 142, 145, 180, 190-191, 193, 195, 203, 118, 220, 234, 237, 254, 306-308, 337

**Coating** 117-119, 122-123, 148, 153, 158, 172, 187, 189, 200

## D

**Decarbonisation, decarbonize** 26, 106, 152, 205

**Deep Learning** 26, 65, 85, 245-246, 248-249, 253, 292-293, 295, 348-349

**Degradability, Degradation, degradable** 86, 93, 123, 147, 169, 192, 197, 218-220, 222-223, 234, 246

**Design** 2, 6, 8, 11, 14, 18-21, 23, 26-31, 34, 36-37, 40-46, 51-53, 58-60, 71-75, 85-88, 91, 93-100, 102-103, 124, 129, 132-133, 135, 140, 148, 152-154, 157-159, 162-164, 174, 176, 180, 188, 197, 199-200, 202-205, 207-211, 213, 215, 220, 222, 224-225, 228-229, 233-238, 240-241, 244, 247, 251, 255-256, 260, 271-272, 275, 277, 279, 284, 286-287, 297, 306-307, 318-320, 322-325, 331, 337, 347, 355

**Diagnostics** 186, 270

**Digitalization** 13, 23-29, 36, 56, 84-85, 88, 91-92, 112, 134, 155, 177, 203, 206, 213, 216, 250, 259-260, 264, 277-278, 312, 317, 340

**Digital Twin** 8, 18, 23, 65-66, 84-85, 88, 90, 92-94, 98, 203, 206-207, 216-217, 277, 290, 317, 323, 349

## E

**Ecology, Eco** 10, 12, 16, 17, 18, 19, 51, 52, 90, 91, 104, 105, 106, 107, 130, 132, 140, 141, 195, 221, 253, 281 > Green

**Economy, economic** 5-6, 8-9, 10-14, 14, 18, 20-21, 23-25, 27, 29, 31, 37-38, 40, 42-43, 49-50, 56, 59, 65, 70, 76, 84, 88-90, 92-93, 98, 103-104, 106-109, 111-112, 114, 118-119, 124, 126, 128, 131, 134-135, 137-142, 146, 148-149, 152-156, 157-159, 166, 173-174, 190, 193, 195, 202-203, 205-207, 212, 215, 218-220, 224, 234-235, 263, 279, 297, 312, 333-334, 236-238, 241, 250, 267, 276, 289, 330, 337, 355-356, 358-359

**Edge AI/Computing/Processing** 7, 9, 35, 64, 150, 152-155, 157-159, 195, 244, 253, 288-289, 292, 295-297, 313, 315, 317, 330

**Education** 5, 8, 24-29, 42, 51, 56, 58-59, 62, 77, 92, 124-126, 170-171, 200, 215-216

**Efficiency, efficient** 6-8, 10-14, 20, 25-26, 31, 37, 47, 65, 71-72, 77, 86, 91, 93, 108, 123, 129, 141, 148-150, 153-154, 158, 191, 195, 236, 247, 256, 259, 261, 278, 283, 289-290, 292, 295-296, 313, 319, 355-356

**Elastomers** 224

**Electrolyser** 107

**Electronics** 11, 13-14, 19, 43, 58, 60, 102, 138, 153-154, 158, 173, 186-189, 196, 199-201, 238, 249, 251, 255-256, 268, 276, 282, 287, 299

**Emotion, emotional** 42, 253, 255

**Energy** 6, 10, 12-15, 20-21, 25-26, 30-31, 38, 43-44, 47-49, 56, 64, 67-68, 76-77, 90-95, 99, 106-112, 118-123, 128, 130-131, 133-134, 140-142, 144, 150, 153-158, 163-166, 170, 172, 176, 180, 190-193, 195, 200, 202, 205-207, 212-213, 215, 218, 224, 226, 230, 234, 236-237, 241, 247, 250-251, 253-254, 255-256, 271, 275, 282-283, 285, 287-292, 294, 297, 300, 303, 306-308, 310, 313, 355, 358

**Engineering** 7-8, 21, 24-29, 32, 35, 39, 51, 58-59, 62, 67, 79, 84, 86, 91-100, 104, 110, 112,

116, 118, 122, 124, 128-129, 131-133, 141, 144, 146, 148, 150, 162, 164, 168-169, 178, 180-182, 185, 190, 195, 202-205, 208-211, 215, 222, 224-226, 228, 233, 235-236, 241, 245-246, 248-249, 257-262, 264-265, 272, 275-281, 288-289, 297-298, 305-306, 310-311, 317-318, 320, 322, 324-325, 343, 356, 358

**Ensembles** 251-252

**Environment, environmental** 5-8, 10-15, 18-21, 24, 26-27, 30, 37-38, 40-43, 46-50, 53-54, 56, 64, 66-67, 69, 79, 86-87, 89-90, 92-93, 95-96, 106, 101, 110-111, 113, 116, 118, 122, 128, 131, 135, 137-138, 146, 148, 153, 155-157, 158-159, 166, 170-171, 181, 186, 188-189, 192, 196, 199-200, 202, 208-209, 215, 218-220, 223, 226, 234, 245-248, 250-254, 256, 263, 266-267, 270-271, 278, 282-283, 285-287, 289, 296, 298, 307, 310, 312, 314, 319, 336-337, 342, 351, 356-357

**Enzyme** 113-114, 116-117, 128-132

**Exoskeleton** 52, 54, 56-57

**Explainability** 65

## F

**Factory** 18-21, 23, 26-27, 30-35, 51, 99-100, 111, 115, 216, 295, 298-299

**Fatigue** 26, 163, 182, 196-201, 208-211, 232

**Fermentation** 112, 114-116

**Finances, financial** 11, 13, 90, 135, 139, 153, 358

**Food** 10, 12, 25, 86, 90, 92, 112, 114-115, 175-176, 212, 251, 312, 315-316, 356

**Fuel Cell** 118, 120-123, 186, 205

## G

**Gaia-X** 330

**Geo-Energy** 306

**Green AI** 250, 253-254

**Green Chemistry** 112-113, 117, 133

**Green Engineering** 124

## H

**Health** 10, 12-13, 20, 52, 54-55, 59, 65, 92, 109, 113, 131, 174, 186, 189, 205, 212, 238, 244-249, 251, 272

**Human-Computer** 46, 51

**Human-Robot** 48-49, 266

**Hydrocarbon** 106-107, 108

**Hydrogen** 13, 74, 77-78, 94, 97, 106-111, 121-123, 129, 131-133, 162-164, 166, 168, 191, 193, 195, 205, 207, 224-225, 227, 237, 241, 306-307

## I

**Identification, Authentication** > Authentication, Identification

**Industry, industrial** 5-15, 18-24, 25-29, 31, 40-44, 46-56, 59-60, 64-65, 67-68, 71, 73, 74, 76-80, 84-86, 88-96, 98-103, 107-113, 112, 114-115, 121-123, 128-132, 134-141, 143, 147-148, 152-155, 157-159, 164-166, 168, 170-171, 173-175, 177, 180-181, 183, 186-187, 189-193, 195-196, 199-200, 202-203, 205-206, 210, 215-216, 222, 224, 226, 231-232, 237, 240, 244-249, 251, 253-258, 260-268, 276, 279, 281-284, 286-288, 291-292, 295-299, 305-306, 310, 312-313, 315-316, 330, 334, 336-337, 343, 345-347, 349, 355-359

**Inelasticity** 324

**Infrared** 110, 172, 288-289

**Interconnects** 196-198, 236  
**Interdisciplinary** 8, 26, 40, 42-43, 51-52, 58-60, 62, 77, 100, 109, 144, 153-155, 170, 174-175, 237, 259, 271, 279, 348, 355  
**Industrial Internet of Things (IIoT)** 5, 7, 12, 35, 159, 202-203, 205-207, 312-313, 315-316, 359  
**Interaction** 40-47, 51-52, 54, 99-100, 116, 154, 162, 164-165, 170-171, 175, 180-181, 187-189, 208, 229, 245, 251-253, 255-257, 267, 271, 276, 278, 291, 307, 318, 323, 338, 343, 346-347, 349  
**Interface** 36, 40-41, 44, 46, 51, 146, 148, 181-182, 190, 201, 230, 235-236, 259, 277, 287, 323  
**Internet, WWW** 7, 19, 31, 46, 58, 134-135, 153, 159, 181, 186, 202, 236, 244, 250-252, 257, 270-271, 274-276, 282, 294, 299, 312-313, 316-317, 337, 340, 354-355, 359  
**Internet of Things (IoT)** 7, 10, 12, 19, 31, 46, 58, 134, 153-154, 159, 186-187, 189, 202, 236, 244, 250, 252, 256, 270-271, 274-276, 282-285, 287, 294, 299, 312-313, 316-317, 340, 354-356, 358-359

## L

**Ledger, Accounting** 18, 86, 354-355, 358  
**Life Cycle** 18, 87, 90, 149, 190, 224, 231, 238, 251, 278-279, 289, 337  
**Life Science** 174  
**Localization** 68, 135, 270-271, 275, 285, 287, 296-298  
**Logistics** 15, 27, 30, 38, 52-53, 64-65, 67-68, 98-100, 139, 251-252, 254, 264, 271, 300, 304, 351, 358  
**Lot Size, Batch Size** > Batch Size, Lot Size

## M

**Machine Learning** 8, 29, 31, 41-42, 46, 78, 85, 93, 95, 128, 154, 163-164, 205, 207, 215-216, 235, 244-248, 251-253, 255-257, 259, 261, 263-264, 267, 271, 274, 276, 283-284, 292, 295, 300, 302, 318-319, 322, 330, 337, 341, 343, 347-350, 352  
**Machinery** 10, 12-13, 28, 35, 43, 52, 212, 215-216, 253, 276, 284  
**Maintenance** 7-8, 11-12, 14, 24, 26, 47, 52, 60, 65, 156-157, 162, 203-204, 206-207, 212-213, 244, 248, 255, 258-259, 262-263, 265, 276, 282-284, 287, 336-337, 342, 347  
**Management** 10, 12, 18-19, 21-22, 25-28, 30, 33-34, 38, 44, 47, 51, 58, 65, 67, 85-86, 88-89, 92, 95, 99-100, 110, 134, 138-139, 142, 146, 154, 157-158, 168, 176, 186, 203, 215, 224-226, 248-249, 251, 253, 255, 257, 265, 277-278, 281, 283, 295, 300, 304, 310, 313-314, 340, 343-345, 347, 353-354, 358  
**Manufacturing** 5-10, 12-15, 18, 20-21, 25-26, 28-33, 35-39, 42-43, 46-52, 54, 56, 58-60, 62, 64, 66-67, 69-75, 90, 98-104, 116, 118-121, 123, 134-139, 141, 152-159, 162-164, 168-170, 177, 199, 202-206, 208-209, 211-212, 222, 225, 229-233, 235, 238, 250-266, 271, 276, 278, 282-284, 287-288, 290, 295, 297, 303, 318, 322, 324-325, 330, 336, 340-342, 345, 347, 349  
**Market, Marketplace** 7-8, 11, 14-15, 20-21, 25, 31, 33-35, 40, 42-43, 45, 48, 59, 70-71, 73, 84, 88, 90-91, 115, 128, 134-135, 142, 148-149, 152, 155, 173, 178, 180, 190, 195-197, 199-200, 236, 244, 255, 262, 277, 282, 284, 295, 332, 335, 356  
**Material** 8, 14, 26, 30, 70, 74, 76-77, 85, 88, 91, 141, 147-148, 153, 162-163, 165, 174, 176, 180-182, 204, 215, 224, 228-230, 234, 236, 250, 288, 325-326  
**MEA (Membrane Electrode Assembly)** 118-119  
**Mechanics** 144, 233, 241, 276, 306, 311, 324-325, 327, 329  
**Media Technologies** 46-47  
**Medicine** 71, 90, 158, 218, 248, 320

**Metal** 62, 66, 68, 69, 70, 72, 94, 95, 99, 100, 101, 106, 150, 154, 155, 156, 160, 162, 172, 176, 179, 195, 200, 201, 211, 262, 302

**Microstructure** 11, 78, 163, 165, 171, 180-182, 185, 204-205, 208, 235-236, 240

**Miniaturization** 253

**Modelling** 28, 51, 78, 80, 93, 112, 129, 138, 149-150, 154, 157, 162, 164, 171, 180-184, 195-196, 202-207, 212, 219, 235, 257, 261, 276-277, 288-289, 320, 325, 327, 329, 346

## N

**Nanoanalytics** 170, 172

**Natural Resources** 10, 12-13, 25, 112, 142, 312

**Network** 10, 12, 29-30, 36, 51, 58-59, 80, 112, 122, 138, 149-150, 168, 177-178, 193, 195, 216-217, 240, 244, 247, 251, 256-257, 267, 270-272, 274-275, 280, 282, 286-289, 292, 294-296, 307, 319, 334, 336-337, 340, 354, 358

**Neural Computing, Neural Network** > Network

**Neutrality** 76-77, 90, 109, 140, 152-155

**NLP (Natural Language Processing)** 99, 244, 258-259, 261-263, 265, 312-315

**Numerical Simulations** 307-308, 324

## O

**Operations Strategy** 134-135

**Optimization** 5, 7-8, 11, 19, 28, 37-38, 44, 56, 65-66, 68, 72, 75, 86-87, 91-92, 94-95, 98, 112, 128-129, 131-132, 138, 150, 153-154, 157, 163-164, 171-172, 174-175, 191, 195, 203, 205-206, 213, 219, 227, 233, 235, 245, 247, 254-255, 259, 263-264, 269, 271, 284-285, 288-289, 295, 300-304, 313, 318-319, 322-323, 336-338, 347-349, 351-353

## P

**Paper & Surface Technologies** 69, 81, 146, 148, 174, 202, 324, 327, 343, 366, 374

**Photoacoustics** 288, 292-293

**Photonic** 58, 60, 200, 288, 291-293

**Photovoltaics** 174, 176

**Physics** 86, 96, 144, 154, 170, 172-173, 181-182, 189, 197, 204-206, 213, 235, 244, 320

**Planning** 19-21, 23, 26, 28, 31, 35-39, 46-47, 51, 64-69, 98-99, 138-139, 205, 225, 252, 264-265, 272, 295, 300, 303-304, 337, 351

**Plastics** 13, 71, 86, 94, 114, 162, 175, 212-213, 215-216, 218-220, 223, 229, 327

**Polymer** 88, 102, 104, 120, 123, 158, 162, 164, 170-171, 175, 187, 189, 212-213, 215-217, 219-220, 222-227, 229, 231, 233, 238, 324

**Power-to-X** 106-107, 109

**Precipitates** 165, 180, 182, 184

**Prescriptive Analytics** 300-302, 304, 336-337, 340, 348-353

**Printing** 28, 37, 42, 45, 60, 70-72, 74-75, 102-104, 119, 134, 139, 147, 153-154, 158, 163-164, 187-189, 222

**Privacy** 34, 46, 86, 136, 244, 254, 333, 348-349, 352, 355-357

**Production** 6-8, 10-14, 18-37, 39, 41-42, 46-48, 51-52, 56, 58-62, 64-68, 70-79, 81, 85-86, 88, 90-91, 93-95, 98-103, 107-124, 126, 128-129, 131-132, 134-135, 137-143, 147-148, 150, 152-159, 162-163, 166, 168, 170-174, 176-177, 180-182, 184, 187-188, 190-191, 195-197, 199, 202-210, 212, 216, 218-220, 224, 231-232, 234-235, 237, 244-245, 248, 250, 253, 255, 258-263, 266, 270-271, 276, 279-280, 282-284, 287-292, 294-298, 300-301, 303-308, 312-316, 324, 327, 330, 336-338, 340-343, 345, 350-351, 354-356, 359

**Product** 6-8, 11, 14, 18-21, 23, 28, 30-35, 37, 41-45, 70-71, 73, 75, 77-79, 85, 98, 108-109, 124, 130, 134-135, 140, 142-144, 148-149, 154-156, 158, 170, 174-175, 178, 193, 199, 202-203, 205, 207-208, 212, 214-216, 219, 224, 226, 228, 238, 250-253, 255, 257, 259, 262-263, 265, 270, 276-279, 282, 289-290, 314, 330, 336-337, 340, 345, 349

**Protein** 112, 114-116, 129, 132-133

## Q

**Quality Assurance** 144, 154, 157, 174, 263, 289

## R

**Reconstruction** 129, 288, 291-293, 323, 344

**Recycling** 6, 11, 13-14, 77-79, 85-86, 88, 92-98, 102-103, 112-114, 116, 129, 140-142, 156, 163-164, 174-175, 177, 190, 195, 203, 212, 215-216, 218, 220, 223, 228, 231, 236-238, 251-252, 255, 276, 356

**Recyclability** 8, 163, 174, 176-177, 235-238

**Regularization** 288, 292

**Reliability** 12, 72, 153, 157, 178, 180, 196-197, 199-201, 203, 207, 215, 224, 232, 244, 252, 270-271, 294-295, 308, 341

**Resilience** 10, 15, 20, 65, 85, 98, 134-135, 139, 152-153, 155, 354

**RFID (Radio Frequency Identification)** 252, 254, 282, 286-287

**Resources** 6, 8-15, 25, 36-37, 47, 51, 60, 64-65, 73, 77, 86, 90-94, 102, 112, 115, 124, 126, 128, 131, 140-142, 146, 152, 154, 156, 170, 177, 180, 191, 219-220, 238, 244, 247-248, 250, 253, 255, 257, 262, 271, 297, 307-308, 311-312, 332, 334

**Responsibility** 5-6, 40, 236

**Robotics** 5, 7, 12, 20, 26-27, 39, 46, 64, 66-68, 152-153, 155, 157, 159, 202, 268-269, 274, 336

## S

**Safety** 7, 10, 20, 30, 35, 43, 45-49, 52-55, 58, 86, 92, 131, 153, 155, 157, 174-175, 177-178, 180, 186, 197, 245, 247-248, 266, 270-272, 282, 289-290, 298

**Sector Coupling** 106-107, 158

**Self-Adaptability** 250-252, 255-257, 312-313

**Self-Organisation** 250

**Semiconductor** 64-69, 107, 138, 197, 200, 265, 295

**Sensor** 45, 60, 64, 74, 98-99, 110, 152-155, 157-159, 186-189, 206, 214, 244, 246, 251-253, 256-259, 261-262, 266-267, 271-272, 275, 282-291, 293-294, 298, 300, 343, 349, 356

**Sentiment** > Emotion, emotional

**Service** 11, 14, 30-31, 33, 37-38, 59, 103, 118, 134-135, 141, 157, 162, 175-176, 180-182, 184, 196, 206, 208, 234-235, 240, 257, 267, 270, 276, 278-279, 289, 294-297, 332, 336-337, 341, 357

**Shared Resources** 36

**Simulation** 11, 14, 30-31, 33, 37-38, 59, 103, 118, 134-135, 141, 157, 162, 175-176, 180-182, 184, 196, 206, 208, 234-235, 240, 255-256, 267, 270, 276, 278-279, 289, 294-297, 332, 336-337, 341, 357

**Smart Building, Smart City** 124

**Smart Manufacturing** 7, 12, 31, 46-49, 51, 152-153, 250-257

**Soft Sensor** 152, 157, 214

**Steel** 76-81, 108, 111, 144, 162, 164, 169, 171, 173, 180, 182-183, 189, 205, 207, 209, 211, 237, 327, 329, 366

**Supply Chain** 10, 25, 36, 48, 70, 73, 135-136, 138-139, 152, 155, 250, 255, 278, 283, 315, 337,



354, 356-358

**Surface & Paper Technologies** > Paper & Surface Technologies

**Sustainability, sustainable** 2, 5-8, 10-15, 18-20, 23-27, 29-32, 35, 38, 40-41, 43, 48, 50-52, 55, 58-59, 64, 76-78, 84-86, 88-92, 95, 98-103, 107, 109, 112-115, 117-118, 120-121, 124, 126, 128-129, 131-132, 134-135, 138-142, 146, 148-150, 152-156, 158-159, 169, 171, 174, 176-178, 190-192, 195, 199, 202-203, 205-206, 210, 212, 215, 218-219, 223, 234-237, 241, 258, 263, 267, 276, 288-289, 295, 297, 312-313, 315, 337-338, 341, 355, 357

**Symbolic Regression** 207, 213-214, 337, 348

## T

**Testing** 9, 41, 43-45, 72, 104, 106, 144, 147, 157, 168, 174-175, 177-178, 181-184, 188, 196-201, 206, 210, 230, 232, 236, 240, 257, 271-272, 274, 279, 288-289, 320

**Thread** 276, 278-281

**Thermodynamics** 292-293

**Thermoplastics** 148, 164

**Timber** 13, 140-141, 144, 146

**Time Series Analysis** 258

**Traceability** 30, 262, 337, 354, 357

**Transducers** 186-189, 197, 299

**Twin, digital** 8, 18, 23, 65-66, 84-85, 88, 90, 92-94, 98, 203, 206-207, 216-217, 277, 290, 317, 323, 349

**Twin Transition** 18, 23, 84, 88, 93, 98, 203

## U

**UAV (Unmanned Aerial Vehicle)** 70-71, 74

**Upcycling** 86, 98

**User Interface** 40, 44, 98-99, 181, 267, 277

## V

**Value Chain** 18, 21, 84-85, 88, 90, 93, 98, 100, 121, 134-135, 146, 153-155, 157-158, 177, 191, 193, 236, 267, 278, 334, 337, 356-357

**Verification** 15, 271-272, 275, 277, 317

**Virtual** 8, 12, 18-20, 26, 28, 34, 41-43, 46-47, 58, 60, 91-92, 134, 155, 157, 199, 244, 250, 252, 276, 278, 283, 293, 295, 324-325, 330, 337, 346

**Visual** 46-47, 51, 254, 259, 264, 266-267, 342-347

## W

**Waste** 6, 10-15, 18, 30, 49, 73, 85-86, 92, 102-103, 108, 110, 114, 116, 119, 128-129, 131, 134, 140-142, 147, 154, 176, 188, 191, 203, 212, 218-220, 223, 226, 237-238, 241, 255, 258-259, 282, 307, 310, 338

**Water** 10, 12, 30, 78, 92-95, 109, 121, 123, 128-129, 133, 156, 187, 220, 223, 228, 237, 307

**Wearable** 20, 40-41, 46, 48-49, 52, 186, 238, 256-257

**Welding** 60, 74, 162-165, 168, 208, 257, 261

**Wireless** 7, 9, 12, 99, 159, 186, 251-252, 255-256, 270-272, 274-275, 282-287, 294-299

**Wood** 140-142, 144-148, 150, 162, 216, 222, 327

**Wood, Timber** > Timber

**WWW** > Internet, WWW

## Authors Index

## A

**Affenzeller, Michael** 348  
**Aichernig, Bernhard** 270  
**Aigner, Wolfgang** 46  
**Amancio-Filho, Sergio** 162  
**Arbeiter, Florian** 228

## B

**Bachinger, Florian** 348  
**Bachlmair, Elke** 40  
**Berger-Weber, Gerald** 222  
**Bernhard, Christian** 76  
**Bernhard, Hans-Peter** 294  
**Bodner, Merit** 118  
**Bögl, Michael** 348  
**Brüggemann, Oliver** 218  
**Brunner, Manuel** 336  
**Burgholzer, Peter** 288

## C

**Cakmak, Umut D.** 224  
**Craß, Stefan** 354  
**Czerny, Bernhard** 196

## D

**Döller, Mario** 70  
**Doe Ocansey, Evans** 258  
**Dhungana, Deepak** 30  
**Domitner, Josef** 162

## E

**Ecker, Jakob** 102  
**Ecker, Werner** 202  
**Eisl, Alexander** 354  
**Elgeti, Stefanie** 318  
**Enzinger, Norbert** 162  
**Erol, Selim** 24

## F

**Falkner, Dominik** 348  
**Felberbauer, Thomas** 46  
**Ferscha, Alois** 4-15, 250  
**Fidler, Franz** 46  
**Froschauer, Roman** 336  
**Frotschnig, Alois** 46  
**Fruhmann, Philipp** 190

## G

**Gansterer, Margaretha** 36  
**Gebser, Martin** 64  
**Geyer, Sebastian** 58  
**Ghafourian, Yasin** 312  
**Gindl, Stefan** 312  
**Grimm, Hanna C.** 128

## H

**Hacker, Viktor** 118  
**Heinzlreiter, Paul** 258  
**Hilber, Wolfgang** 186  
**Hingerl, Kurt** 170  
**Hirner, Heimo** 58  
**Hlawitschka, Mark W.** 92  
**Holom, Roxana** 258  
**Horn, Martin** 270  
**Hulla, Maria** 18  
**Hultsch, Boris** 146

## J

**Jakoby, Bernhard** 186  
**Joanneum Research** 152  
**Jodlbauer, Herbert** 336

## K

**Kaiser, Stephan** 140  
**Khatibi, Golta** 196  
**Kiener, Daniel** 234  
**Kloiber, Karin** 84  
**Korak, Gernot** 58  
**Kraler, Anton** 140  
**Krenmayr, Bernhard** 180  
**Kritzinger, Stefanie** 348  
**Kourist, Robert** 128  
**Kumar, Mohit** 348

## L

**Lehner, Markus** 106  
**Leitner, Martin** 208

## M

**Major, Zoltán** 224  
**Matković, Krešimir** 342  
**Mehofer, Christoph** 58  
**Michelic, Susanne** 76

**Mingler, Bernhard** 58  
**Mitterer, Christian** 234  
**Monturo, Alessio** 348  
**Moser, Thomas** 46

## **N**

**Nimmervoll, Florian** 40

## **P**

**Paireder, Elmar** 276  
**Pappler, Udo** 174  
**Parragh, Sophie N.** 292  
**Paulik, Christian** 84  
**Pedarnig, Johannes D.** 170  
**Pernkopf, Franz** 234  
**Petutschnigg, Alexander** 124  
**Pinter, Gerald** 228  
**Pitzer, Erik** 348  
**Poletti, Cecilia** 162

## **R**

**Raffaseder, Hannes** 46  
**Ramsauer, Christian** 18  
**Reiner, Gerald** 134  
**Riedlsperger, Florian** 180  
**Römer, Kay** 270  
**Romaner, Lorenz** 234  
**Roßbory, Michael** 348  
**Rückert, Elmar** 266

## **S**

**Schenk, Johannes** 76  
**Schlund, Sebastian** 98  
**Schmermbeck, Katharina** 52  
**Schmid, Christian** 70  
**Schmidt, Johanna** 342  
**Schnöll, Hans Peter** 18  
**Singewald, Tanja** 190  
**Slatner, Matthias** 112  
**Sobieczky, Florian** 348  
**Sommitsch, Christof** 162  
**Sonderegger, Bernhard** 180  
**Springer, Andreas** 294  
**Stampfl, Jürgen** 102

## **T**

**Tauber, Markus G.** 312  
**Tschabuschnig, Günther** 330

## **U**

**Ußmüller, Thomas** 282

## **V**

**Valtiner, Markus** 190  
**Vetyukov, Yury** 324

## **W**

**Wagner, Stefan** 348  
**Walpot, Martin** 112  
**Walter, Thomas** 196  
**Wartner, Sandra** 258  
**Weidner, Robert** 52  
**Witrisal, Klaus** 270  
**Wögerbauer, Martin** 312  
**Wolf, Matthias** 18

## **Y**

**Yoshioka, Keita** 306

## **Z**

**Zenisek, Jan** 348  
**Zeppetbauer, Mario** 40  
**Zuderstorfer, Gerold** 180





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