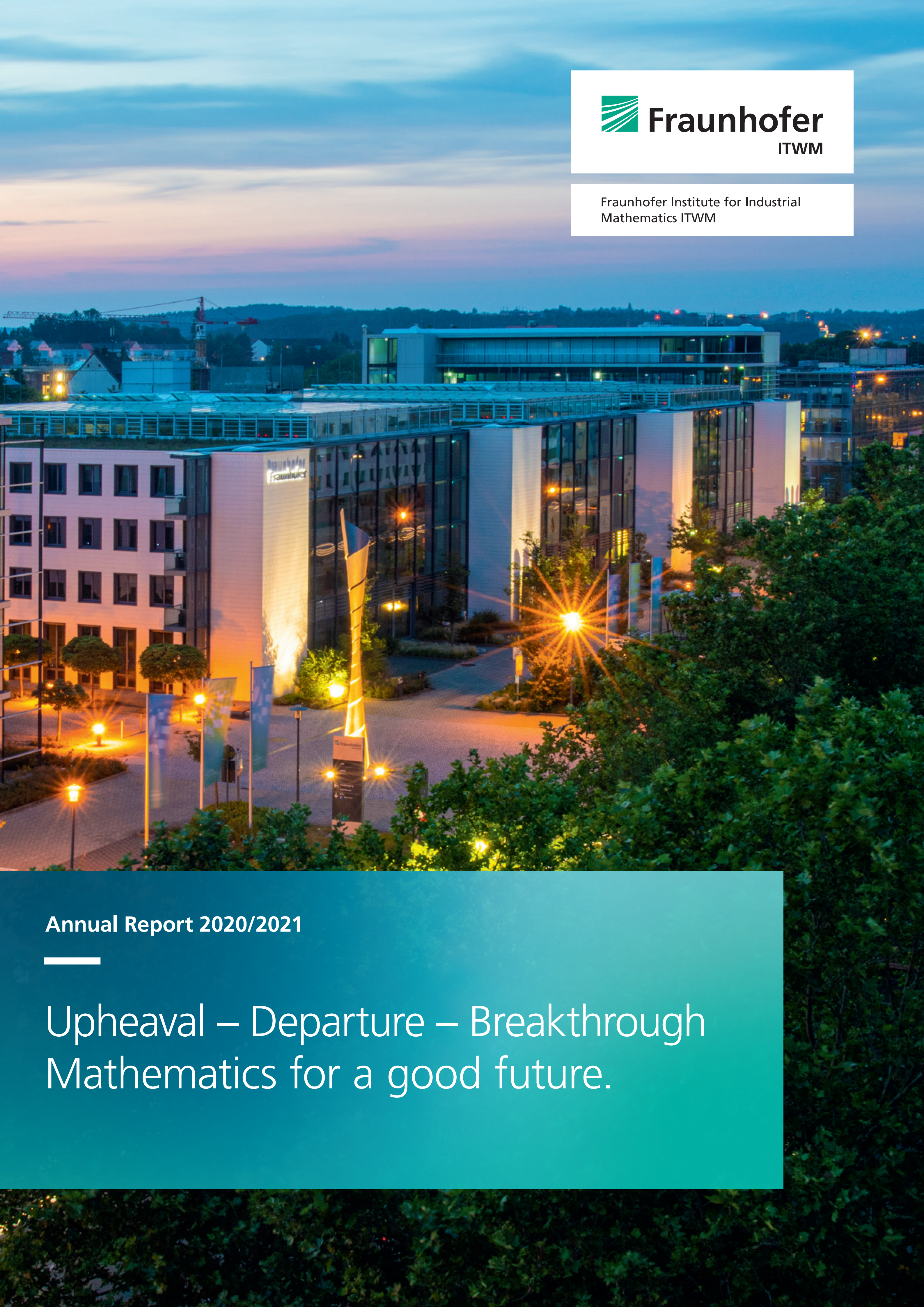


Fraunhofer
ITWM

Fraunhofer Institute for Industrial Mathematics ITWM

Annual Report 2020/2021

Upheaval – Departure – Breakthrough
Mathematics for a good future.

Cover

For the cover picture, we captured a special moment in the blue hour with a view of the Fraunhofer ITWM. The annual report looks back at special moments and highlights in 2020/21.

Annual Report 2020/2021

Upheaval – Departure – Breakthrough
Mathematics for a good future.

2020 Upheaval – Departure – Breakthrough

Mathematics for a good future.

Dear readers,

In our Annual Report 2020/21, we look back on a year of upheaval that confronted everyone with unimagined challenges. Privately and professionally, many things had to be improvised, rethought and organized from one day to the next. I am therefore even more proud of what we have achieved at Fraunhofer ITWM under the extraordinary conditions of a worldwide pandemic.

It was an enormous effort to equip all employees for working at home within a very short period of time, and it was challenging for all of them to adapt to a new way of working as quickly as possible in order to continue to work seamlessly. Despite adverse conditions, many of our researchers have been extremely committed to contributing their expertise to the fight against Corona. They have lived up to their scientific and social responsibilities and thereby demonstrated the values for which the research activities of Fraunhofer-Gesellschaft research stand.

This annual report is still dominated by the Corona pandemic. But it also aims to show that Corona did not overshadow everything – many exciting projects were completed or newly started. The mathematical expertise of the researchers at Fraunhofer ITWM is in demand in numerous industries and thus shapes the future of all of us in very different areas.

In 2020, Fraunhofer-Gesellschaft has redefined its research structure – a departure into the future. Seven Fraunhofer Strategic Research Fields (FSF) set priorities in the research portfolio; in addition, eight lead markets have been defined. By focusing research activities on these focal areas and markets, specific goals are being pursued: affordable health, completed energy transition, digitized value creation, holistic circular economy, as well as security and a resilient society. The innovation and industrial sites of Germany and Europe are to be strengthened in this way in the long term.

With its research work, Fraunhofer ITWM provides solutions that have an impact on many lead markets and is actively involved in several FSFs. In order to make clear how our institute fills the “Fraunhofer Powerhouse” with life, we have restructured the content of our annual report. Instead of being divided by our different departments, the individual chapters are subdivided by the FSF and lead markets and visually designed according to the new Fraunhofer corporate design for the first time.

In this annual report, we want to make clear how versatile mathematics is, how it supports numerous fields of research and how it drives innovation in various industries. We want to make the people behind “the big topics” visible and offer exciting insights into the multifaceted daily lives of our researchers. One of my major concerns is to make artificial intelligence (AI) more accessible across disciplines.

As the AI pilot of Rhineland-Palatinate, I have been the contact person for companies on AI issues since 2020, and at ITWM, we provide advice on the application of AI technologies – you will also find information on this in this annual report. We also have a lot to offer in terms of content in next generation computing and quantum computing at the institute, and I am involved in the coordination of these initiatives at Fraunhofer-Gesellschaft in order to push the breakthrough of the transfer into practice.

At hardly any other time has science received so much public attention as it has since the beginning of the Corona pandemic. It experienced much appreciation, but also criticism. Our expertise has been requested more frequently than ever before. Not only have we seen increased media interest, but we have also intensified our political contacts at various levels.

An extraordinary 2020 lies behind us. It has shown us the enormous importance of science, and research has achieved a lot in a short time. You will find out what we, at Fraunhofer ITWM, have contributed to it on the following pages.

I wish you an entertaining read and would like to encourage you to feel free to contact the listed persons for the individual topics if you have any questions.

Best regards

A. Schöbel

Prof. Dr. Anita Schöbel

Director of Fraunhofer Institute for Industrial Mathematics ITWM

Content

The Institute in Profile

Computer simulations are indispensable in the design and optimization of products and processes. Real models are replaced by virtual models. The mathematics is playing a fundamental role in the design of this digital world. It is the technology with which these images are generated and efficiently converted into software, the raw material of the models and the core of every computer simulation.

225 industrial projects with 143 partners realized.

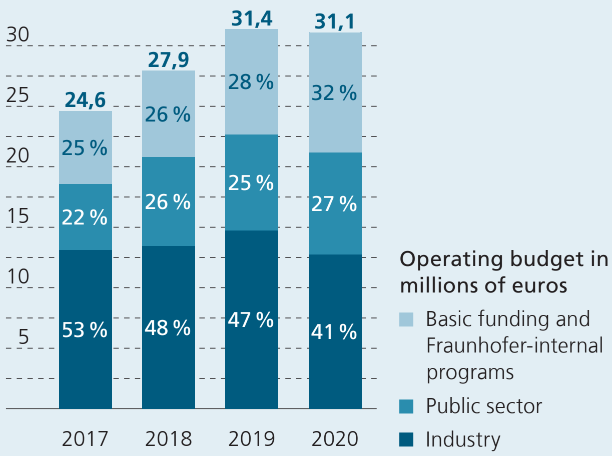
Applied mathematics as a key technology

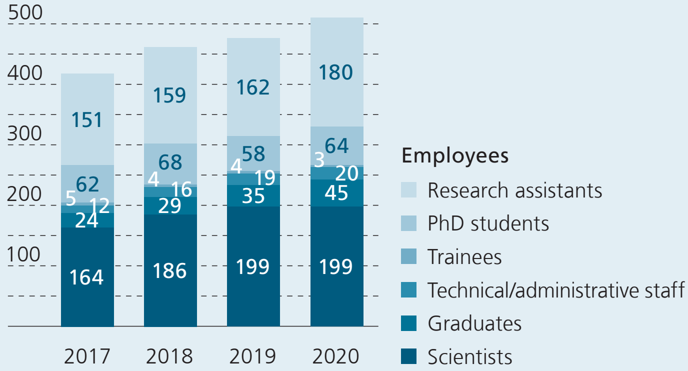
Many small and medium-sized companies use simulation to reduce costs. We support these companies in particular with consulting and computing power. They profit on the market through the use of simulation in terms of innovation and quality assurance of products. Of course we also work with large companies, especially in the automotive industry, mechanical engineering, the textile industry, microelectronics, the computer industry and in the financial sector. Integral components of our research and development projects are consulting and implementation, support in the application of high-performance computing technology and provision of customized software solutions. We not only use simulation software, but develop it ourselves, often in cooperation with leading companies.

Our versatile core competences

- Processing of data from experiments and observations
- Setting up mathematical models
- Conversion of the mathematical problem solutions into numerical algorithms
- Summarizing data, models and algorithms in simulation programs
- Optimizing solutions in interaction with the simulation
- Visualize simulations in pictures and graphics

As Fraunhofer ITWM we do not only want to be the bridge between the real and the virtual world, but also to build a link between university mathematics and its practical implementation. Therefore, the close connection to the Department of Mathematics at the University of Kaiserslautern plays a special role.





Industries – who do we work for?

The methodological competence of our departments and the broad spectrum of their application fields are used in numerous industries.

With our core competencies in the areas of modeling and simulation, optimization and decision support, data analysis and visualization, we address companies and organizations in the following industries:

- Process engineering, Mechanical/plant engineering
- Automotive industry and suppliers
- Medicine and medical technology
- Energy and raw materials industry
- Technical textiles
- Information technology
- Finance industry

Through many years of cooperation with our regular customers, we have strong domain competence in subsectors of certain sectors of industry. To mention industries such as the automotive industry, process engineering and the energy sector.

For all industries, the following applies: The modeling and simulation competence of the Fraunhofer ITWM generates real competitive advantages on the market.

Networking and Cooperation within the Fraunhofer-Gesellschaft

65

joint projects with other Fraunhofer-Institutes

A large network and smart minds are crucial for the success of projects. Our specific mathematical competences make the Fraunhofer ITWM a sought-after and appreciated cooperation partner within the within the Fraunhofer-Gesellschaft.

The "Powerhouse" represents the organizational and funding structure of the Fraunhofer-Gesellschaft. In the following, we will show how the Fraunhofer ITWM is involved on all levels:

Fraunhofer Groups

Institutes with related expertise organize themselves in research groups and appear together on the R&D market. They play an active role in corporate policy as well as in the implementation of the functional and financial model of the Fraunhofer-Gesellschaft. The Fraunhofer ITWM is a member of the:

- Fraunhofer ICT Group
- Fraunhofer Group for Materials and Components (guest status)

Fraunhofer High-Performance Centers

High-Performance centers organize the shoulder-to-shoulder cooperation of research with industry. Universities, colleges, Fraunhofer institutes and other non-university research institutes work together with companies and civil society actors on specific topics at a single location in order to bring innovations quickly into application. They stand for excellent infrastructure, training concepts and know-how that can be used across organizations. They bring together suitable partners and accompany ideas all the way to the market.

Kaiserslautern is home to the High-Performance Center "Simulation and Software- based Innovation", which is under ITWM management.

Fraunhofer Cluster of Excellence

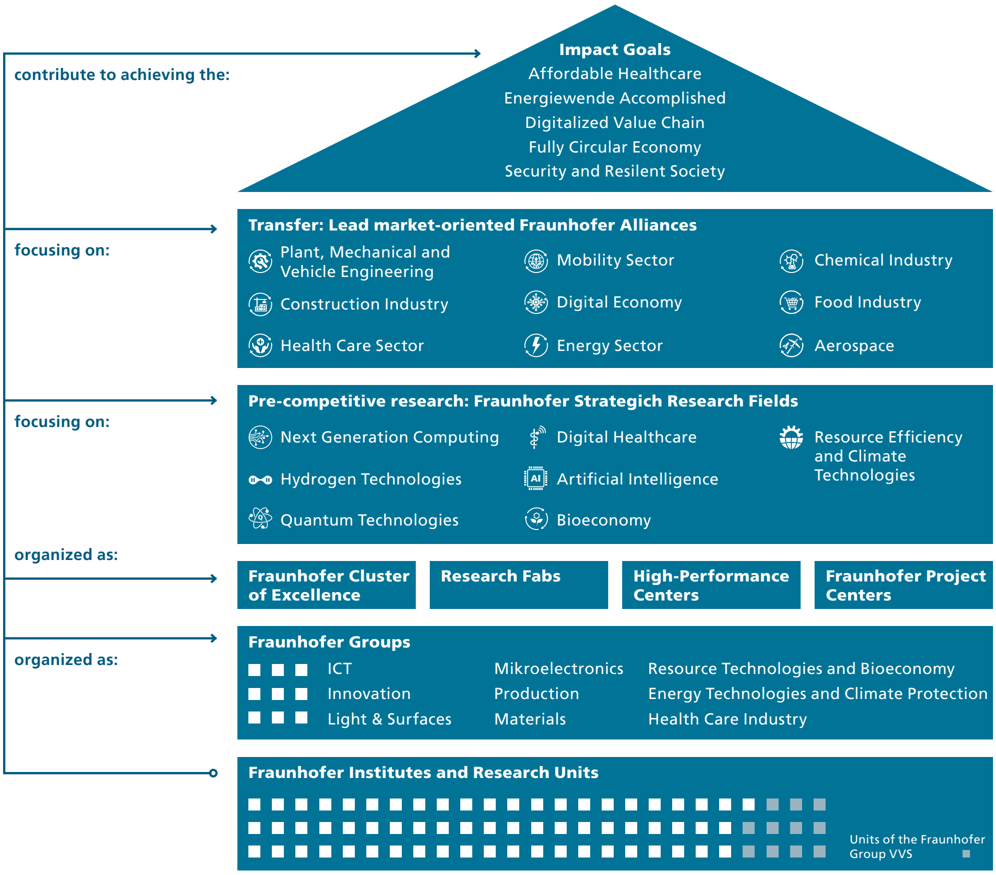
These clusters promote the cooperative development and processing of system-relevant topics by means of a cross-institute research structure. Organizationally, the research clusters correspond to a virtual institute which is distributed over several locations. We are involved in these clusters:

- Advanced Photon Sources CAPS
- Cognitive Internet Technologies CCIT
- Programmable Materials CPM

Fraunhofer Strategic Research Fields

The Fraunhofer Strategic Research Fields (FSFs) define the portfolio-defining priorities of the Fraunhofer-Gesellschaft and bundle the essential future fields of application-oriented research. They provide an overarching strategic focus on key challenges in line with the goals set.

Our institute director Prof. Dr. Anita Schöbel is spokesperson of the FSF "Next Generation Computing" and together with Prof. Dr. Manfred Hauswirth (Fraunhofer FOKUS) responsible for the topic "Quantum Computing" at Fraunhofer. At our institute, the Rhineland-Palatinate competence center with the focus on "Quantum High Performance Computing" is located.



The "Fraunhofer Powerhouse" illustrates the further developed structure of the Fraunhofer-Gesellschaft. Our institute is actively represented at all levels. This annual report is based on this structure.

Lead market-oriented alliances

With the lead market-oriented alliances Fraunhofer's goal is to target sectors that are highly relevant for innovation – the Fraunhofer lead markets – and to create added value by offering system solutions and cross-institutional transfer. We are involved in the following lead markets:

- Plant, mechanical and vehicle engineering
- Health care sector
- Chemical industry
- Mobility sector
- Digital economy
- Energy sector

Fraunhofer lead projects: preliminary research in a network

Thematically, the Fraunhofer lead projects are oriented toward the current needs of the industry and combine the expertise of various institutes for efficient preliminary research. The aim of the program is to exploit the synergy potential by bringing together the competencies of several institutes to provide solutions to the challenges of the German industry. Lead projects with ITWM participation are:

- ML4P – Machine Learning for Production
- QUILT – Quantum Methods for Advanced Imaging Solutions
- COGNAC – Cognitive Agriculture
- ShaPID – Shaping the Future of Green Chemistry by Process Intensification and Digitization

FCC – strong partner in Sweden

One of our most important international partners is the "Fraunhofer-Chalmers Research Center for Industrial Mathematics", FCC for short, founded in 2001 by the Fraunhofer-Gesellschaft and Chalmers University in Gothenburg. In 2020, 65 employees worked on topics such as multiphysics simulation, geometry, modeling of biological systems and data mining. The budget was seven million euros.

High Performance Center Simulation and Software-based Innovation

HIGH PERFORMANCE CENTER
SIMULATION AND SOFTWARE-BASED INNOVATION

Stable network at the site

Five years of successful research and transfer work can be followed by more: the high performance center "Simulation- and Software-based Innovation" in Kaiserslautern will initially receive funding until the end of 2021. But it also looks good for the time after that.

The success story began in 2016, when the cooperation of the Kaiserslautern Fraunhofer Institutes with both the Technical University and the Kaiserslautern University of Applied Sciences and the good collaboration with industry was bundled in the high performance center. Also involved from the beginning are the German Research Center for Intelligence (DFKI) with its location in Kaiserslautern and the Leibniz Institute for Composite Materials IVW. In the meantime, the performance center established itself as the digital transfer center of the region with an increasing focus on methods of artificial intelligence (AI), next generation computing (NGC), and quantum computing.

Funding secured for 2021

That is why this offering is to be maintained: The German Federal Ministry of Education and Research (BMBF) and the Fraunhofer-Gesellschaft are providing two million euros for the current year. "The competencies of our industry-oriented transfer centers are of particular benefit to chemical process engineering, the automotive industry and the IT and energy industries," says Dr. Konrad Steiner, head of department at the Fraunhofer ITWM and at the same time managing director of the performance center. "In the current funding phase we want to establish and expand future topics and strengthen the transfer to industry and society." From the outset, the center has received accompanying funding from the state of Rhineland-Palatinate, which is currently focusing on the future topics of quantum computing, energy industry and the use of hydrogen.

Long-term monitoring

The long-term design of the center is based on a transfer roadmap that has been coordinated at the site. In this roadmap the goals and current measures are specified; they are reviewed on an ongoing basis.

The high performance center is divided into research and development labs and transfer centers. The R&D labs are methodologically oriented; they develop concepts and algorithms that are available as basic technologies for the following transfer centers. The "MSO-based process engineering" focuses on modeling, simulation and optimization (MSO) in process engineering. The Center "Digital Commercial Vehicle Technology" has its main focus on commercial vehicle technology and the "Smart Ecosystems" are concerned with smart energy, smart health, Green by IT, and adaptive and open systems.

Contact

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More information at www.leistungszentrum-simulation-software.de/en

Spin-offs and Other Collaborations

Spin-Offs of the Fraunhofer ITWM

- **Math2Market** – The digital material laboratory with extensive software service for companies
- **fleXstructures** – specific engineering projects and services for the simulation of flexible components
- **Sharp Reflections** – Big Data computing technologies for the future of seismics
- **ThinkParQ** – Fast and scalable solutions for all performance-oriented environments such as HPC, AI and Deep Learning
- **Product Information Agency for Pensions PIA** – Neutral agency for the risk-reward classification of subsidized pension products
- **Wendeware AG** – Software ecosystem for the energy transition

Networking in the promotion of young talent

The **Felix Klein Center for Mathematics (FKZM)** is an institutional connection between the Department of Mathematics of the TU Kaiserslautern and the Fraunhofer ITWM. The focus is on the promotion of young scientists, for example, with modeling weeks for schools, scholarships, and a mentoring program for mathematics students. Scholarship holders not only receive financial support, they can also combine practice and theory. Students in advanced semesters and doctoral students can take part in advanced training courses lasting several days as well as lectures by top-class researchers. The monthly "Thinking outside the box" event of the Felix Klein Center provides interesting insights into various topics from science and culture.

The Competence Center for Mathematical Modeling in MINT Projects in schools (KOMMS) is aimed primarily at teachers. It is located at the TU Kaiserslautern and combines the areas of school projects, education and training as well as research.

The national **excellence school network MINT-EC** aims to get students interested in MINT subjects. As part of this cooperation, events such as the Math Talent School are offered.

Further networking at the site

Die **Science and Innovation Alliance Kaiserslautern (SIAK)** forms a network for digital transformation, innovation and interdisciplinary research. Through its members from science (universities and research institutes) and business, especially from small and medium-sized enterprises, it is regionally anchored.

Networking in Europe

Im **European Consortium for Mathematics in Industry (ECMI),** scientific institutions and industrial companies in Europe have joined forces with the aim of integrating mathematical modeling, simulation and optimization even more strongly into economic application. An important role is played by the training of industrial mathematicians, because their expertise is needed in particular.

6

Spin-Offs founded since establishment of the Fraunhofer ITWM.

More information at www.itwm.fraunhofer.de/networks

Review: Highlights 2020

There has not been an atrium this well attended since March 4, 2020

Terahertz Conference - last attendance event 2020

Few would have suspected it at the time: The "9th International Workshop on Terahertz Technology and Applications" was the last attendance event of the year 2020 at our institute! The workshop took place on March 3 and 4, 2020.

As every year, it provided a forum for representatives from science and industry to exchange experiences. The focus was on applications, non-destructive testing, security and communication technology as well as new developments in terahertz system technology. They demonstrated the great potential of the technologies for analysis, testing and measurement tasks. The program was characterized by the contributions of renowned speakers from all over Germany and international researchers, including Dr. Peter Uhd Jepsen from the Technical University of Denmark and Dr. Tadao Nagatsuma from the Osaka University. In addition to people from science and research, we were also able to welcome numerous participants from industry.

More information at www.itwm.fraunhofer.de/terahertzworkshop

In demand as an advisor in the crisis team: Division Manager Karl Heinz Küfer

Support in pandemic management

Is it possible to predict the development of a pandemic? This was the question addressed by our researchers in the EpideMSE project: With the help of statistical methods and data-based modeling, they developed a mathematical forecasting model that supports policymakers at the local level in pandemic management. "Similar to weather forecasts, our model makes it possible to make short-term predictions so that developments can be identified early enough and the course can be better assessed," says Prof. Dr. Karl-Heinz Küfer, head of the "Optimization" department.

Parallel to this, research is also being conducted on an agent-based social simulation model, SoSAD, at the branch office of the German Research Center for Artificial Intelligence in Trier (DFKI). Both research projects were merged in the project SEEvacs – Simulation-based Evolution and Evaluation of Vaccination Strategies in Covid-19-pandemics to provide sustainable decision support on the macro and micro level. The city of Kaiserslautern is taking advantage of this knowledge: on February 22, 2021, it gave the go-ahead for a joint expert opinion on the impact of the opening of the open-air swimming pool on the city's infection incidence. Our researchers were also often in demand as interview partners in the media and helped to classify current developments for the public in a comprehensible way. Numerous media publications have appeared.

More information at www.itwm.fraunhofer.de/dfki-pm

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Two female Fraunhofer institute directors in the NFDI Senate

Appointed to scientifically renowned posts: Anita Schöbel (left) and Claudia Ecke

In December 2020, our institute director Prof. Dr. Anita Schöbel was appointed to the Senate of the National Research Data Infrastructure (NFDI). The NFDI is intended to make data and research results, which were previously stored decentrally at the respective institutions, accessible to the scientific community. In addition to Anita Schöbel, the board includes another institute director: The Joint Science Conference (GWK) of the German federal and state governments appointed Prof. Dr. Claudia Eckert, director of the Fraunhofer Institute for Applied and Integrated Security AISEC, to the organization's Senate.

The two researchers have the opportunity to help shape the content and strategic direction of the NFDI. "There is a lot to do. In Germany, Europe and internationally, researchers are waiting for scientific results from different sources, locations and organizations to be made more accessible," says Anita Schöbel.

More information at https://s.fhg.de/nfdi

Alumni meetings – also possible digitally

Raise your cups! Virtual instead of together on site.

Like so many events of our institute, the alumni network meeting in December 2020 had to take place virtually. Nevertheless, many former ITWM members had registered and, after two hours, were again up to date on the research status of their former employer. This included, of course, research projects on the topic of "Fraunhofer ITWM vs. Corona"; the focus was on "EpideMSE", "AVATOR – aerosol dispersion in indoor environments", and "modeling of moisture propagation in face masks". Another focus was on quantum computing: researchers from the departments "Financial Mathematics", "Flow and Material Simulation", and "Optimization" took the opportunity to present their projects. For a sense of community despite the physical separation, all participants received a package with a cup, tea and chocolates before the alumni meeting – relaxed networking also works digitally!

More information at www.itwm.fraunhofer.de/itwmalumni

Promoting and Recruiting Young ITWM Talents

The promotion of young scientists is a particularly important topic at the Fraunhofer ITWM. The activities of the Felix Klein Center for Mathematics, a joint institution of the Department of Mathematics of the Technical University of Kaiserslautern (TUK) and our institute, should be emphasized here. However, we also reach young people by participating in other programs, events, and formats and show them where mathematics, research, and our institute can lead them.

What career opportunities does applied mathematics offer? The Math Talent School provides answers.

Math-Talent-School 2020: Get to know the professional world and work in teams

In the annual Math-Talent-School event format, 23 young people from schools of the national excellence school network MINT-EC had the chance to immerse themselves in the working world of mathematicians from March 2 to 6, 2020. Selected students from all over Germany took the opportunity to learn what is meant by applied mathematics in practice.

The focus of the days at the Fraunhofer ITWM was on group work. The teams worked on different questions with the help of mathematical modeling and computer simulation – actively supported by researchers of Fraunhofer ITWM and the Technical University of Kaiserslautern (TUK). Among others, the groups dealt with the "development of a pedometer" or "choreography for music fountains". In addition, an exclusive guided tour through the institute and the department of the TUK was part of the colorful program. The Math Talent School is organized annually by MINT-EC in cooperation with the "Felix Klein Center for Mathematics".

More information at www.itwm.fraunhofer.de/math-talent-school-2020

Save the research results! Exciting mission at Digitaltag 2020.

Digitaltag for the first time with Fraunhofer Escape Game @Home

Mastering challenges digitally in a team and realizing your own ideas at the same time is not possible. It is! The Fraunhofer Escape Game @Home presented students with new challenges on June 19, 2020 – for the first time in purely digital form.

In teams of four to five people, they were able to show what they were capable of and solve various tasks together in a virtual room. The online game was convincing with an exciting case. The task was to save endangered research results of the Fraunhofer-Gesellschaft. This gave the participants an insight into the world of work and research. In addition to team spirit, skill and creativity, analytical skills were also required to find a solution. The digital games event was part of the Germany-wide Digitaltag, sponsored by the "Digital for All" initiative, which is to be held annually.

More information at www.itwm.fraunhofer.de/digitaltag2020

Doing a PhD in different worlds: Math connects internationally

Armin Bosten on site at the institute – he does research here and at the University of Liège.

In 2020, 64 PhD students are doing their doctorates at the ITWM. They are doing research on exciting topics, working in different departments and in the most diverse programs. Two international colleagues, for example, are working on their doctoral thesis in our department "Mathematics for Vehicle Development":

Davide Manfredo joined our institute on April 1, 2020. He came to Kaiserslautern with a master's degree in mathematics for the biological sciences from the University of Trento in Italy and is a participant in a very special program in which the EU is funding 14 doctoral positions across Europe for three years: "THREAD – Joint Training on Numerical Modeling of Highly Flexible Structures for Industrial Applications". With the help of financial support from the EU, THREAD aims to promote the international exchange and mobility of young scientists. However, mobility was rather difficult in 2020. Instead of Kaiserslautern, Davide Manfredo initially sat in his home office with his parents in Turin. Later, more mobility was possible again. "THREAD" offers a unique network of universities, research institutions and industry in eight European countries. This is a very special training environment, because in addition to working on application-oriented dissertation topics, the PhD students are also allowed to complete a three-month internship in an industrial company – including fleXstructures, a successful ITWM spin-off. The focus of the research projects is on the question of how thin, flexible structures such as ropes, cable bundles, or hoses can be better modeled and simulated in the computer in the future.

Armin Bosten is also working on similar topics. The Belgian native has been a doctoral student in the field of "Mathematics for Vehicle Development" since November 2019. Bosten is doing his PhD in the team "Mathematics for the Digital Factory" with a scholarship from ITWM. At the same time, he is supervised by Prof. Olivier Brüls of the University of Liège (French: Université de Liège). In practice, this means for him that he is always on site in Kaiserslautern and Belgium alternately for a few weeks. Both young mathematicians have an exciting professional life as ITWM PhD students – not only between cables and tubes, but also between different countries.

More about THREAD and Davide Manfredo: www.itwm.fraunhofer.de/threadphdprogram

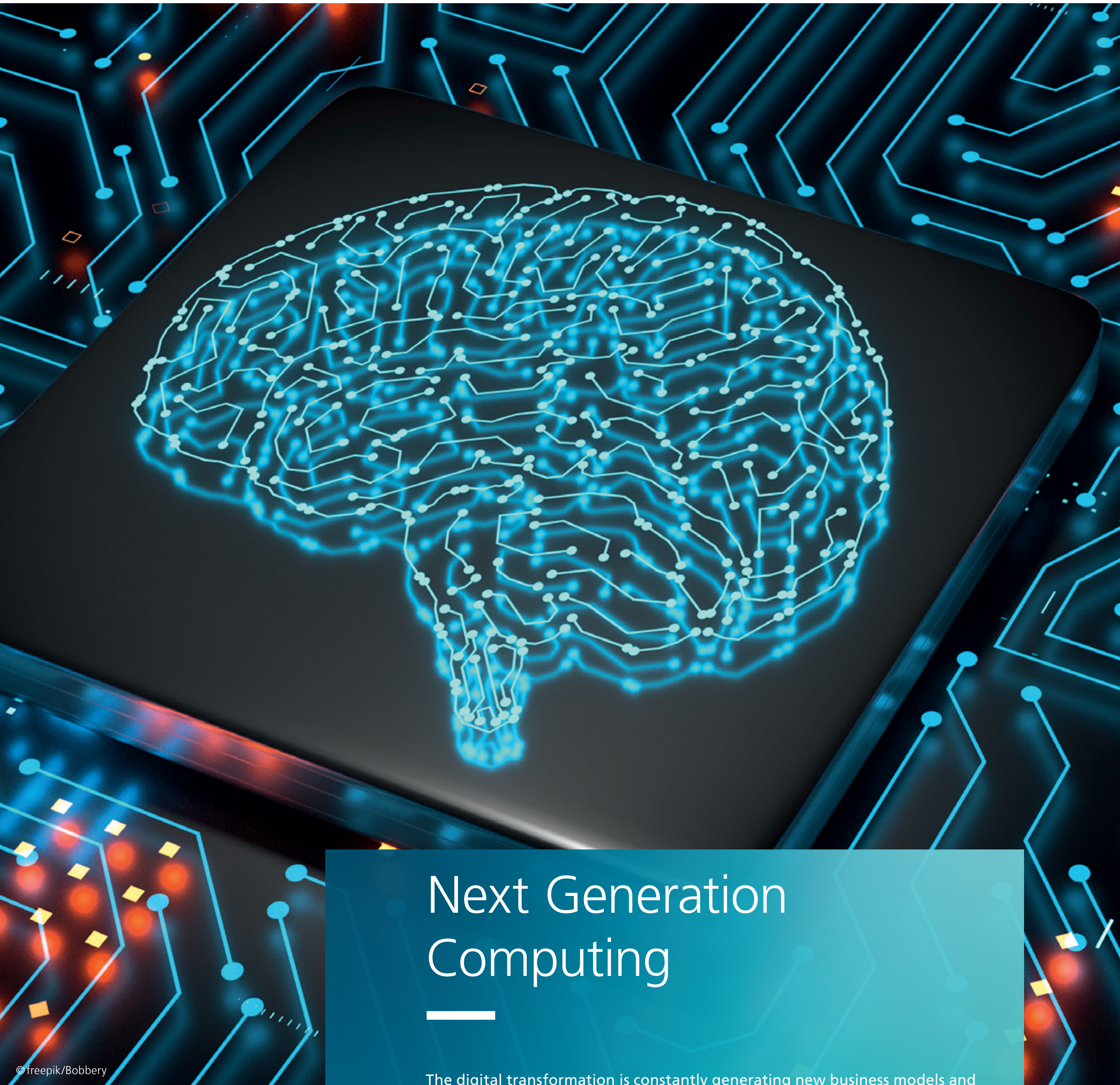
Interview with Armin Bosten: www.itwm.fraunhofer.de/interview-bosten

European Career Fair 2020: International Career Fair with the ITWM

Recruiting in the USA: Nicole Cumia (Fraunhofer headquarters) and Dietmar Hietel on site at the ECF.

The European Career Fair (ECF) takes place every year at the renowned Massachusetts Institute of Technology (MIT). It is the largest European career fair in the USA and offers American students the opportunity to get in contact with European companies, universities, and organizations – in 2020 also with ITWM researchers. The target groups are especially graduates, PhD students, and postdocs of the universities on the American East Coast, including MIT, Yale, and Harvard. Dr. Dietmar Hietel, head of the department "Transportation Processes", was on site in February 2020 and conducted interviews with students who were interested in a career at Fraunhofer ITWM. So maybe more international young talent from the USA soon?

More information at www.itwm.fraunhofer.de/jobs-career



Next Generation Computing

The digital transformation is constantly generating new business models and innovations. However, conventional computing technologies are reaching performance and energy efficiency limits: Time for Next Generation Computing! Time for a new hybrid computing generation! Fraunhofer is driving the development of hardware and technologies for the next generation of computing and is setting priorities in high efficiency trusted computing, neuromorphic computing and quantum computing. The goal is to develop trustworthy, highly perfomant and efficient hardware and software solutions.

Next Generation Computing is Based on Three Pillars

Dr. Jens Krüger from our "High Performance Computing" department is a Fraunhofer consultant for the strategic research field "Next Generation Computing". He ventures a look into the future and describes which computing technologies will shape the way we work and perhaps even our everyday lives.

The next generation of computing will be diverse. It stands on three pillars: the first pillar is based on traditional architectures as we know them today, but specialized. The second pillar represents neuromorphic technologies, which function similar to our brain, and the third pillar is quantum computers. Together with IBM, the Fraunhofer-Gesellschaft has been operating the IBM System One quantum computer near Stuttgart since June 2021.


© IBM

The cool beauty of quantum computing: The System One from IBM is the fastest quantum computer in Europe.

What are the distinguishing features of high efficiency trusted computing?

The core is based on highly efficient trusted microelectronics. On the one hand microelectronics that are protected against hacker attacks on infrastructures and prevent the decryption of data communications on the other hand architectures that are designed to be very efficient. Such types of microprocessors are also to be developed in Europe. One example is EPI, the European Processor Initiative, in which 28 partners from ten European countries are jointly developing the high-performance computing processors and accelerator units. E.g. the Stencil and Tensor Accelerator (STX) is designed to support scientific computing applications – such as weather forecasting – and data analysis in an highly efficient way and involves the accelerator architecture and software ecosystem. We are focusing on the use of European technologies and are aiming for an energy-efficient processor technology with application in a European pre-exascale and exascale system.

What challenges can we meet with the next computer generation?

Digitization presents us with major challenges in the areas of health, mobility and the energy transition – continuously more data must be processed at ever increasing efficiency. One solution is neuromorphic computing, in which computers imitate the human brain. This is extremely efficient in processing information and very good at pattern recognition; at the same time, it is also extremely energy-efficient. We want to mimic this functionality of the brain by processing data in a network of neurons and synapses, rather than data transport from memory to the processing unit and specific instructions. A major advantage is the minimal energy required, because only the neurons of a network that are actually needed are activated.

More information at www.itwm.fraunhofer.de/EPI_en

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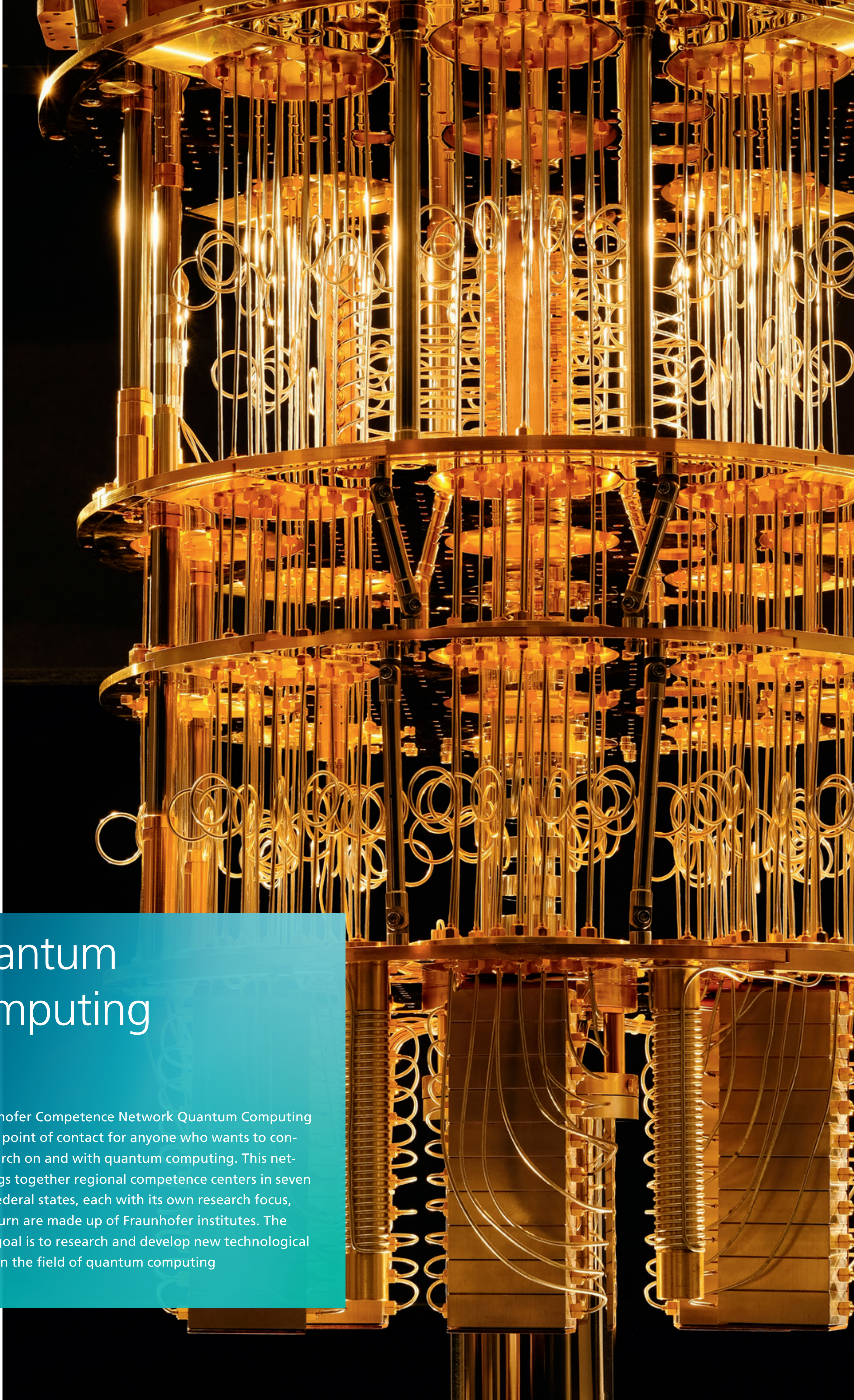
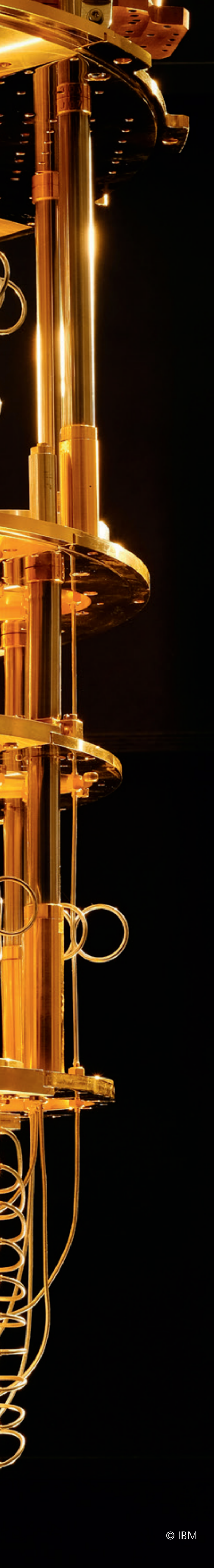


Quantum Computing

The Fraunhofer Competence Network Quantum Computing is the first point of contact for anyone who wants to conduct research on and with quantum computing. This network brings together regional competence centers in seven German federal states, each with its own research focus, which in turn are made up of Fraunhofer institutes. The common goal is to research and develop new technological solutions in the field of quantum computing



Quantum Computing – The Future Calls

A "game changer" – the potential of quantum technologies can hardly be predicted. Compared to traditional computing, quantum computing promises an exponential acceleration of selected algorithms as well as the possibility to deal with complex problems. Together with Prof. Dr. Manfred Hauswirth, Director of Fraunhofer FOKUS Institute, ITWM Institute Director Prof. Dr. Anita Schöbel is responsible for the topic of quantum computing at Fraunhofer. In cooperation with IBM, a national competence network has been established to develop quantum-based computing strategies for the next generation of high-performance computers.

Competence network with Rhineland-Palatinate participation

The Rhineland-Palatinate competence center "Quantum High Performance Computing" was opened at our institute in August 2020. We contribute our expertise in the fields of mathematics, physics and high performance computing as well as our good networking with industry. Among other things, the competence center will assess the conditions under which practical problems can be solved on quantum computers and applied in the industry. In addition, new quantum-based technologies, application scenarios and algorithms can be tested through cloud access to IBM quantum computers. We focus on quantum chemistry, finance and energy as well as material simulation, quantum image processing and quantum machine learning.

Fraunhofer operates "Quantum System One"

However, quantum computing has also been possible in Europe since June 2021: Together with IBM, Fraunhofer operates the quantum computer Quantum System One under local data protection law. It is available to companies and research organizations to develop and test quantum algorithms in an application-oriented manner and to build up know-how.

Solutions for imaging and energy

The Fraunhofer lead project "QUILT" (Quantum Methods for Advanced Imaging Solutions) already started in 2018. In close cooperation with industry, six Fraunhofer institutes are jointly researching imaging methods in the terahertz spectral range based on quantum optics. Initial successes, the generation of suitable photon pairs, have already been recorded and the next steps planned. Researchers from our institute play a key role in the project in modeling, simulating and optimizing quantum-based contact-free methods.

Another project is the joint project "EnerQuant". It uses the advantages of quantum computing for optimization problems in the energy industry. Funded by the German Federal Ministry for Economic Affairs and Energy (BMWi), researchers are developing algorithms for qubit-based quantum computers and quantum simulators. These are to be used to solve a fundamental model of the energy industry with stochastic influencing variables.

More information at www.itwm.fraunhofer.de/quantum-computing

EnerQuant: Quantum Computing for the Energy Industry

Complex optimization problems with many variables are difficult for classical computers to solve. Only recently have certain quantum computers achieved promising results in solving optimization problems – with the potential to handle even discrete variables. In the joint project "EnerQuant: Energy Economics Fundamental Modeling with Quantum Algorithms", our researchers from the departments "Financial Mathematics" and "High Performance Computing" are exploiting advantages of quantum computing for the energy industry.

Optical system for laser cooling and control of ultracold sodium atoms in the laboratory at the Kirchhoff Institute for Physics Heidelberg

"In short, in the EnerQuant project we are developing algorithms for qubit-based quantum computers and quantum simulators for the solution of a fundamental model of energy economics with stochastic influencing variables," explains Kerstin Dächert, member of the "Financial Mathematics" department at Fraunhofer ITWM and project coordinator. Together with colleagues from the department "High Performance Computing", she and her team are conducting research in the joint project with universities and companies from industry.

As a basis, the researchers define a simple fundamental model that can be translated into a quantum mechanical problem and realized on a quantum simulator. This is implemented in a prototype made of cold atoms and tested for its performance in order to successively further develop the fundamental model and quantum simulator. The long-term goal is to model the German electricity market with sufficient stochastic accuracy.

Exploiting new potential

EnerQuant makes it possible to exploit the potential of new computing technologies for energy-economy modeling. The researchers show how fundamental models can be formulated to use the computing power of quantum simulators and thus make a long-term contribution to the further development of energy system modeling. The results will be incorporated into the software platform of the partner JoS QUANTUM and will be available to industry after the end of the project. Furthermore, EnerQuant provides an analysis of the potential of quantum computers and compares their efficiency with classical hardware and alternative approaches to solve optimization problems.

EnerQuant started in September 2020 with a duration of three years and is funded by the German Federal Ministry for Economic Affairs and Energy (BMWi). In addition to Fraunhofer ITWM, Fraunhofer IOSB-AST, the Universities of Heidelberg and Trento, and Jos QUANTUM are also part of the network.

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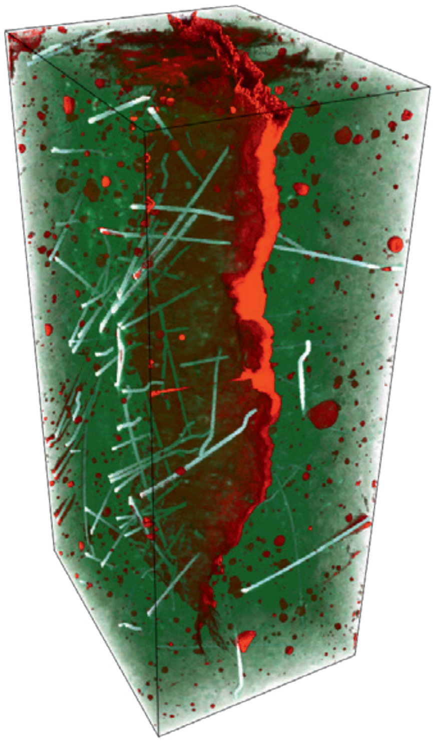
Observing the Inner Structure of Concrete Beams During Bending – Quantum Computing Accelerates the Evaluation of CT Data

Higher resolution, faster and new acquisition methods – the amount of image data is growing faster than the speed of analysis methods. This poses new challenges for industrial image processing. Quantum image processing promises a remedy. One example is computed tomography during mechanical tests.

Gulliver, the computed tomography portal of the TU Kaiserslautern, is a unique experimental facility that will make it possible to image the internal structure of concrete beams during bending tests. Gulliver generates approximately 120 GB to 2 TB of image data per experiment. The aim of the current research is to analyze the structural changes like crack initiation and growth while the test is in progress.

Bringing theory and practice closer together

Skillful use of the special properties of qubits makes it possible in principle to represent such large image data with just a few qubits, e. g. 1024 × 1024 pixels with 21 qubits. If the currently used processing and analysis algorithms were replaced by quantum counterparts or quantum physical pendants, more efficient processing of enormous amounts of data as produced by Gulliver would be possible. Theoretically, both storage and computational requirements could be reduced exponentially.



3d rendering of cracks in a concrete sample with reinforcing steel fibers.

Practically, encoding the image and running algorithms require a huge number of individual quantum operations. The results of simple image processing steps on small images are therefore often noisy beyond recognition at present. Like in quantum computing in general, noise models and algorithms that require as few basic operations as possible are therefore the subject of current research.

More information at www.itwm.fraunhofer.de/surface-and-material-characterization

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Health and Medicine

Improving health care, increasing the chances of healing, supporting diagnoses – these are some of the goals that Fraunhofer-Gesellschaft aims to achieve with results in medical, environmental and nutritional research. Intelligent, assistive systems that provide support in preventive health care, diagnostics, therapy and nursing care and make a significant contribution to safeguarding society's future are intended to help achieve these goals. We are focusing, in particular, on tools to support decision-making in therapy planning and to strengthen resilience.

Health 4.0: Accelerating the Development and Production of New Medicines

In the Fraunhofer Innovation Cluster "Production for Intelligent Medicine", research is carried out on how gene or cell therapeutics as well as vaccines can be produced in large quantities in an automated, fast, and cost-effective way. 23 Fraunhofer institutes are involved, including the "Optimization" department of ITWM.

Innovative advanced therapy medicinal products (ATMPs) represent a new, promising class of therapeutics as "living medicines". They have the potential to offer new therapeutic options to people suffering from diseases that have so far been untreatable or insufficiently treatable. This applies to some cancers, some of which even have a chance of being cured by such new therapies. However, the production of these cell-based, new therapeutics has so far been highly manual, making them time-consuming and expensive and limiting their availability to patients.

Combining Industry 4.0 with Health 4.0

To further develop this promising approach, Fraunhofer researchers from different disciplines want to fundamentally redesign the production of such ATMPs. In the cluster, experts from biological and medical research have worked closely with their colleagues from the fields of automation, process control, quality management, robotics and mathematics to set up the processes for high throughput and reasonable manufacturing costs in the future. In the first phase of the project, a modular pilot plant was designed for the automated production of therapeutics.

To this end, a team led by department head Prof. Michael Bortz modeled bioprocesses that can now be optimized virtually. Researchers led by Dr. Heiner Ackermann were responsible for questions relating to the capacity planning of production plants. The aim is to maximize throughput at the lowest possible cost. Dr. Neele Leithäuser and colleagues developed methods for analyzing data streams (time series) that are continuously collected for monitoring production processes.

More about the innovation cluster at s.fhg.de/pharmaproduction

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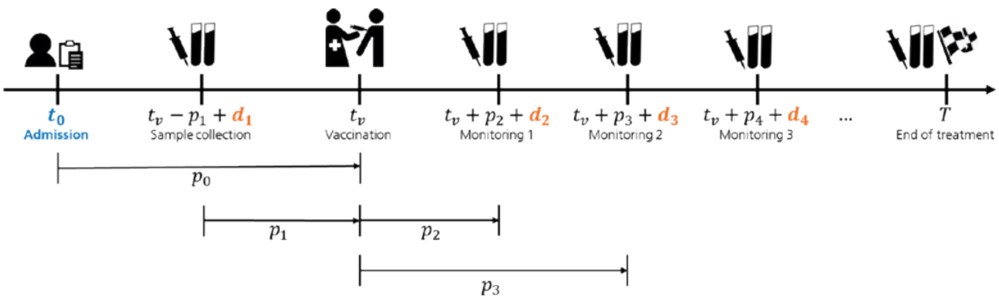
Making Uncertainties Plannable

Testing the efficacy of new medicines or therapies on humans is an important part of biomedicine and pharmaceuticals. However, the path of patient samples to those who process them is riddled with uncertainties.

A pharmaceutical company needs patients who are willing to participate in a study for a new drug. "The uncertainty already starts with the question whether enough patients can be enrolled in the participating clinics during the planned study period," says Dr. Sandy Heydrich, who heads the process planning team at Fraunhofer ITWM. "There's a lot of stochasticity in workload generated by the clinical trial," says Dr. Heiner Ackermann, deputy head of department "Optimization – Operations Research".

The daily workload of those who process the samples is often uncertain because it depends on the number of incoming samples, some of which have to be processed within a certain



During a drug trial, there are several sources of uncertainty: the start of the trial, samples arriving too early or too late, or treatment ending prematurely.

the process. This is because not only is the enrollment of individuals in clinical trials to some degree subject to chance, but the arrival of samples for study is also stochastic.

Goal: Predict workload in the laboratory

The "art of guessing", the basis of stochastics, accordingly characterizes the work in this environment. On behalf of a biotechnology company, the team at Fraunhofer ITWM is looking for mathematical solutions to make the entire process more predictable, up to and including personnel scheduling. "If there were no uncertainties, we could calculate the arrivals of the samples individually and determine the period of time due to their shelf life. The more accurately it is predicted how many samples will arrive and when, the better the workload in the lab can be planned. The team led by Heydrich and Ackermann aims to use a mathematical model to provide answers to many questions, such as: Is the current staff sufficient for the workload that will be generated?

Making every day more predictable

he project partner's goal is to optimize staff scheduling based on the samples that are likely to be received. For this purpose, the researchers are developing a simulation tool that provides a forecast of the number of sample arrivals for each study day. The core of the

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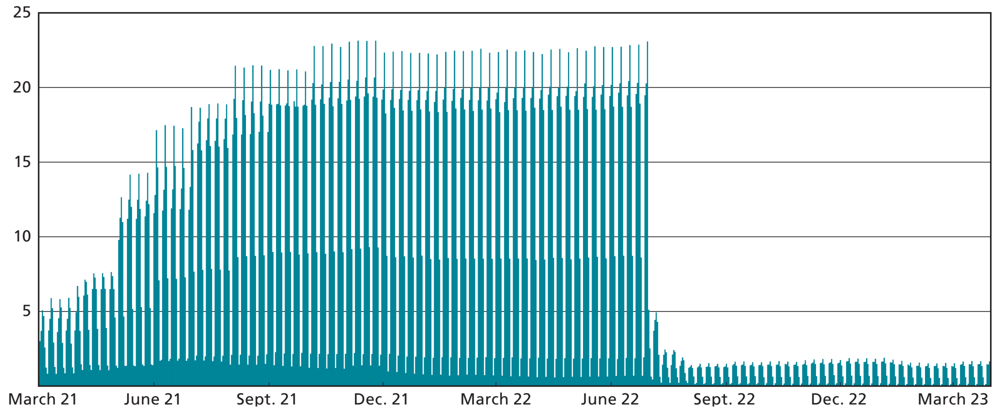

Our researchers have developed a simulation tool that uses several parameters to predict the number of sample arrivals on each day of the time horizon. These results are used to perform a what-if analysis, which is used to optimize staff scheduling.

model is a Monte Carlo simulation to estimate the number of sample arrivals at the production site for each day in the time horizon of the study. The influencing parameters are taken into account, but also different scenarios are represented, such as the fluctuating number of patients. The variable level of detail of the model optimally supports the planning process in every phase.

More information at www.itwm.fraunhofer.de/layout-cutting-problems

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Energy-Efficient AI Chips for Atrial Fibrillation Detection

A system for the reliable detection of atrial fibrillation that is as energy-efficient as possible – that was the task of the pilot innovation competition of the German Federal Ministry of Education and Research (BMBF).

AI systems can improve healthcare, increase patients' chances of recovery and support doctors in their diagnoses. But they may also require high amounts of energy. Together with the Fraunhofer Institute for Integrated Circuits IIS, a working group from our High Performance Computing department was awarded first prize. Our project HALF (Holistic AutoML for FPGAs) is a holistic approach to the optimization of artificial neural networks and FPGA (Field Programmable Gate Arrays) architectures. For the competition, the neural network not only had to consider performance, but also had to be supplemented by the factor of energy efficiency, so that the dangerous atrial fibrillation is detected with maximum efficiency to allow longer runtimes for mobile ECG devices.

AI model decides on the energy consumption of the hardware

But how exactly do you find the networks that meet the defined requirements and specifications? "There are various search strategies here, and we use an evolutionary approach. We start with ten different randomly selected networks, train and test them. Then we select the two best networks and mutate them, creating ten new network variants," explains Dr. Jens Krüger. "We repeat this process with a unique approach for the selection and mutation until we find the best network. This is a process of automated machine learning – or AutoML."

In search of the ideal network

The researchers are extending this process to include a holistic approach that looks not only at the neural network but also at the hardware, since the AI model affects the hardware's energy consumption. To do this, they use FPGAs as a form of a programmable chip. An FPGA can be reprogrammed any number of times – very helpful in finding the optimal neural network mapping.

This has now resulted in a new unifying methodology that is energy efficient, reduces development time for optimal neural network topologies, and enables appropriate FPGA implementations. These software tools are suitable not only for FPGAs, but also for a wide variety of chips and system architectures, and enable the analysis of patient data even on mobile devices. This potential has been recognized and awarded by the BMBF a resulted in the Neural Architecture Search Engine (NASE) Tool.

Further information at www.itwm.fraunhofer.de/HALF_en

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New Approaches for Radiotherapy

With the approach of viewing radiotherapy as a multi-criteria optimization task, our researchers have significantly advanced the medical treatment of cancer in recent years. The "Patient Positioning" project aims to set further standards in the fight against cancer. An interview with Dr. Philipp Süss, from the "Optimization Technical Processes" department.

Why does the project put "Patient Positioning" to the test in radiotherapy?

The planning of radiation therapy begins with a detailed computed tomography (CT) scan. The treating physicians use this CT image to plan the dose with which they will irradiate a tumor. The problem is that the location of critical organs and tumors on the day of treatment are no longer identical to those on the plan CT, for example because the stomach or bladder fill varies. Reconstruction is very difficult, but significant in determining the dose the person will receive on the day of treatment. Many therapy devices nowadays offer the possibility of recording a less detailed CT immediately before the start of radiation in order to adjust the position on the day of treatment as close as possible to that of the previous recording.

Can the treatment be adjusted at such short notice?

Yes, the planned daily dose can be adjusted according to the acute condition of the person to be treated. The dose becomes more important than the image. This is exactly where we come in: We want to ensure more effective treatment by shifting the focus away from the image to dose control. To do this, we are developing a software solution that compares the current image with the previously acquired one and formulates an updated recommendation for the radiation dose. Currently, hospitals are looking at how to correct the patient setup based on

The software developed by ITWM researchers shows the calculated dose in color, which can be optimized with a slider.

the difference between the current CT image and the planning CT. We are trying to reconstruct the planned dose.

What stage is the project at?

Quite far along. Our industrial partner Varian Medical Systems has commissioned a software prototype, and the basic feasibility is given. The software is now being tested at Rutgers University Hospital in New Jersey using image data from past patients. In this way, we want to verify that the method brings the desired benefits, but also to test the workflow. For staff performing radiation, the usual workflow changes when they use the software to look at the dose rather than just the image.

More information at www.itwm.fraunhofer.de/radiation-therapy

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Fraunhofer ITWM versus Corona

The year 2020 will always be inextricably linked with the Corona pandemic. The new kind of virus shook all areas of public life. Its worldwide spread was declared as a "public health emergency of international proportions". The pandemic changed people's everyday lives and suddenly presented companies, the economy and the global economy with unexpected challenges. Fraunhofer immediately initiated the "Fraunhofer vs. Corona" action program in order to make scientific findings applicable as quickly as possible in the fight against the pandemic. Fraunhofer ITWM contributed to the fight against the virus with mathematical methods and is one of the institutes with the most anti-corona projects.

Using Mathematics Against COVID-19

In the fight against the Covid-19 pandemic, our experts have been involved in various research projects from the very beginning. They are supporting society and industry in a number of ways and in different areas in coping with the Corona crisis using mathematical methods. A selection of our activities at a glance:

EpiDeMSE – Support for decision-makers

Providing decision-makers at the local level with the best possible support in planning measures – that is the goal of the EpiDeMSE project (Epidemiological Modeling, Simulation and Decision Support). In April 2020, researchers within the framework of the Fraunhofer-Gesellschaft's Anti-Corona Program began working on a tool that provides forecasts of epidemic progression straight away. The model uses time-varying parameters that are estimated from the collected case numbers and compared with other statistical data. In this way, the effectiveness of the measures on the infection rate can also be assessed.

Site planning for vaccination centers

Even before a vaccine against the SARS-CoV-2 virus was available, researchers at Fraunhofer ITWM were already working together with the Robert Koch Institute and Technical University of Kaiserslautern on the site planning for vaccination centers. Answers to questions with many unknowns had to be found: How many vaccine doses are available? Who will be vaccinated first? Where should vaccination take place? In their publications, the researchers looked at different location scenarios and evaluated, among other things, the number of physicians needed, the distance of the population to the vaccination centers, and the number of locations.

Cooperation with the DFKI

Pooling expertise to achieve more together: Together with the German Research Center for Artificial Intelligence (DFKI), researchers at Fraunhofer ITWM have developed a model that simulates and examines possible opening scenarios. EpiDeMSE was used for this purpose. The result is a clear and easy-to-understand visualization of the infection situation and a forecast of future regional developments.

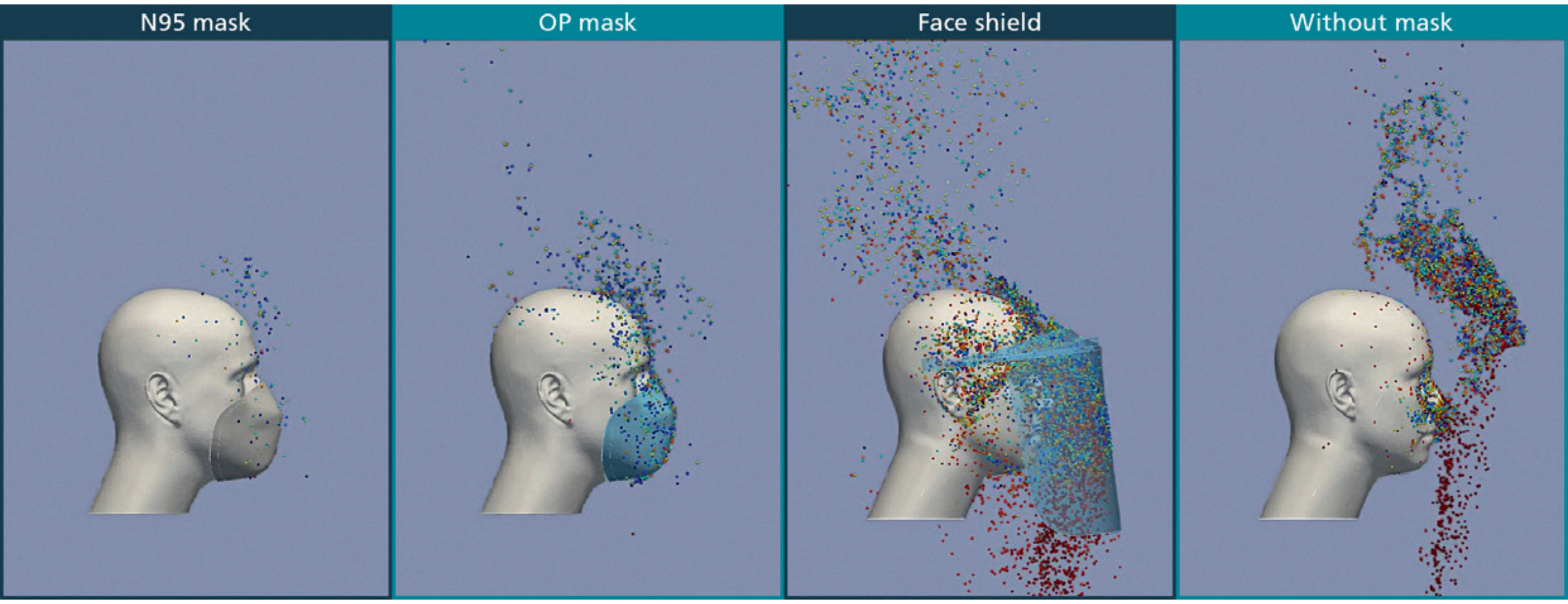
Scatter plot: Blog and podcast

Since the beginning of the pandemic, the statistics blog "Streuspanne" has been devoted to questions and statistical parameters that have shaped the discussion about Corona. In addition to a three-part mini-series on Corona testing, blogging mathematicians and statisticians Dr. Sascha Feth and Dr. Jochen Fiedler also address mutant Corona viruses and conspiracy theories. In the podcast of the same name, the two scientists can also be heard making statistics understandable for laypeople.

More information at www.itwm.fraunhofer.de/itwm-vs-corona

All social media activities under the hashtag #ITWMvsCorona

AVATOR – How Do Aerosols Spread Indoors?



Different types of protective mouth-nose coverings prevent the spread of aerosols to varying degrees.

The Covid-19 pandemic has made many people aware that infectious aerosols play a major role in the spread of disease. In the project "AVATOR" (Anti-Virus Aerosol: Testing, Operation, Reduction), several Fraunhofer institutes are investigating ways to assess the risk and reduce the danger of infection by aerosol-borne viruses. For this purpose, an interdepartmental team at ITWM is developing a multiscale simulator which calculates the aerosol propagation in indoor environments.

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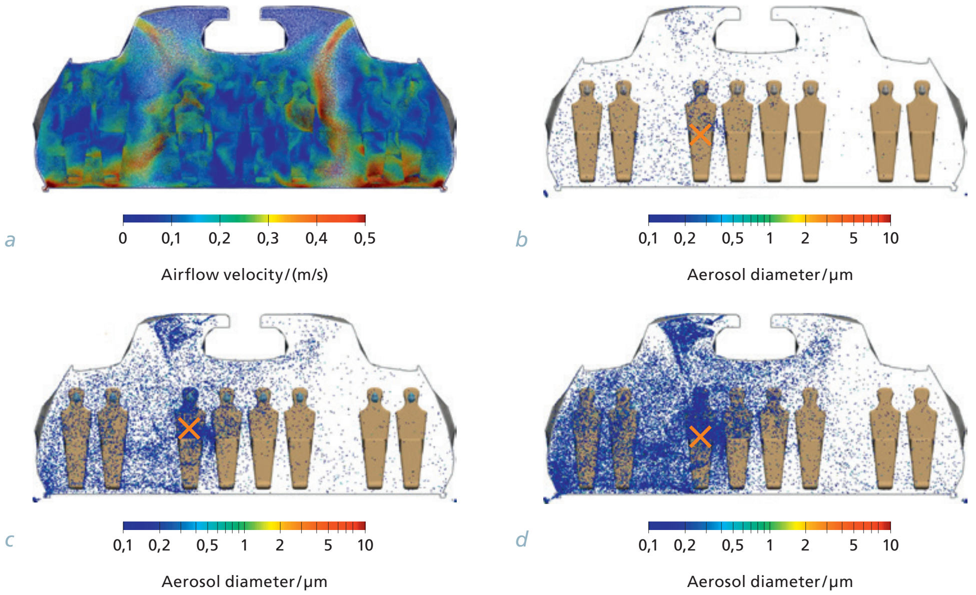
Ventilation to fight Corona? SARS-CoV-2 can be transmitted via aerosols – airborne droplet nuclei smaller than ten micrometers. This is also possible in certain situations over greater distances, for example when many people congregate in insufficiently ventilated indoor spaces.

Digital twins simulate situation and form basis for concepts

Against this background, distance, the number of people in rooms, and indoor air hygiene and ventilation are important building blocks in the pandemic. Especially for educational institutions, hospitals, care facilities, hotels, airplanes or trains and offices as well as production facilities, the researchers in the project are looking for answers to hygienic questions as well as practical solutions to prevent the spread of aerosol infections.

In indoor environments, aerosols do not simply disappear, but spread throughout the room over time. In addition to cleaning technologies for indoor air, AVATOR also investigates the spread of aerosols and derives hygiene concepts for specific applications. The researchers are modeling the dispersion mechanisms using ITWM simulations



Simulation scenario airplane – How do aerosols disperse in the interior? Aerosol dispersion starting from the marked person with different masks: a. Airflow velocity; b. N95 masks; c. OP masks; d. without masks

ITWM expertise of many years helps with implementation

Dr. Ralf Kirsch, team leader "Filtration and Separation" of the "Flow and Materials Simulation" department, adds: "In our work, we at ITWM benefit greatly from the fact that we can draw on a broad spectrum of expertise – in this case, our many years of experience in the field of modeling and simulation of filters are very helpful."

Multiscale approach takes several somponents into account

The multiscale approach also incorporates fine details into long-term observations – such as the type of individual protective equipment. Which mouth-nose covering protects how? The researchers then use the simulation results to derive a risk assessment that can be used to compare different indoor air concepts for each scenario.

In parallel to the simulation-based assessment procedures for air dispersion, the participating institutes are developing various air purification technologies. These findings are finally tested in laboratory environments as well as validated in real environments. The project results will then lead to new concepts for reducing the risk of infection with SARS-CoV-2.

In this way, sensible hygiene measures can be developed and the effectiveness of existing ones validated. AVATOR is part of the Fraunhofer Society's "Fraunhofer versus Corona" program and runs until September 2021.

Detailed information about the project including simulation videos
www.itwm.fraunhofer.de/avator_en

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Meltblown: Less Clouds in the Simulation Sky

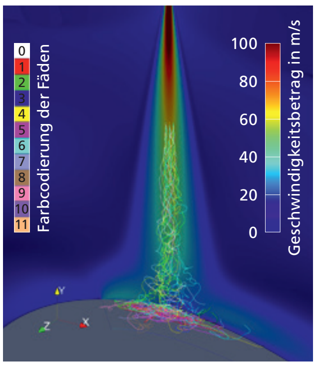
Nonwoven production is getting more attention than ever from the general public in Corona times, because nonwovens are crucial for infection control. Mouth guards, disposable bed linen, surgical gowns, wound protection pads and compresses are just a few examples. The ultra-fine nonwoven products are manufactured in so-called meltblown processes. ITWM simulations help to better understand the production processes and design them more efficiently. Researchers of the "Transport Processes" and "Flow and Material Simulation" departments provide support with their expertise.

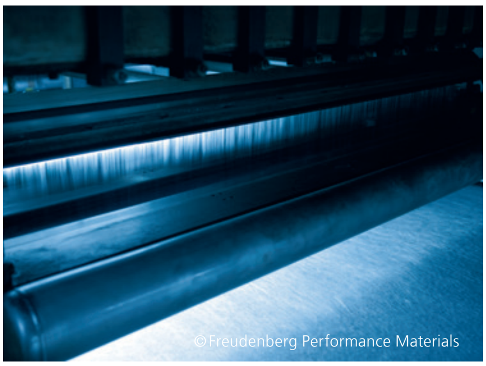
For example, in the Fraunhofer-internal project "ProQuIV", the entire production chain of infection protection is optimized in this way. The abbreviation stands for "Production and Quality Optimization of Nonwoven Infection Protection Clothing". This is because bottlenecks in the production of these materials were observed at the beginning of the crisis. For the class of meltblown nonwovens, increasing the efficiency of production is particularly difficult because these processes react very sensitively to fluctuations and material impurities.

Digital twin optimizes meltblown process

"Meltblown" is the name of the industrial production process whose ultra-fine fiber nonwovens are responsible for providing the crucial filter function in face masks. In this process, the molten polymer is forced through nozzles into a forward-flowing, high-speed stream. It is dispersed and cooled in a highly turbulent air flow. This is how the individual fibers (filaments) are formed. They swirl under the air flow, entangle and stretch, and fall more or less randomly onto a conveyor belt, where they solidify further as they cool.

In this process, a key factor is the behavior of the filaments in the turbulent, hot and fast air flow. The filaments' properties are affected by this air flow. "The complex process poses a great challenge in simulation," explains Dr. Walter Arne of Fraunhofer ITWM. He has been working at the institute for years on the simulation of various processes related to filaments, threads, and fibers. "This is because the quality of the filaments, and thus in the end of the nonwovens, is influenced by many factors. For example, by an aspect we call cloudiness." In the graphic on the right, it is clear what is meant by this: How homogeneous is the nonwoven? "Product quality can be greatly improved if non-uniformity is optimized. Our simulation helps with figuring out how to do that," the researcher adds.

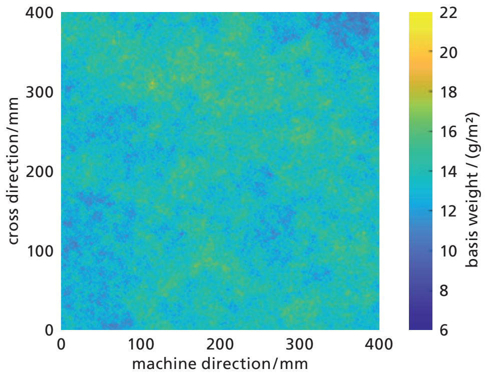




Left: Simulation of filaments in the meltblown production process. Right: Production of nonwovens using the meltblown process in Kaiserslautern.

Top: Quality control of a meltblown material in the clean room area. Bottom: Cloudiness: How homogeneous is the nonwoven? Simulated basis weight distribution as a measure of the homogeneity of the nonwoven.

This is where ITWM software comes into play. "With our Fiber Dynamics Simulation Tool FIDYST, the movements of the fibers, their stretching, their falling, and the orientation with which they land on a conveyor belt are predicted. Depending on the process settings, specific turbulence is created and thus nonwoven qualities that differ, for example, in structure, cloudiness, basis weight and strength," explains Arne.



Simulation across the entire process chain

Digital twins and calculations from Fraunhofer ITWM help to simulate and better understand the processes. The production of technical textiles thus not only becomes more efficient, but the nonwovens can be developed virtually without having to realize this in advance in a test facility. In this way, production capacities can be increased while maintaining quality. Simulations save experiments, allow new insights, enable systematic parameter variations and solve upscaling problems that can lead to bad investments in the transition from laboratory to industrial plant.

However, the virtual implementation of the meltblown process also opens up new opportunities for optimization at other levels: In the upscaling of industrially relevant processes, such as mask production, the ITWM expertise concerning filters is also used. The "Filtration and Separation" team headed by Dr. Ralf Kirsch has been working for many years on the mathematical modeling and simulation of various filters.

More information, including simulation video, at www.itwm.fraunhofer.de/meltblown-process-simulation

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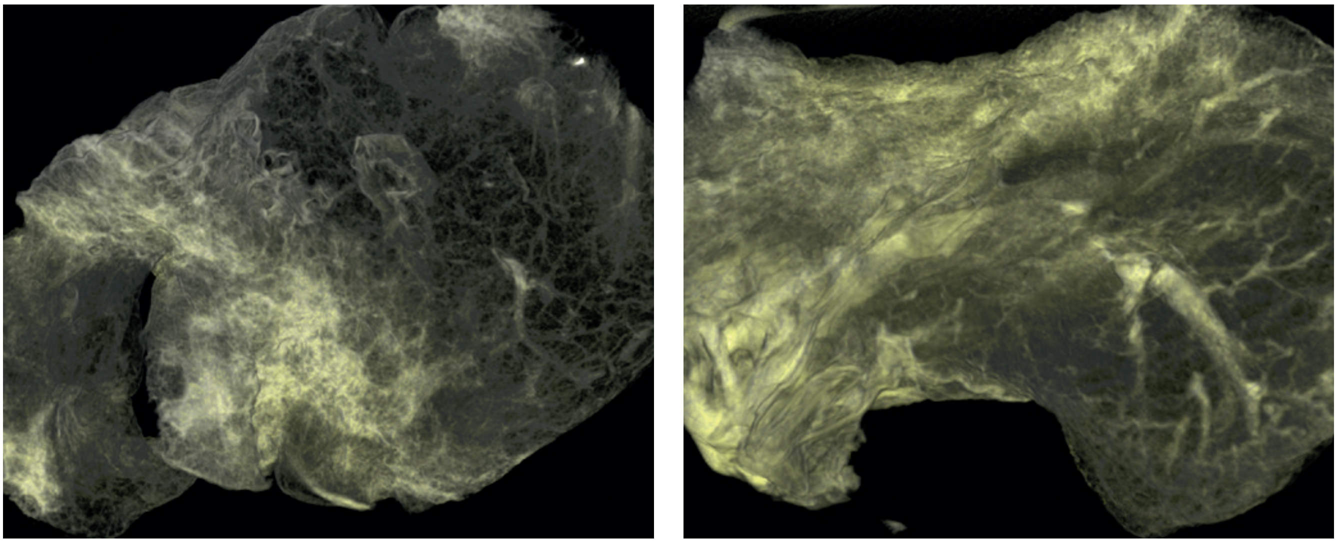
Better Understanding Lung Damage from COVID-19

How exactly does the Sars-CoV-2 virus damage the lungs? To answer this question, medical researchers have looked deep into the microstructure of the lungs. Changes caused by Covid-19 can be easily detected with traditional X-rays or thoracic computed tomography. However, to understand the microstructural changes and pathophysiology of Covid-19-induced cardiopulmonary failure, they need microradiological studies. The image analysis algorithms of Fraunhofer ITWM help the Heidelberg Clinic to analyze the image data.

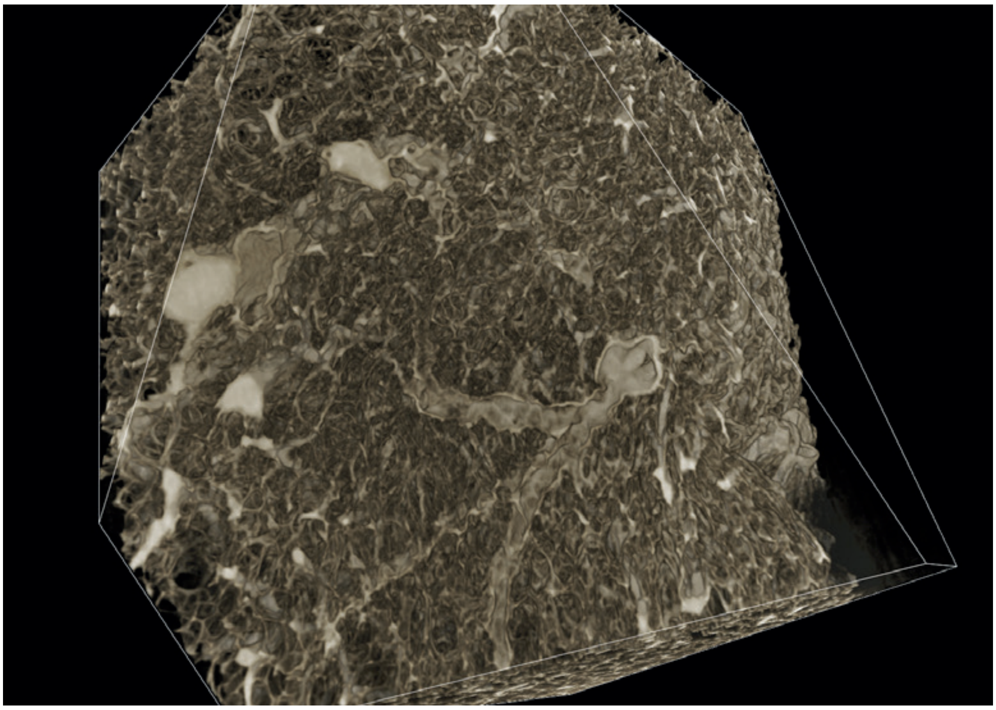


Volume visualizations from the left upper lobe of the lung; sections of size 14 cm × 14 cm × 1.4 cm are shown here.

The University Hospitals of Göttingen and Heidelberg are investigating lung tissue from patients who died of Covid-19 using computed tomography with synchrotron radiation (SRµCT). Thanks to the high resolution and good signal-to-noise ratio, capillary vessels can be visualized and analyzed in the SRµCT volume images. "However, this produces very large amounts of data on very different scales; we can analyze and interpret these with our methods," says project leader Dr. Katja Schladitz.

Similarity between mice and humans – at least in lung tissue

Years ago, the Image Processing department developed algorithms to analyze capillary vascular systems in SRµCT images of prepared mouse lungs and observed regenerative growth at different stages. Typical signs of vascular growth were detected and quantified in 3D images for the first time. In the case of Covid-damaged lungs, the goal is to uncover the



A high-resolution image section from the visualization of the lung tissue of 5.4 mm × 5.4 mm × 4.5 mm: The vascular wall system is visible; the alveoli can be guessed as pores.

causes of typical changes observed on clinical CT: Is local compaction due to tissue scarring, congestion, or hemorrhage? Does the morphology of the vessels change? Which vessels are damaged and how? The answers to these questions help to better understand the disease process and typical symptoms and specify treatment options for Covid-19-induced pneumonia.

"Fraunhofer vs. Corona"

Fraunhofer-Gesellschaft reacted very quickly to the pandemic and launched the "Fraunhofer vs. Corona" action program as early as April 2020. Experts worked, and are still working, at the forefront of the fight against the pandemic, supporting industry and society in coping with direct effects and later consequences. The focus is on anti-Corona projects in the medical and health sectors, such as vaccine development, innovative diagnostics and drug development, but also in the provision of IT capacities. Fraunhofer also provides technological support in the production of components for protective equipment. Accompanying preliminary research also paves the way to a more resilient society.

Fraunhofer ITWM successfully participated in the action program with eight project proposals – the Covid-19 analysis for synchrotron images presented here is one of the funded projects.

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Mobility

Mobility determines a major part of life, globally and locally. Appropriate technical and conceptual solutions are needed to guide traffic, make it safer and conserve resources. With our partners in the automotive industry, we focus our activities on vehicle-environment-human interaction and develop software tools for virtual product development and product creation in the digital factory.

The ITWM Technical Center – Experiments and Simulations Consolidated

Simulations have long played a major role in mobility research and are becoming increasingly important, especially in virtual product development in the vehicle sector. This is the focus of our "Mathematics for Vehicle Development" division, which combines the necessary technical testing facilities in its technical center. Here, we develop our own measurement and simulation techniques, which are built hand in hand with the modeling and simulation methods as well as software tools.

Hardware and ssoftware as the technical bedrock of our research

The simulator center includes the robot-based driving simulator RODOS® (RObot based Driving and Operation Simulator), the static driving simulator VI-Grade compact DIM and the virtual reality laboratory. The measurement technology is provided by REDAR (Road and Environment Data Acquisition Rover) – a 3D laser scanner vehicle – and the highly automated measurement machine MeSOMICS® (Measurement System for the Optically Monitored Identification of Cable Stiffness). It is used to determine cable stiffness.

Virtual environment for cars and commercial vehicles

The RODOS® driving simulator represents the largest of the facilities at the technical center and allows the exploration of situations right up to the moment before a crash in a detailed, highly reproducible and risk-free environment with the aid of interactive simulation. With a payload of 1000kg, the robot arm allows the use of standard tractor and excavator cabs as well as real car bodies. Inside a spherical projection dome measuring ten meters in diameter, 18 projectors create a seamless projection of an interactive scene, whereby, for example, driver-vehicle-environment interactions are studied. RODOS® is currently the most powerful driving simulator of Fraunhofer society. We also use the static simulator VI-Grade compact-DIM for model development as well as for cooperative driving simulation and mapping of complex mixed traffic situations. This system is optimized for the interactive simulation of passenger cars and is used in particular for the development of our CDTire/Realtime software

VR Lab for people in complex environments

The Virtual-Reality Lab opens up the possibility of placing people in complex environments and scenarios. Applications can be found in driving simulation, production and factory planning as well as visualization. One or more people can experience a virtual reality as a pedestrian in our laboratory, on a surface of ten by six meters. Human reactions can also be studied in highly complex traffic situations by interfacing with the simulation environments of RODOS® and VIGrade compact DIM via a real-time data interface.

More information at www.itwm.fraunhofer.de/technikum_en

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CDTire – Reinventing the Tire with Simulation

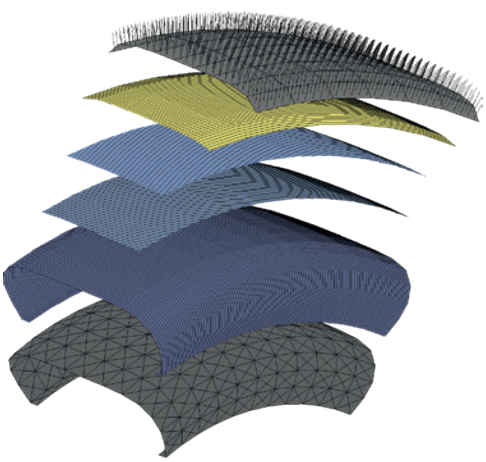
The tire modeling software has long been an integral part of the product range in the field of "Mathematics for Vehicle Engineering". In an interview with Dr Manfred Bäcker, head of the "Tire Modeling" group, we wanted to find out the unique selling points of CDTire:

CDTire is a tool for the simulation and development of tires. What does it do and who works with it?

Historically, tire simulation models such as CDTire were first used by the automotive industry. They were needed to enable full vehicle simulations on digital (measured) test tracks in the virtual vehicle development process in order to obtain statements about comfort, operational stability and driving dynamic properties of a development status early in the development process and to further improve it. The tire industry, on the other hand, uses detailed tire models, which, however, are not applicable due to their very high computational simulation cost. Moreover, they are not readily made available to third parties, i. e. not even to customers in the vehicle industry, because they also contain design details which are regarded as proprietary know-how. That is why the automotive industry has always has always been dependent on tire models developed outside the tire industry. Because of the demand for low computational cost, these very much simplified models were inferior to the finite element (FE) models of the tire industry.

And this is where CDTire comes into action?

Exactly! With the CDTire model generation, developed between 2010 and 2012, we have provided simulation models of tires for the first time that are accepted and used as development tools in both the automotive and tire industries. The key to this success is a model framework which simulates tire geometry and structure with similar accuracy as the tire industry's FE models – but at hundred times the computational speed.



CDTire/3D: Functional layer concept

What does CDTire do in the virtual pre-development of tires? What do the individual process steps look like?

Since CDTire/3D is suitable for all applications from driving dynamics to comfort to "Noise Vibration Harshness", the software suite allows evaluations for these development criteria at a very early stage. In addition, since 2018, we have established a new method for the subjective evaluation of tires on driving simulators in cooperation with the tire manufacturer Goodyear via corresponding pilot projects with vehicle manufacturers such as Maserati. For this, we use the real-time capable CDTire/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Realtime, which is derived from CDTire/3D. This innovation is so important because the subjective evaluation of a tire by professional test drivers is still the pinnacle of the development process: Only their OK releases the tire. However, this usually requires many iterations and a corresponding tire prototype must be produced in each iteration. Vehicle prototypes must also be available, of course. The goal is to complete 90 percent of this time-consuming and cost-intensive process on the driving simulator using virtual tire and vehicle prototypes, so that ideally only the final acceptance has to take place on the real test track. This can save immense costs and development time.

What were the biggest challenges in software development in recent years?

We have consistently designed the new generation of CDTire as a “multi-physics tool”. Thus, the actual structural mechanical tire model has been extended in recent years by a thermodynamic model (CDTire/Thermal) for the simulation of temperature propagation within the tire and also by a model for the air flow within the tire – the so-called cavity model. These different physical sub-models require a high degree of modularity in software development and also pose a challenge to the numerics of the overall model, because the structural model, temperature model and internal air model naturally interact with each other. The overall model thus becomes a so-called “multi-scale model”. The computational step sizes of the sub-models are on different scales and must be coordinated against each other to achieve good overall performance. The modularity and extensibility in the sense of a multi-physics tool with simultaneous high computing speed is the greatest challenge.

CDTire contains a whole family of tire models that are used by both tire and vehicle manufacturers. What new properties will be considered in CDTire in the future?

We achieved the greatest development progress and at the same time the greatest success in attracting new customers by adding the dynamic inner air model. The new application allows a good prediction quality for full vehicle simulations in a frequency range up to 300 Hz. Pilot users were Audi and Maserati, which we were able to win as customers. In the near future, the prediction quality is to be further increased by linking the tire model to a flexible rim model. Furthermore, CDTire is to be extended for the “Air-Borne Noise” application. Here, we simulate the transfer of structural vibrations of the tire surface into the outside air and their feedback via the body into the vehicle interior.

More information at www.itwm.fraunhofer.de/cdtire_en

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Making Better Use of Data – AI and ML in Vehicle Engineering

Whether measured in test vehicles or recorded in modern vehicles during operation: In the automotive sector, the availability of data has been increasing for years. This also applies to quantity and quality of environmental data: digital maps, climate, topographical data and even socio-economic information are flowing into the growing data pool. The technologies used to collect and process this data are also constantly being improved, which is why methods of artificial intelligence (AI) and machine learning (ML) can be used very efficiently and effectively today, to extract valuable information from the sheer volume of data.

Modern vehicles are bubbling sources of data. AI methods help to use and understand the flood of data.

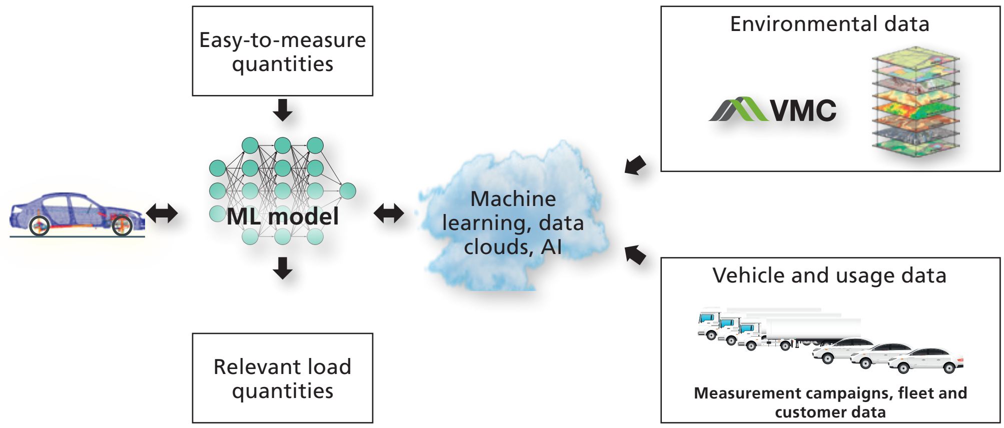
©istockphoto/metamorworks

In our department "Mathematics for Vehicle Engineering – Dynamics, Loads and Environmental Data", such methods are used to incorporate the knowledge gained in the process into the vehicle development process at an early stage. For example, in the form of the Virtual Measure Campaign VMC® software suite: Its aim is to compile and maintain environmental data in a geo-referenced database covering as much of the world as possible and to link it with mathematical analysis tools. With the help of driver, vehicle and environment models, VMC® can predict traffic-dependent speed profiles thanks to efficient simulation technology and – based on this – derive statements about vehicle loads and energy demands.

Another profound benefit for the entire development and safeguarding process arises in the next step through the combination of usage data on the one hand and vehicle and environmental data on the other hand.

From the vehicle directly in the cloud

Modern vehicles reveal a lot about their use because they record numerous condition variables; commercial vehicles are also often equipped with a telematics system that sends the collected data to a cloud at regular intervalsFor commercial vehicles, especially for agricultural and construction machinery, the usage



Environmental data, vehicle data and models support the development process of modern vehicles and their operation.

variability is very high, depending on the customer group and region of use: For example, a truck in the mountainous regions of the Caucasusis exposed to very different loads than a truck that transports its load mainly in mainly in central Europe. Or an excavator in a sand pit compared to an excavator that crushes construction debris and separates it into "metal" and "concrete".

For the development process, it is therefore of particular interest to know as much as possible about the actual use of a vehicle in order to set the right design and testing criteria.

AI recognizes type of use

To draw the right conclusions from the data at hand, AI and ML come into the game. "At this point, we use an ML-based detection algorithm that recognizes the type of use, for example 'digging' in the case of an excavator," explains Dr. Michael Burger, deputy head of the "Dynamics, Loads and Environmental Data" department. "Once an appropriate ML model is trained, we can derive very accurate and very efficiently usage profiles, specific to groups of people and their respective regions of use. However, equipping a large number of commercial vehicles with sensors that are precise and sensitive requires a lof of effort and a robust operation is usually costly and time-consuming. "As an alternative or complementary approach, we also use data-based and hybrid models that predict relevant internal quantities, such as internal component forces. For this purpose, we use easily measurable external quantities such as accelerations at axles or on the frame," says Michael Burger. This makes it possible to avoid numerous sensors and complex measurement technology.

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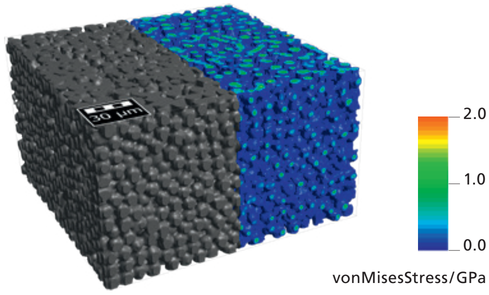
DEFACTO – E-Mobility Gains at the Cellular Level Are Picking up Speed

Revolutionizing european battery cell production

The EU's DEFACTO project has set an ambitious goal: to develop a modeling toolchain for e-mobility batteries that describes all relevant aspects ranging from battery materials, the manufacturing process to the macroscopic cell behavior. These tools are expected to improve understanding and lead to faster, more favorable development processes for novel cell types and to extended lifetime of the batteries. The ITWM team under Dr. Jochen Zausch is focusing on the modeling and simulation of cell performance and aging mechanisms.

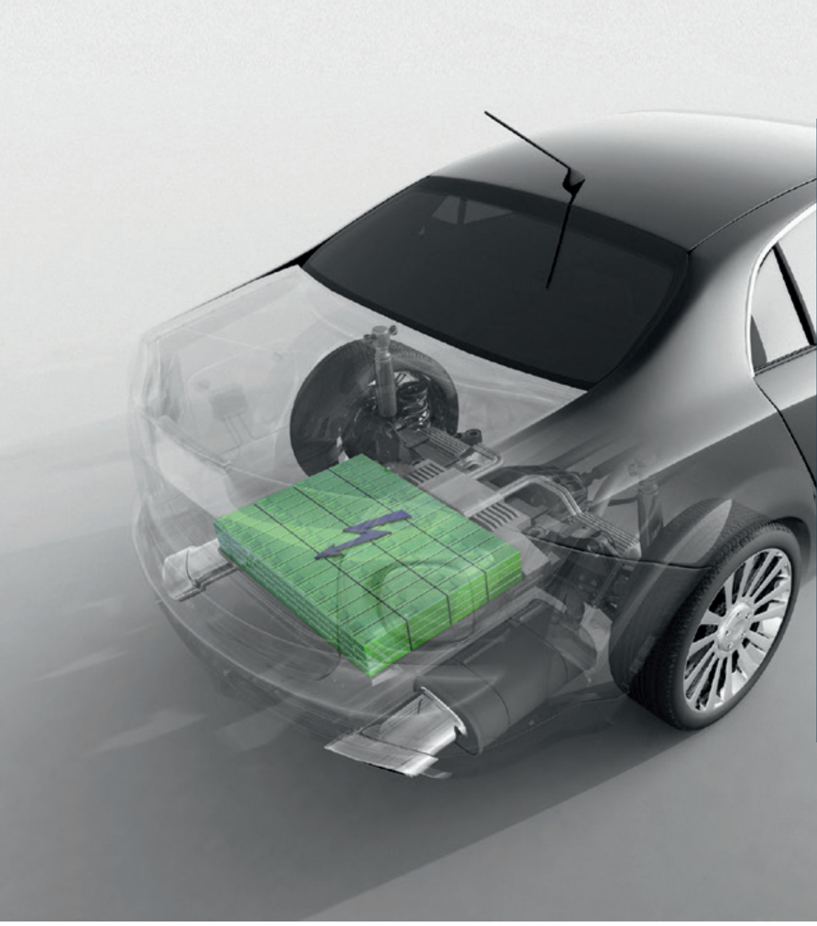
The basic components of batteries for e-mobility are complex electrochemical cells. "In our contribution to DEFACTO, we are concentrating on the mechanical aging of the cells, which is caused by volume changes of the battery electrodes," says Dr. Jochen Zausch, head of the "Electrochemistry and Batteries" team in the "Flow and Materials Simulation" department.

The promising, high-capacity, silicon-containing anodes degrade quickly after only a few charging cycles. The reason for their short cycle-life is the silicon particles in the anode, which expand and contract. This process, which is called "cell breathing," increases wear due to



Simulation: Calculated mechanical stresses in a compression experiment of a virtual battery electrode

cracks and damage. The mechanical stability of the electrodes and thus the charging capacity are gradually reduced. Simplified, these



"Structure.e": Faster Charging

Another current e-mobility project that involves the BEST simulation software from ITWM is "Structur.e". Its goal is to put an end to long waiting times for electric vehicles at charging stations. In this project, which is funded by the German Federal Ministry for Economic Affairs and Energy, Zausch and his team are researching methods that improve the performance and charging capability of lithium-ion batteries. In a large project consortium coordinated by Volkswagen AG, ten companies and research institutions are not only working on the development of new electrode concepts, but also on suitable characterization methods. The work is supported by computer-based simulations, which are developed at ITWM.

new materials increase the range of the electric vehicle, but at the same time the lifetime of the cells is less than a typical car would require.

Understanding cell material behavior with ITWM simulations

Zausch and his team get to the root of such problems with the ITWM tool "BEST", which they use to simulate the electrochemical behavior of the cell. "The big challenge isn't only about calculating the ideal battery behavior,. We also want to provide for more realism by predicting how the battery properties change over the cell's lifetime," says Zausch. This will be achieved by linking and enhancing two ITWM software tools: BEST (for electrochemistry) and FeelMath (for structural mechanics). "Ideally, this microscopic view can then be transferred to the macroscopic scale. We want to deepen our understanding with regard to material selection, electrode production and processing at the European level." To promote innovation in e-mobility, the European Commission is funding the DEFACTO project with a total budget of around six million euros. The initiative's consortium of 13 companies and research institutes from Belgium, France, Germany, Greece and Spain will pursue this ambitious goal through June 2024, with the aim of increasing the competitiveness of European industry.

For more information, visit our website at www.itwm.fraunhofer.de/defacto_en

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Digitization

Every day, large volumes of diverse data are generated at high speed all over the world – in companies, urban infrastructures and private households. The volume is growing constantly and processing and analyzing these huge volumes of data is becoming a key competence for high-tech countries. We provide companies with advice and support in building up know-how and developing solutions for business processes such as production and logistics. Equally, we emphasize feasibility, cost-effectiveness as well as data protection and security.

Europe-Wide Congress: Trust in AI

Can We Trust Artificial Intelligence (AI)?

This was the question posed by participants at the Europe-wide digital congress "Trust in AI. Responsible AI for Science and Society" on November 26, 2020. Broadcast from the Fraunhofer Center in Kaiserslautern, the German Research Center for Artificial Intelligence (DFKI) together with the two Fraunhofer Institutes ITWM and IESE were able to reach more than 650 interested parties and present current examples from research practice. The Rhineland-Palatinate Initiative for the Future (ZIRP) also invited participants to the conference in the context of the German EU Council Presidency, which was attended, among others, by Minister President Malu Dreyer: In her welcome address, Dreyer highlighted the contribution of Rhineland-Palatinate researchers and companies to responsible AI. Katarina Barley, Vice President of the European Parliament, also had her say, as did the then Rhineland-Palatinate Science Minister Prof. Dr. Konrad Wolf. Institute Director Prof. Dr. Anita Schöbel emphasized the application aspect of AI, especially in the areas of mobility, health and production. AI, especially in the areas of mobility, health and production.

Discussion with Prof. Dr.- Ing. Martin Ruskowski (SmartFactoryKL, DFKI), Prof. Dr. Anita Schöbel (Fraunhofer ITWM) and Prof. Dr. Peter Liggesmeyer (Fraunhofer IESE)

Information on the congress at www.itwm.fraunhofer.de/trustinai_en

Anita Schöbel Becomes AI Pilot

A highlight of 2020: On November 16, former Science Minister Konrad Wolf appointed our Institute Director Anita Schöbel as the first AI Pilot of Rhineland-Palatinate. "She is an internationally renowned expert in the field of Artificial Intelligence and mobility and can already point to a large number of innovative projects. Ms. Schöbel will give a further boost to the application of artificial intelligence in Rhineland-Palatinate," the science minister said at the appointment. As part of the AI agenda of the state of Rhineland-Palatinate, the AI pilots are intended to act as a link between science and industry in order to leverage the potential of AI for companies and businesses. Anita Schöbel herself focuses her activity as an AI pilot primarily in the area of consulting and is available as a contact person for experts and users. In order to enable the use of AI where it can offer added value, lectures on the topic of artificial intelligence are also held at the institute.

The press release is available at www.itwm.fraunhofer.de/ki-lotsin-en

Researchers in Financial Mathematics Calculate Smart Solvency Capital

Insurance companies must regularly present the so-called solvency ratio to the public. This is intended to provide indications of how crisis-proof the providers are. The calculation is very complex and specific, and many companies only perform it once a year. Financial mathematicians are helping to calculate the solvency ratio using artificial intelligence (AI). What this means is explained in an interview with Dr. Stefan Mai, business unit developer "Retirement Provision" in the "Financial Mathematics" department:

Solvency ratio: greater transparency, but also increased complexity. AI provides a remedy.

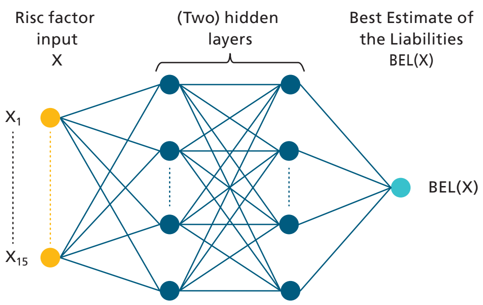
First of all, we should clarify the current meaning of the solvency ratio for insurance companies and how it is dealt with.

The new European supervisory regime Solvency II has been in force since January 2016 – with the aim of avoiding insolvency of insurance companies or ensuring that companies can fulfill their commitments even under extreme circumstances such as crises. Solvency capital is calculated in different ways, with the calculating company having to take into account all risk scenarios relevant to it in each case. Examples of major crises can be natural catastrophes, stock crashes or a strong demand for health insurance services due to epidemics/pandemics. The solvency ratio is a point of reference for the precautions taken by the insurance company.

From our discussions with insurance companies, we know that the decision-makers would like to use a neural network that enables a sensitivity analysis of the solvency capital in "real time". Our research concept: The neural network is trained on existing data and the company's internal model. Here, the award-winning ITWM software tool NASE can also be used to determine the optimal architecture of the network. With my colleague Dr. Roman Horsky, I am constantly in discussion about the contribution that quantum computing could make in the context of such a research project, but this is a dream of the future. In any case, as a result, decision-makers should receive information not just once a year, but in "real time" for more precise control - for example, to optimize the return on investment for customers.

What support can our expertise provide?

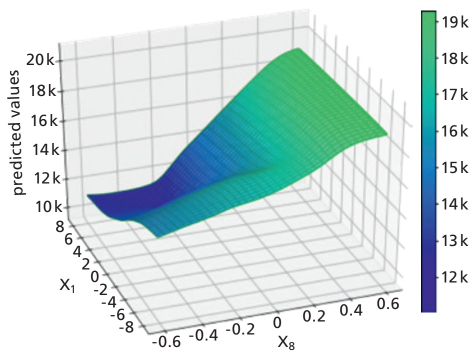
The Solvency II calculations in the area of life insurance are not only required by law, but are also extremely time-consuming, as every single contract is calculated in at least 10,000 future capital market scenarios until expiry. Because of the effort involved - many insurance companies manage millions of contracts in their portfolios - calculations are usually performed only once a year.



Schematic neural network for calculating the available capital (© https://doi.org/10.3390/risks8040116)

What does that mean in practical collaboration? How can I imagine this?

The starting point are discussions in the form of an intensive workshop to understand the parameters, models and variables on the asset and liability side of the insurance. Subsequently, the data basis is jointly reviewed and the processing effort of the preparation is estimated. Only then do we move on to the actual development and evaluation. Here, we are supported in particular by Dr. Stefanie Grimm as an expert in data science. Finally, the software is jointly integrated into the company system. In all process steps, we proceed according to the principles of agile collaboration. This means that we work flexibly with customers to address changed or additional issues. Collaboration can take place in a joint innovation lab. Here, employees of our department cooperate with employees of the company in a team. Regular consultations ensure a direct flow of information and thus lead to the best possible project result.



Behavior of a neural network with Variation of the risk factors X1 and X8. (© https://doi.org/10.3390/risks8040116)

In such an industrial project, we can leverage our unique selling proposition in the market, an exclusive combination of domain knowledge in financial and actuarial mathematics, combined with methodological expertise in data science and quantum computing.

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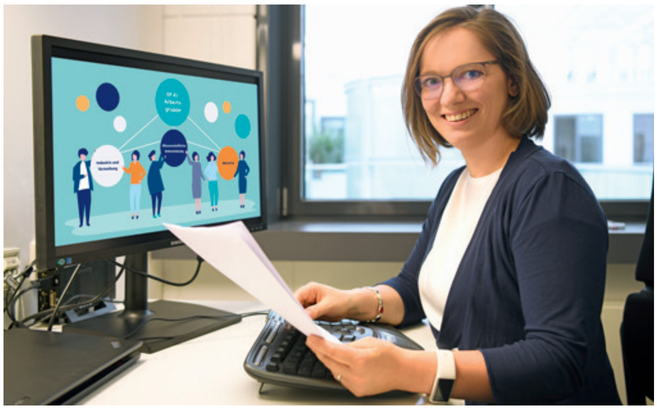
Tracking Down Fraud with Algorithms and AI



Over the past few years, the “Billing Audit and Conspicuity Detection” business area has developed a level of expertise that is probably difficult or impossible to find elsewhere. Two scientists play a special role in this: Dr. Stefanie Schwaar, Business Unit Developer “Billing Verification” and Dr. Elisabeth Leoff, Deputy Head of the “Financial Mathematics” department. Their work focuses on traditional methods and modern AI or machine learning for detecting anomalies.

The young team is working on sophisticated methods and software tools for auditing accounts and has already established itself in sectors such as the automotive industry, care and health, and public administration.

Research project: an AI tracking dog for billing in the care sector

Billing fraud and corruption in the healthcare sector cause major damage to social insurance schemes. This results in enormous costs of several billion euros per year for the taxpayer. Up to now, it has been very time-consuming to accurately check the accounts of care services and contract physicians, and detecting fraud has involved a great deal of complex, manual paperwork. At the same time, due to the particular situation in care (dementia patients, many “small” services), it is difficult to prove a complaint for individual services. In the joint project “PflegeForensik – Effektive Strafverfolgung bei Pflegebetrug durch automatisierte Bildverarbeitung” (Care Forensics – Effective Prosecution of Care Fraud by Automated Image Processing), which is funded by the BMBF within the framework of the “Forschung für die zivile Sicherheit” program, ITWM researchers from two departments support prosecution with modern algorithms of artificial intelligence (AI) in the field of image as well as text recognition. It is carried out in cooperation with the Leipzig Police Department and the General Prosecutor’s Office in Dresden.

The core objective of the project is to develop algorithms for the automatic scanning and intelligent evaluation of mountains of paper. This is because every nursing service has its own paper documents, they are structured differently and often not everything is available digitally. Some of them are handwritten, some are tables, some are not. So automated checking is a real challenge. “So far, the various documents have been manually transferred to tables and checked. Image processing can automate a lot of this. Intelligent algorithms can capture both the document

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structure and the content. For example, signatures can be found in documents and assigned to the correct employees," explains Dr. Henrike Stephani, deputy head of the "Image Processing" department at Fraunhofer ITWM.

Machine learning method supports smart fraud detection

The accounting documents are an interplay of performance records, tour and duty schedules and other documents. These have to be combined during the inspection in order to detect fraud. "A conspicuous feature can be, for example, that many of the nurse's services were billed at the same time in the service record, but the duty roster only lists a short assignment. We need to find such peculiarities in an automated way," Leoff said.

Machine learning (ML) methods are used in the research project – more precisely, deep learning methods. With the help of so-called "supervised learning", the algorithm learns from a mixture of real and artificially generated data to first recognize crucial information and then detect anomalies. To train these AI algorithms, the ITWM team designs a database and fills it with data. This means that several thousand documents must have been created by humans and marked with properties in order to make the algorithm intelligent at all. The algorithms are programmed and tested again and again with data from real investigation procedures. The evaluation is then based on the analysis of the documents and conspicuous features are automatically searched for.

But the work is not done with algorithms only: "In the end, we want to provide investigators with a software tool that helps to systematically uncover fraud cases more quickly. It must be easy for the public prosecutor's office and the police to use and deliver results that are as reliable as possible. In addition, the computing time must not take too long, as the police should be able to retrain the software independently for unknown formats. Which can often still be difficult with deep learning methods today," Leoff emphasizes.

AI competencies are constantly being expanded

The business area is complemented by the six-member EP-KI team (EP-KI: AI decision support for business processes) around Stefanie Schwaar. This team also takes care of the development of smart AI processes for applications, but with a different target group. Many decisions in companies and administrations today are still based on manually evaluated data sets. The knowledge of many employees in companies remains with them and is rarely taken into account for future decisions. At the same time, public administrations, in particular, are facing a major technological upheaval which is leading to the digitization of numerous other processes. In this context, the AI junior research group supports companies and administrations.

The group, which is funded by the German Federal Ministry of Education and Research, focuses its research on future-oriented issues and their solution through application-friendly processes.

The fields of application are not limited to billing verification and fraud detection. Here, methods of explainability (Why is a bill conspicuous?) and prognosis (How is the development to be expected?) are also considered. They share more about their work and activities on the team's website and blog.

More information on the "Accounting Audit" business unit www.itwm.fraunhofer.de/accounting-audit

To the EP-KI team blog www.itwm.fraunhofer.de/epki-blog_en

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Tarantella Spins Fast Networks – Computing Power for Deep Learning

The development of tools that facilitate Deep Learning users' entry into High Performance Computing was the goal of a BMBF project; the share of the "High Performance Computing" department is explained by project manager Dr. Peter Labus.

Your team has developed the Tarantella framework – an unusual name for a piece of software. How did it come about? And how dangerous is Tarantella?

Tarantella enables artificial neural networks to be trained on high-performance computers. This makes the time-consuming process faster because more data can be processed at once. The artificial neurons are activated more frequently – so they start dancing, so to speak. Tarantella expresses this very well because it is a boisterous Sicilian dance that is danced in large groups. So a spider metaphorically spins the neural web, which is why it's in our logo. And of course completely harmless!

What can Tarantella do?

Besides the already mentioned feature that neural networks can be trained faster with more computers, we also support the training of arbitrarily large neural networks. This was previously not possible due to the limited memory of a graphic card. Now, even deeper neural networks can be trained, which can learn more complex mathematical functions and thus solve more difficult problems. We were supported on the one hand by the German Research Center for Artificial Intelligence (DFKI), which dealt with the issue of partitioning the neural network among the various computers of the supercomputer. Support for the performance evaluation of our software came from the Center for Information Services and High Performance Computing (ZiH) in Dresden. And finally, the University of Heidelberg: The team dealt with application scenarios of particularly large neural networks, for whose training Tarantella is needed.

So the framework is ready to use. What application areas have emerged?

Neural network training is becoming increasingly relevant as the computing time invested in AI grows exponentially. This has enabled many breakthroughs in speech and image processing, which we are already using in social media, online shopping, but also in the smart home. Science also benefits from the use of large neural networks, e.g. cosmology, climate research, particle physics. Our goal was to make supercomputers usable by Deep Learning users without assuming knowledge of these systems (or of parallel programming), thus democratizing the development of new AI solutions. Tarantella makes this possible by building on one of the most widely used Deep Learning frameworks – TensorFlow – and its interface. Existing AI applications can be ported to run on a high-performance computer with minimal changes due to Tarantella.

Further information www.itwm.fraunhofer.de/HP-DLF_en

Tutorials on our website www.tarantella.org

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Customized Digital Planning Processes

The digitization of planning processes is intended to help manufacturing companies get the optimum out of their processes. A team from the "Optimization" department provides support with the development of customized software.

Questioning existing planning processes is often the task of researchers in the field of "optimization" in their industrial projects. In many cases, commissioning companies are convinced that they know the bottleneck in their own process. The experience of the researchers shows: A different picture often emerges through process simulation.

Mathematically imitating the way experienced workers think

A team led by Dr. Heiner Ackermann and Dr. Elisabeth Finhold is helping companies get started with digital production planning. "In any production, there are many tasks that need to be highly coordinated. In such a case, we look closely at the setting and questions: How are individual processes coordinated? What is happening on which machine? How well are they utilized?" is how Finhold describes the first phase of such a project. "Then it gets mathematical: We develop algorithms that are specifically tailored to the complex rules of the company."

The goal is to customize planning processes. With customized algorithms, the project team replicates to a certain extent what experienced production planners do in their everyday work. "Those who plan production know the working environment very well and have a lot of know-how. We are trying to imitate how these employees structure their tasks," explains Ackermann and emphasizes: "This is also about knowledge management and the digitization of knowledge. We can help automate a high proportion of routine tasks." This would relieve specialists and at the same time create resources for special tasks.

Increase of production efficiency

The software, which has been specifically developed to meet a company's needs, can then be used to explore which variants are possible in the process. Potential for improvement comes to light and there are suggestions as to how production as a whole can run more effectively.

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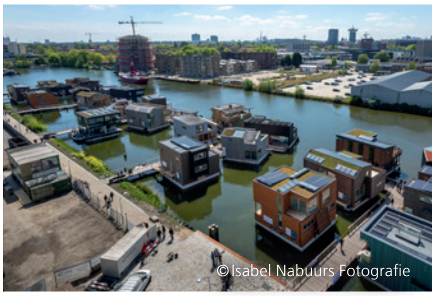
Energy

Our focus is on renewable energies, efficiency technologies, smart grids and the digitization of the energy industry. Small and medium-sized enterprises, as well as industry and the energy sector, have access to a wide range of research and development services. The focus is always on secure, sustainable, economical and socially equitable supply.

Smart Software for Managing Fluctuating Energy Production

In the "High Performance Computing" department, sustainability and the smart use of energy have had a high priority from the very beginning – as can be seen in the "Green by IT" group formed back in 2009. The commitment has resulted in a coporate spin-off, Wendeware AG, in 2019. Matthias Klein-Schlößl, head of the "Green by IT" group, outlines some of the highlights:



Floating residential and energy community with ITWM technology: Amperix controls the energy flows in Schoonschip.

We have been researching software and hardware solutions for the energy transition for many years. This has resulted in the energy manager Amperix and the platform myPowerGrid, which coordinates many decentralized energy managers as a combined virtual unit. Wendeware AG is now marketing our products and further develops these technologies. Since mid-2020, Wendeware has been partnering with an anchor customer: a leading German battery system manufacturer. They use our energy management system to record and monitor energy flows in plants and to intelligently control the storage system and other generators and consumers in a property.

Good winter for Schoonschip

"Green by IT" has been accompanying Schoonschip, a floating residential quarter in Amsterdam North, for quite some time. The energy community did really well over its first winter. To understand what we have achieved, you first need to know that 30 houses (47 residential units) share a very small electricity grid connection with a maximum output rating of around 150 kilowatts while being heated with heat pumps. This means that in winter, a high power consumption is to be expected, and at peak times this consumption would actually be too high for the grid connection.

All houses are equipped with battery storage. Our energy community control system uses these storage units for coordinated support of the grid connection, a process we call "peak shaving". At peak times, the storage systems supplied a total of up to 63 kilowatts of electricity. The shared grid connection was held close to its maximum due to the power consumption of the heat pumps, while the battery storage systems protected it from overload. During sunny periods, the storage systems are used for day-night buffering.

The technology is being used in another residential project: "Wohnen mit Freu[n]den" in Oggersheim. In addition to the main meters, we have equipped an apartment building (which also forms an energy community) with all kinds of technology for measuring electricity, water and heat, a practice known as submetering. This provides energy transparency for the residents and serves as a basis for billing. An evaluation of the key figures shows that "Wohnen mit Freu[n]den" already covers about 60 percent of its electrical energy requirement from its own combined heat and power plant (CHP) and, on balance, generates more than twice as much electricity as the residents consume. For this reason, it may make sense to couple the CHP with a battery storage system to further increase self-sufficiency.

For more information, visit www.itwm.fraunhofer.de/greenbyit_en

Our cooperations at www.wendeware.com/ueber-uns

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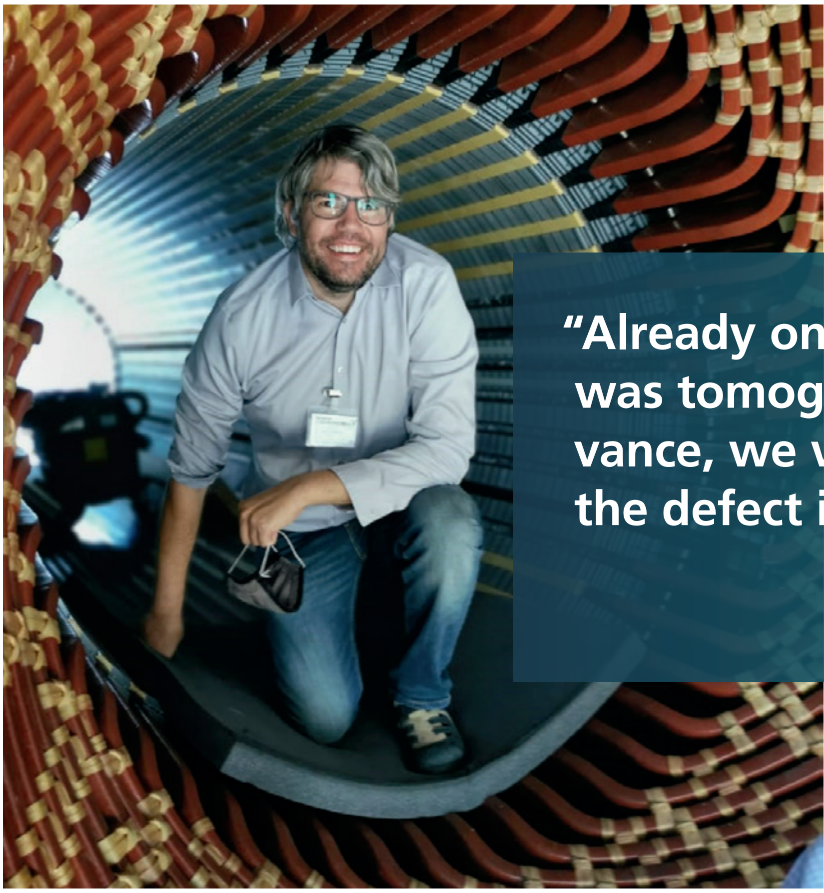
Keeping the Current Flowing: Non-destructive Testing of Power Plant Generator Rods



Preliminary examination: Dr. Friederich in the power plant generator, whose mica insulation, which is sometimes difficult to access, can be examined using terahertz technology.

The inspection of power plant generators is a complex undertaking, partly because of the sheer size of the generators and partly because of their structure. Not all locations are accessible and space for the use of measurement technology is often limited. In recent years, however, many terahertz and millimeter-wave technologies have evolved from scientific backgrounds into specific industrial applications, including non-destructive testing for defects below the surface in quality control and product maintenance. Together with Siemens Energy, we were able to prove the applicability of the new technology for the inspection of power plant turbines in several feasibility studies.

The mica insulation of current conductors in the generator was investigated. Early detection of defects and cracks in the insulation is crucial for the functionality and running time of the generators. The goal was to detect internal defects before the surface material ruptures. Camera-based inspection methods only detect defects on the surface and are therefore not an option on their own. This is because it is too late for maintenance and timely repair. The defects must be detected before they are visible from the outside.

> **“Already on the first specimen, which was tomographically recorded in advance, we were able to recognize the defect in the terahertz image.”**
>
> **Dr. Andrey Mashkin**
> Siemens Energy

Radar-based measurement technology combined with terahertz waves

“Imaging-based terahertz testing is particularly well suited for this purpose,” says project manager Dr. Fabian Friederich from the “Materials Characterization and Testing” department. “Radar-based approaches, in fact, enable the acquisition of depth information and simplify the differentiation of individual features of the measured object.” Corresponding terahertz imaging systems are often based on quasi-optical lens systems that offer a certain degree of flexibility, e.g., with regard to the choice of focal length and thus working distance. The quasi-optical components for the terahertz range are usually quite large and are therefore not suitable for the inspection of generator rods. The remedy here is a combination of radar-based measurement technology and the use of a type of endoscope, which is guided between the generator rods. This consists of a plastic waveguide as a near-field antenna in conjunction with a terahertz radar sensor.

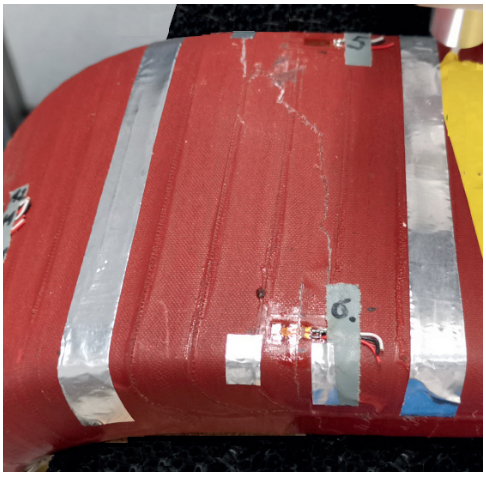
Promising test measurements

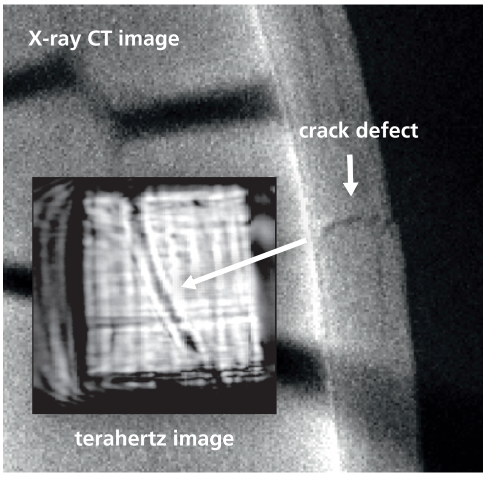
The measuring tip was first tested on a defective generator rod in the laboratory. It was guided over the surface in the area of the defect and the surface of the generator rod was scanned point by point to generate a volumetric image of the area. Comparative images with X-ray CT were used to detect and rule out the defect characteristics. The investigations led to very promising results, so that in the next step, specific approaches for the application of the method in typical interstices of the generator rods were tested.

For this purpose, the ITWM experts first investigated suitable materials for the guidance and influences due to bending of the measuring tip, in the form of further comparative measurements on the generator sample taken. On the basis of these findings, adapted measuring tips were subsequently worked out on plastic plates and combined to form an endoscope. Finally, exemplary measurements were carried out on assembled generator bars to validate their suitability for use.

What is next?

In the next steps, other aspects of the measurement geometry are investigated; for example: What is the influence of the angle of incidence on the measurement signal? Other approaches to solving the problem of the measuring tip in the field are also being examined. “We want to realize a fully adapted measurement system that can be used routinely to check generator rods on this basis,” says Dr. Fabian Friederich.





The photo on the left shows a section of a generator rod. The X-ray CT image of the sample cross-section shown in the background on the right shows a crack inside the insulation. The embedded terahertz image has a different perspective that shows that the crack extends over the entire width of the generator.

More information at www.itwm.fraunhofer.de/terahertz-testing

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FlexEuro: Flexible and Smart Management Wins in the Energy Market

The manufacturing industry needs a lot of electricity. Energy and electricity usage are therefore often decisive cost factors in the industrial sector. At the same time, flexibility in the power supply system has become the slogan of the day. After all, those who respond smartly to fluctuations on the market and manage their power consumption benefit from it. In the BMWi-funded FlexEuro project, researchers from the "Financial Mathematics" and "Optimization" departments are developing models and methods for the optimal marketing of load flexibilities in various electricity markets.

So-called supply-dependent power generation was unimportant in the past for nuclear and coal-fired power plants, but is now crucial for the price in the electricity mix. This means that due to renewable energies, such as wind and solar power, electricity production is increasingly dependent on the weather and also fluctuates over the course of a day, sometimes every hour or even every second. However, it is not just generation that has an impact on markets and prices, but also varying levels of demand. Companies that respond to such flexibility when purchasing electricity are going to have decisive advantages in the future, especially energy-intensive companies. At the same time, they relieve the burden on the energy network.

Smart control of aluminum production

These industrial processes with particularly high energy consumption include, for example, the production of aluminum or, more precisely, aluminum electrolysis. TRIMET Aluminium is on board as an application partner in the FlexEuro project. Everything revolves around light metal products in the medium-sized family business. "At the kick-off to the project, we were also shown the impressive manufacturing processes in the electrolysis furnaces during a tour of the plant. That definitely increased our understanding. They have to run 24/7 so that in the end the output does not suffer," says Dr. Neele Leithäuser. That takes a lot of energy. Some of the furnaces are already designed to compensate for deviations in power input by controllable heat exchangers without interrupting production.

"TRIMET also calls these flexible furnaces a virtual battery," explains the deputy head of the "Optimization – Operations Research" department. The special feature: In the converted cells, production can be ramped up and down depending on the weather. When the sun is shining and the wind is blowing, the furnaces can melt up to 25 percent more with surplus green electricity. If it is dark or there is no wind, they ramp down production by up to 25 percent. This is highly complex, because electrolysis requires a constant operating temperature of 960 °C. Even 10 degrees above or below that is not good for the end product. The aim of the project is to control electricity consumption in such a way that the electricity required on the market can be used as efficiently as possible.

Mathematics keeps an eye on short-term marketing options

"Here, we focus on short-term marketing options for flexibility," explains Elias Röger, ITWM expert in financial mathematics. Röger cites the so-called day-ahead-market as an example. "Always at noon of each day, the stock

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Flexible electrolysis furnace at TRIMET Aluminium SE.

Short-term Marketing Options

- The balancing power market: Balancing power, also referred to as reserve power, ensures supply in the event of unforeseen events in the power grid. It is provided by certified market participants and remunerated by the grid operators.
- The day-ahead auction: trading of electricity for the following day. There is one price for each of the different delivery periods, which becomes known at the end of the auction.
- The intraday market: It refers to the continuous buying and selling of electricity that is delivered on the same day. Electricity can be traded back and forth until shortly before the delivery date, which allows speculation. Positions from the day-ahead auction can be changed again here.

market determines the electricity price for each hour of the following day. This result depends on the level of expected consumption and the forecast generation from renewable energy sources.” The different characteristics and restrictions of the markets require an individual combination of mathematical models for each marketing option (see info box for differences between the markets). In TRIMET’s practice, this can mean that the furnaces then use less electricity in a “more expensive hour” in the best case and continue to ramp up in less expensive hours. The project is now halfway completed and the researchers are drawing up an initial interim balance.

Leithäuser summarizes: “In the first one and a half years, we at ITWM dealt intensively with marketing on the day-ahead-market. For this purpose, the possibility of flexible consumption was modeled as a multicriteria optimization problem. Mathematical forecasts were then used to calculate optimal load schedules for the coming day. Here we were able to show that flexibility is very profitable economically.”

FlexEuro will run until August 2022 and the end result should be specific recommendations for practical action. The plan is to bring the developed models and methods into use as software prototypes at the project partner.

More information at www.itwm.fraunhofer.de/flexeuro_en

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Industry 5G – Not Just Dreams of the Future Due to Mathematics Expertise

Dr. Paulo Renato da Costa Mendes brings 5G and Industry 4.0 closer together in his team; especially when it comes to the topic of flexibility and renewable energies.

Slogans such as the Internet of Things (IoT) or Industry 4.0 are ubiquitous in the media. It seems clear that in the future, more and more machines, systems and devices will be networked with each other, especially in production. Everyone is also talking about 5G, which is considered the successor to 4G (LTE). But the fifth generation is much more than just a new mobile communications standard. 5G is opening up entirely new perspectives for Industry 4.0 as it is aimed specifically at communication between machines. The "5Gain" project, funded by the Federal Ministry for Economic Affairs and Energy, forms a core of the ITWM activities on the topic of 5G.

The team led by Dr. Paulo Renato da Costa Mendes and Dr. Christian Salzig is dealing with very practical problems and Industry 4.0 in the field of energy, more specifically with "5G infrastructures for cellular energy systems using artificial intelligence". In the interview, Paulo Renato da Costa Mendes explains to us what the 5G developments mean:

5G is considered a future technology par excellence. Siemens and Handelsblatt are already talking about "Industrial 5G". What advantages will 5G bring in the area of Industry 4.0? And when is that even foreseeable?

5G is considered to be ten to 20 times faster than 4G, as well as more flexible, autonomous, secure and efficient. It enables higher data transmission rates and shorter latencies. Depending on the application, the advantages cannot be fully exploited simultaneously in one and the same network. The consumer sector may need rather high data rates to stream videos on the go, for example.

For industrial applications, reliability and lowest latency are important. Particularly where the level of industrial automation is already high, 5G offers rapid opportunities to turn Industry 4.0 into Industrial 5G. 5G is still largely a pipe dream. But we are talking about a relatively near future. In three to five years, some things will be realistically feasible.

How can mathematics, or we at Fraunhofer ITWM, support this in practice? What challenges arise in the project and what expertise do we bring to the table?

Especially our years of experience and methodological competences in the field of machine learning qualify us. We develop AI algorithms for a wide variety of areas. This paves the way for optimally exploiting the potential for 5G. In the "5Gain" project, this helps when coupled with our project experience in the monitoring and control of energy networks. AI methods for the distributed control of cellular energy systems are just as much in demand as forecasting models. These are to predict communication requirements based on demand. The solution path is mathematics with the goal of developing intelligent grid control.

It can be explained more precisely like this: Due to the decentralized expansion of renewable energy sources with controllable loads and storage (e.g. electric mobility), the control of energy systems is becoming increasingly complex. Most electricity from renewables is weather-dependent. It is produced independently of demand, when the wind blows or the sun shines. More flexible thinking is needed. At the same time, the power grid should be expanded as little as possible. Our solution approach: dividing the energy grid into regional cells. Each cell has different participants and characteristics and performs decentralized load management, feed-in management and marketing. We develop adaptive methods (e.g. reinforcement learning) that learn the control of such individually present energy grids.

That means AI and machine learning are used. And what does that mean for 5G in the end?

The regulation requires a communications infrastructure that provides the necessary data rates, response times and resources for different numbers of participants, and does so flexibly and quickly in every situation. All this lies dormant in the advantages of 5G. We are working on the further development of various system components and testing them with our partners, also in real environments. For example, in the real lab of the city of Dortmund and with partners from the consumer side or energy producers.

However, other areas in which 5G creates completely new opportunities are of course also exciting. Another application example in the near future could be the remote maintenance of plants via 5G networks, so that 5G will also play an important role in our predictive maintenance application field in the future. There will certainly be other exciting projects to research and develop in the future.

More information on our website at www.itwm.fraunhofer.de/5gain_en

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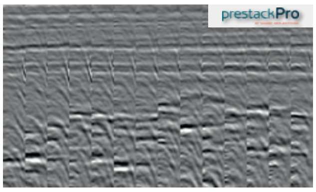
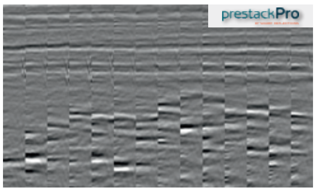
Deep Learning Speeds up Seismic Data Processing





Seismic gathers after prestack depth migration. Curved events (upper image) originate from multiple reflections and are recognized as such by the ML software and eliminated (lower image).

The energy supply of industrialized nations is increasingly based on a mix of different sources. Despite their diversity, they have one important feature in common: the nature of the earth's subsurface. Whether it is locating oil and gas fields, siting offshore wind farms, or identifying areas suitable for geothermal energy: Seismic data sets are measured, processed and interpreted to identify the geology of the subsurface. A research project of the "High Performance Computing" department investigates how Deep Learning methods can support this process.

Deep Learning (DL) has proven its usefulness in many application areas. For seismic data, however, the application is more difficult because the data originates from the unknown and inaccessible subsurface. DL methods that accelerate seismic interpretation are sought; most current methods are too complicated due to many parameters. The working group around Dr. Norman Ettrich has now achieved an important step: They have developed machine learning (ML) methods that do not require parameters. The subjectivity of human data interpretation is also eliminated.

Training through Supervised Learning

The basis is the training of deep neural networks. This is not uncommon, but so far the networks are trained on only part of the data and the learning steps are applied to the entire data set bit by bit. A neural network learns quickly what a cat looks like because it can be trained with photos of cats. This is completely different with seismic data: here there is no clear target image. That is why it trains on synthetic data that reflects the wide variety of real-world data.

"We train exclusively on synthetic data and transfer what we learn to arbitrary field data sets," says project leader Dr. Norman Ettrich. "This is successful because our data modeling excellently reflects the properties and diversity of real measured data. Our methods are used in processing. In simple terms, the input is data with interfering signals, the output is cleaned data. In other words, data without interfering signals, which makes interpretation much easier."

Enormous reduction in computing time

The newly developed methods simplify the seismic work chain. Above all they shorten the required working time by days and even weeks – in each case depending on the amount of data. And this can be huge, because areas of 1000 to 10,000 square kilometers are considered!

The new ML methods were integrated into the ALOMA software, which was also developed in the "High Performance Computing" department. The result is a software package for parallel ML-supported processing of seismic data.

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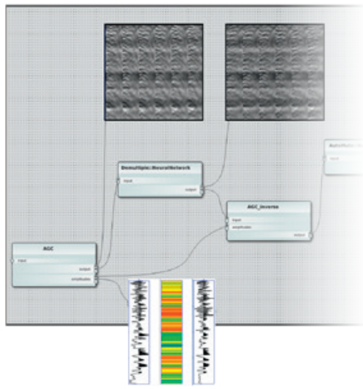
ALOMA: A Parallelization Framework – Not Only for Seismic Applications

One of the challenges of Big Data is to correctly execute complex computing operations on growing volumes of data. It can only be mastered with the massive parallelization of computers and computing power.



Section of an exemplary workflow with ALOMA

Researchers in the High Performance Computing department have been using GPI-Space for years as a programming platform for high-performance systems. What makes GPI-Space so special is its user-friendliness: Customers do not need to acquire any special HPC knowledge, because the software system takes care of the efficient execution of the algorithms. This also applies to the specialized version ALOMA.

ALOMA detects data dependencies

The tool is primarily used in seismics. However, it is designed as a general framework for the execution of workflows on distributed systems, because ALOMA recognizes dependencies in the data sets that are supplied as input – regardless of the data source – and answers the following questions: How is the data distributed? Which data can be processed simultaneously and independently? Where can the data be processed?

"In order to identify dependencies and answer these questions, ALOMA must have or generate appropriate information about the individual modules and their combination in the workflow. For this workflow, we use a representation as a Petri net, which the internal workflow engine can analyze accordingly," explains project manager Dr. Dirk Merten. To do this, users only have to connect outputs of algorithmic modules with the inputs of further modules in a graphical workflow editor. Information about the individual modules is provided when they are integrated into ALOMA. This information includes the number and types of the modules' input and output data, as well as their granularity. These are values specific to seismic (e. g. "Seismic Data" or "Velocity Model") and the granularities "Trace", "Gather" or "Inline".

Traditional algorithms and ML

In addition to the granularities typical for seismics, ALOMA also supports data splits from pattern recognition and machine learning. This means that modules derived from Deep Learning can also be integrated. In an exemplary workflow, a volume of input data can be corrected multiple times, stacked into one volume, and analyzed for error patterns. Processing and analysis modules for traditional algorithms and neural network inference are easily combined in one workflow. ALOMA automatically handles the parallelization of all modules within the workflow.

With ALOMA, seismic experts can integrate new traditional or machine learning-based algorithms and prototypes within a very short time, combine them with existing algorithms in workflows, and test them in parallel on realistic data sets and under everyday conditions.

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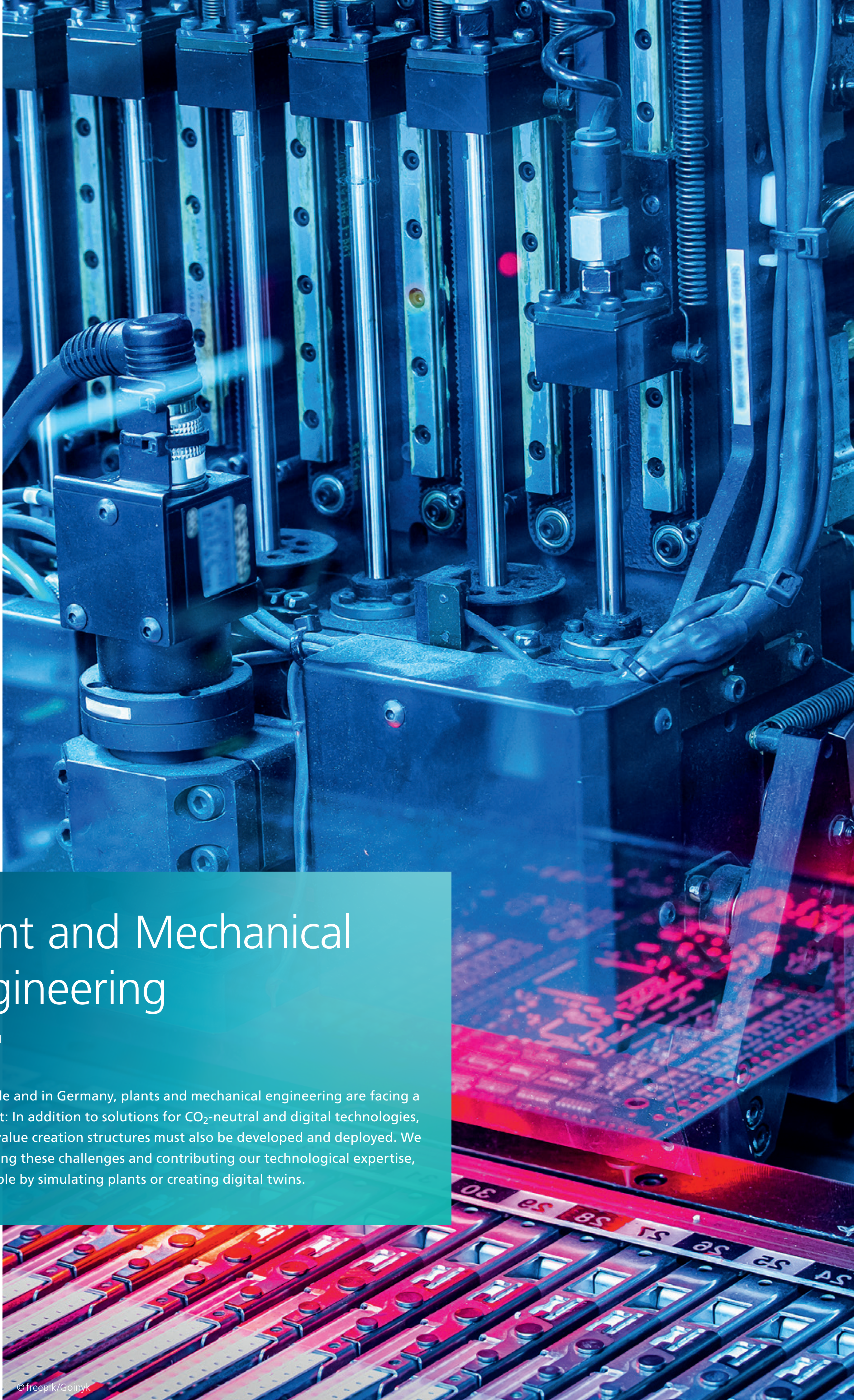

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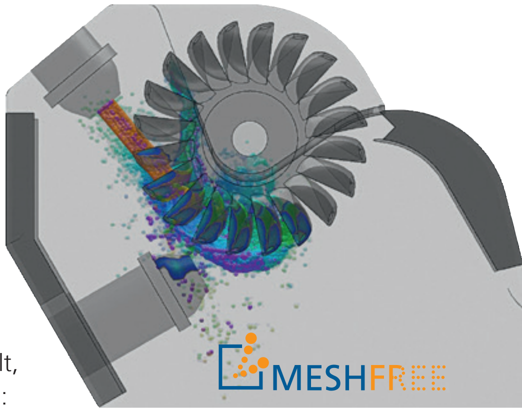
Plant and Mechanical Engineering

Worldwide and in Germany, plants and mechanical engineering are facing a major test: In addition to solutions for CO_2-neutral and digital technologies, resilient value creation structures must also be developed and deployed. We are meeting these challenges and contributing our technological expertise, for example by simulating plants or creating digital twins.

MESHFREE – Process Simulation to the Point



The simulation with MESHFREE shows the flow behavior and abrasion (wear) in a Pelton turbine.

How does water behave when a car drives through a puddle? How efficient is a water jet turbine? What happens during machining or during the filling of a beer glass? These are all complex questions to which there is an innovative ITWM answer in the field of simulations: MESHFREE.

The interdisciplinary team around Dr. Jörg Kuhnert and Dr. Isabel Michel now consists of seven members and is developing meshfree simulation as a key solution for a wide variety of application fields. Their MESHFREE software combines more than 15 years of expertise from the Fraunhofer Institutes ITWM and SCAI.

Simulating dynamic processes

"For a long time, a computational grid was first placed over every geometry in the simulation process. This is and was usually expensive, tedious and also not optimal for many processes in terms of results," says Kuhnert. "Our simulation method eliminates the need for such computational grids. Instead, we use the finite pointset method (FPM) approach. This uses point clouds in which each point can be freely positioned." This offers decisive advantages over traditional methods and more and more cooperation partners are now taking notice.

"In the automotive sector, we have been providing support with simulations for some time now. MESHFREE makes processes more understandable digitally," explains Michel. Specifying material properties is sufficient to predict behavior with MESHFREE. The user exports the geometry from common CAD tools. "As we continue to develop our methodology, we work hand-in-hand with the industry. Examples include multiphase simulations or 3D-2D transitions. In the same way, we are exploring the interaction of fluids and solids. As a result, the demands on simulations are growing: MESHFREE is becoming more efficient and more accurate, and at the same time we want to make it easier to use. Smaller companies should also benefit from the solution."

New boost for turbines

One of these practical examples is hydropower turbines, or more precisely Pelton turbines. "In a project that we are implementing with Voith Hydro, among others, different model approaches are intertwined," Kuhnert reports. "We are investigating the water flow in interaction with the air as well as the behavior of the complete flow. Wear, known as abrasion, is also mapped by MESHFREE."

The example of abrasion illustrates how important simulations are because, above all, they can save time and money, Kuhnert emphasizes. "The surface of a turbine runner is damaged over time by sand or stone particles contained in the water. This leads to changes in the flow and the turbine becomes weaker. The runner will eventually need to be replaced," the team leader explained. "If modernization does occur, the team assists in optimizing the turbine," he continued. "Simulation is a great tool for predicting flow, the formation of water layers and material wear – in plant design even long before a prototype is built.

Further information on the project page www.meshfree.eu

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Smart Monitoring, Automated Foresight

"Condition monitoring", permanent monitoring of the machine condition, and "predictive maintenance", machine-learning-based prediction on the basis of data – the team around Dr. Benjamin Adrian has built up expertise in these focal areas. Here, mathematics and AI provide tailored solutions. One practical example is the collaboration with Berger Holding (Memmingen Allgäu), where everything revolves around ball screws.

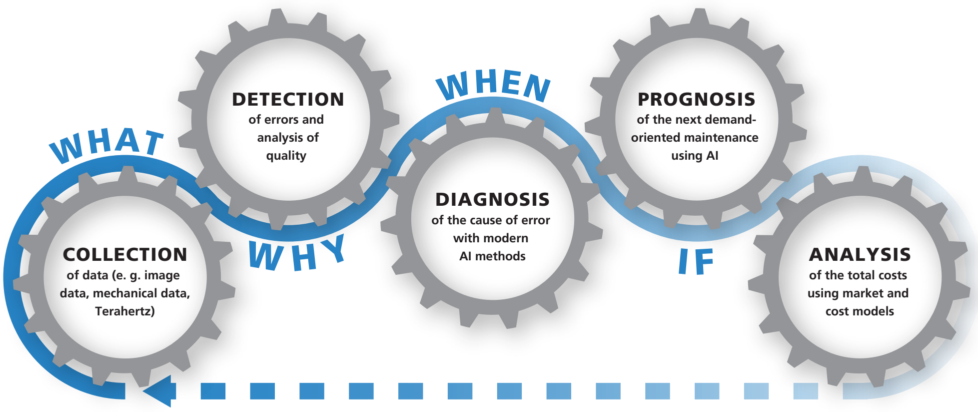
Predictive maintenance is the optimal maintenance strategy.

A ball screw is installed in machine tools, for example, and is used in the automotive industry, measurement technology, medicine, and aerospace. Large forces act on the component and the service life is related to the load on the balls. Maintenance and avoiding failures are production goals – preferably automated and smart.

In the project, this means proceeding step by step for the team: "Based on sensor data and their complex analysis, we calculate the profile, virtually the fingerprint of each ball screw in as-new condition," explains Adrian, project manager at the "System Analysis, Prognosis and Control" department. This profile serves as a reference. Ball screw operators can then perform comparative measurements or have them performed automatically and observe how the profile has changed. This data answers questions such as: Is the ball screw installed correctly? How does the condition change? When does the ball screw need to be replaced?

Goal: A ball screw that controls itself

"We are not just looking at data itself, but examining where it comes from. We want to understand exactly what the data is telling us and how it is created. Also with our experience around sensor technology." Based on this, the testing station and measurement technology are being expanded and a concept for moni-



Condition monitoring and predictive maintenance: data acquisition, analysis, prediction and evaluation from a single source.

“We will be able to improve our quality control through the cooperation with Fraunhofer ITWM and save our customers rejects and unplanned machine downtimes.”

Dr. Martin Körner
Development engineer at Berger Holding

Project example Berger: Digitization of a ball screw. A ball screw translates rotational motion into translational motion and vice versa.

toring is being developed (condition monitor). In Berger’s case, this now means its own software.

Berger is pushing ahead with this further development of ball screws as part of the “Pay-per-Stress” project sponsored by the German Federal Ministry for Economic Affairs and Energy. The goal is to introduce a new leasing model for machinery and equipment whose rates are calculated not only according to useful life, but also to actual wear and tear. This requires a reliable wear model for each critical machine component, such as the ball screw. This increases the transparency of costs and reduces risk surcharges in the leasing rate. This makes the concept equally attractive for small and medium-sized companies with limited financial resources. The end user also recognizes faulty assemblies or where problems need to be fixed and can look ahead to see when they need to renew or replace a part (predictive maintenance). Berger’s major goal is a ball screw that monitors its own wear.

Further information on our website at www.itwm.fraunhofer.de/en/predictive-maintenance

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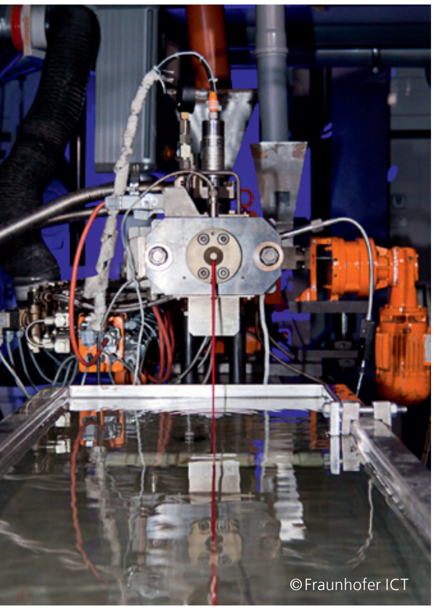
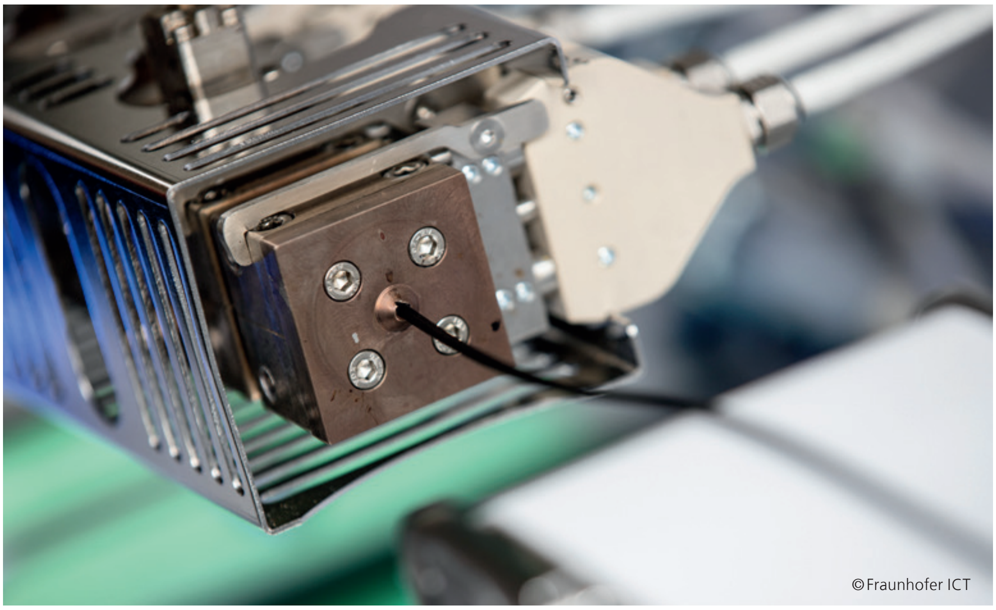
Hybrid Backward Computing for the Plastics Industry

In the Fraunhofer-internal project HyTwin, the ITWM team around Dr. Alex Sarishvili is developing a hybrid digital twin together with researchers from the Fraunhofer Institute for Chemical Technology ICT. Using machine learning (ML) methods, this twin supports companies in the optimization and control of their plastics processing, more precisely their extrusion processes.





A test setup based on real production processes and equipped with extensive measurement technology is being created in the Fraunhofer ICT laboratory.

Extruder, additives, twin screw, nozzle – these are all technical terms from the world of plastics processing, although there are of course many complex variants of production. However, the extrusion process is common to all of them. Here, plastic is pressed as a tough mass under high pressure and high temperature through a shaping opening. At the end, the company receives as a product, for example, thermal insulation panels or plastic granulate for further processing into PET bottles or plastic pipes. "Extrusion is a highly complex physical-chemical process in which hundreds of parameters play a role and which is accordingly difficult to model and optimize," explains Sarishvili. Almost all plastics processed into a product pass through such a step in the process chain.

In the plastics industry, optimizing this still often means using "trial and error" to test how the quality of a product can be improved and optimized by varying individual parameters. Necessary material parameters are determined and tested anew for each material mixture of the real process. This is time-consuming and cost-intensive.

©Fraunhofer ICT

Fraunhofer ICT has a modern pilot plant with twin-screw extruders from 16 to 43 mm as well as versatile metering options at its disposal.

Smart modeled and calculated backwards

Computer simulations or digital twins offer the possibility of optimizing almost the entire extrusion process based on simulation. The project team is taking a hybrid approach: They are developing a digital twin that is both data-based and model-based, which uses AI to predict and optimize. In the best case, the digital twin thinks about the end first and calculates backwards: What product properties or quality do I want and what parameters do I have to set for this? Machine learning processes need masses of data if they are to function properly. At the beginning of the project, therefore, real test data was initially generated at Fraunhofer ICT. They are adapted to a physical-chemical process model and a data cloud of measurement and simulation data is generated. The AI then learns from this.

The expertise of the researchers at Fraunhofer ITWM lies particularly in mathematical modeling and simulation of technical processes. "For many years, (deep) machine learning methods have also been developed at our institute. We are responsible for smart algorithms," says Sarishvili. This has resulted, for example, in the Design for Quality Prediction software tool, which provides essential functions for creating simple data-based models for extrusion processes. As a result, the digital twin should then make it possible to achieve, among other things, higher production speeds, greater flexibility and higher product quality at the lowest possible cost. And not only that, at the end of the project, the goal is an easy-to-use software platform that can also be used by small and medium-sized enterprises (SMEs).

The team also has new projects lined up already: The ENERDIG project, promoted by the Federal State of Rhineland-Palatinate with funds from the European Fund for Regional Development (EFRE), just for starters. The focus here is on determining and optimizing the energy flexibility of extrusion processes.

More information on process analysis using machine learning at www.itwm.fraunhofer.de/process-analysis

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EMMA Learns to Drive – Dynamic Human Model for Autonomous Vehicles

5

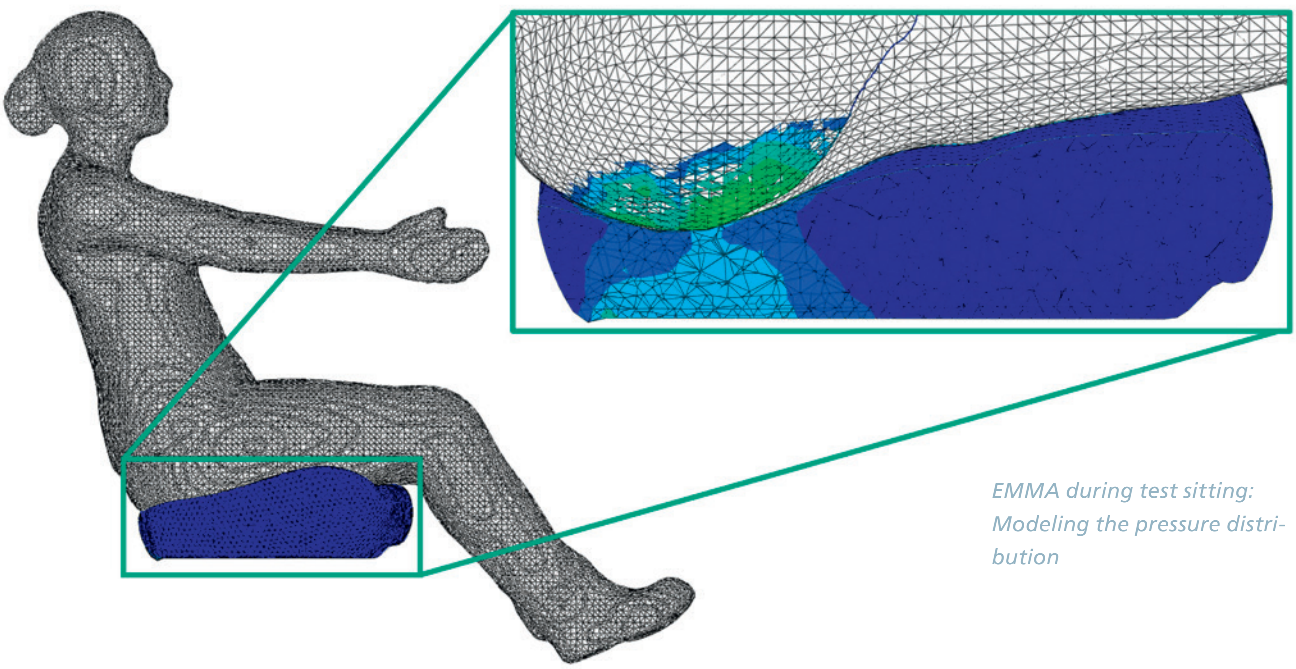
Five disciplines combined in EMMA4Drive: mechatronics, ergonomics, psychology, automotive engineering and techno-mathematics

In order to understand the expectations of customers of autonomous vehicles, to strengthen their trust and to prove safety, new digital tools are needed for research, development and validation of the technology. With the EMMA4Drive project, researchers in the division of "Mathematics for Vehicle Engineering" are further developing the dynamic human model EMMA-CC for use in fully or partially autonomous driving vehicles.

EMMA-CC stands for "Ergo-dynamic Moving Manikin with Cognitive Control" and is an old acquaintance: In the MAVO project of the same name, six Fraunhofer institutes had collaborated on digital human modeling for the simulation-based ergonomic design of workplaces. The further development EMMA4Drive now virtually takes a seat in the car and dynamically simulates the interaction of human body parts and the vehicle seat during driving maneuvers. The resulting software prototype will serve as a digital twin of the occupants, helping to analyze and evaluate new seating concepts in the passenger compartment in terms of safety and ergonomics during driving maneuvers.

Motion sequences instead of quasi-static tests

So far, human models have mostly been used in crash simulations to estimate the risk of injury. However, detailed, computationally time-intensive models for calculations in the millisecond range are used here, which are not suitable for the simulation of dynamic driving maneuvers, since longer processes have to be simulated here. Another field of application for digital human models are ergonomics analyses in assembly planning. The models used for this purpose often only represent postures of the human body or quasi-static motion sequences by means of highly simpli-



EMMA during test sitting: Modeling the pressure distribution

Precision work during the cabin change: For the next test cycle, a car chassis is lowered into the projection dome of the RODOS.

fied multi-body kinematics. Such models do not take dynamic effects into account and the analysis of physical loads is hardly possible, since pure kinematics models can provide little information about biomechanics..

Sit better, operate more comfortably

“Our human model, on the other hand, uses an optimization algorithm to automatically calculate new body postures and entire motion sequences over a longer time window with the associated muscle activities,” explains project manager Dr. Marius Obentheuer. “This means that the simulation model can also be used to investigate the effect of dynamic driving maneuvers on humans and their (reaction) behavior – for example, in the design of assistance systems or control algorithms for (partially) autonomous driving.” EMMA4Drive thus enables comparatively simple implementation of new movement patterns and efficient virtual investigation of safety, comfort and ergonomics in (partially) autonomous driving.

EMMA on RODOS®

And before EMMA is allowed on the road, she must of course pass her driving test – virtually in our interactive driving simulator RODOS® (RObot based Driving and Operation Simulator). But first, a real human takes a seat there to collect physical measurement data and provide input for the simulation software. The interaction between the driver and the seat is investigated, for example the pressure distribution. This data should help to better answer fundamental questions about autonomous or semi-autonomous driving: How quickly should the tilted backrest of a seat be raised again with the integrated electric motor system? Does the turned seat return to its original position? How long does it take for the human to take the wheel again when the vehicle signals “Danger from the right, please take over!” in semi-autonomous mode?

The driving simulator is a central component of the technical center in the division “Mathematics for Vehicle Development” and allows the use of different production cabs and real car bodies mounted on a strong robot arm. Currently, the researchers are working on a combined biomechanical-mechatronic model of the coupled seat system, which can be used to parameterize and calibrate the simulation software developed in the EMMA4Drive project.

Fewer hardware conversions required

This means that in the future, certain tests that are primarily aimed at physically stressing the occupants can also be carried out purely virtually, in addition to individual RODOS® simulator studies in a real driving cabin. When testing new concepts or comparative investigations of alternative variants, this saves time-consuming hardware modifications. However, for studies in which psychological aspects of the driving behavior are in the foreground, the simulation with RODOS® in a realistic cabin environment remains indispensable, since it is crucial for achieving a perfect immersion of the human being into the driving situation.

Further information can be found at
www.itwm.fraunhofer.de/emma4drive_en

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Virtual Vision Is Better: New Approaches in Image Processing

What makes a good inspection system for the industrial production process? First and foremost, the lighting and camera setup, because depending on how the light beam falls on a surface, defects such as dents or scratches become more apparent. Of course, the properties of the material to be inspected also play a role. Plastic has a different optical behavior than metal.

Here you can clearly see that certain areas in the image are overexposed. Reliable defect detection is not possible there.

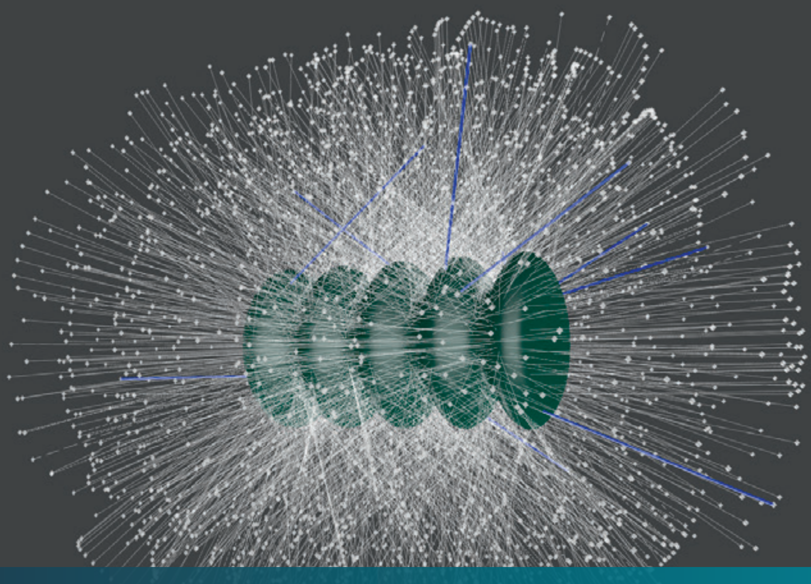
As long as the geometry of the test object is simple, such as rubber seals, tablets or metal plates, the setup can be adapted in just a few steps. The situation is quite different with complex geometries: If one takes, for example, a commercially available bulbous thermos made of aluminum with a handle made of plastic, it is almost impossible to develop a machine for fully automated inspection. If a robot is used to precisely maintain the angle between the surface and the illumination, this fails at the handle at the latest. In addition, aluminum and plastic exhibit different reflective behaviors. The angle of the illumination and camera must therefore be changed during the inspection.

Image processing, computer graphics, robotics: Together to the goal

So what to do? One solution would be to construct the entire inspection in the computer and physically simulate it – in other words, virtual image processing. Interdisciplinary work is being done on this at the Department of Computer Science at the TU Kaiserslautern and at Fraunhofer ITWM: Using existing computer graphics methods such as ray tracing, material models, CAD, and camera models, the team generates synthetic images and tests image processing algorithms on them. In addition, it implements methods to determine the optimal positions of the camera and lighting.

The first research result is an algorithm that calculates which surface areas can be safely inspected at all. For this purpose, it uses a 3D model of the test specimen and takes into account camera positions and illumination angles. This also resulted in a demonstrator consisting of a robot with camera and illumination.

However, simulating an entire inspection system and then modeling its effectiveness is a much more complex task. That is why the researchers asked themselves: How do you calculate optimal camera or illumination positions in relation to the inspection object? And they were able to answer it in part – with another algorithm. This method uses the 3D model to scan the entire surface and uses the local curvature to calculate which surface points are



Based on the geometry of the inspected object, our software creates a list of viewpoint candidates (white) and reduces them to a set of viewpoints needed to cover the most important areas (blue). A viewpoint marks a physical point in space, relative to the object, where the camera must be positioned during the inspection.

"In addition to computer graphics and visualization, we also need modeling based on physical principles for a viable simulation. With the V-POI planning tool, we are taking a big step in this direction"

Prof. Hans Hagen
Department of Computer Science at the TU Kaiserslautern

potentially important and thus must be in the camera's field of view. These positions are used for path planning of the robot or even fixed camera positions.

Learning system: Viewpoint of interest V-POI

The V-POI planning tool developed by the project team already copes well with component geometry and surface properties and has also learned to recognize potential problem areas during analysis. In order for the inspection system to know what a good part should look like, it is first "fed" the CAD data of a workpiece. The software is designed to calculate individual scan paths for objects placed on a turntable, for example, based on the specific product.

Goal: Manufacturer-independent system

The research objective is a software infrastructure that simulates the complete inspection environment, i.e. both the properties of the test specimen and the properties of all hardware components (illumination, camera, optics, etc.). The architecture of the software is to be designed in such a way that commercial suppliers of sensors, lighting, etc. can enter their product-specific properties, e.g. camera parameters, without having to disclose sensitive know-how. The system will therefore be manufacturer-independent.

Further information at www.itwm.fraunhofer.de/virtual-inspection-planning

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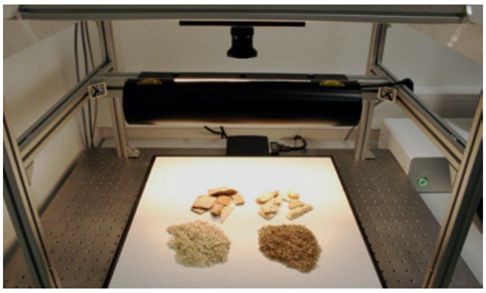
RGB Becomes Hyperspectral: Seeing More Than the Eye Allows

The monitoring of individual steps and parameters in production has been advanced with a great deal of energy for years in the context of "Industry 4.0". Through the development of new, efficient sensors and measuring systems, data is collected, evaluated and used to optimize production. In the field of optical sensor technology, hyperspectral imaging is an important building block for capturing information that initially remains hidden to the eye.

Hyperspectral image data in the infrared wavelength range can be used, for example, to identify wood species in production in real time, thus ensuring the correct composition, and ultimately quality, of the products. One important application is chipboard production.



Hyperspectral camera with illumination unit: The camera captures the wood samples as if on an assembly line – up to 300 line images per second.

It is all in the mix – even with chipboard

The composition of the processed wood chips plays a crucial role in the strength of the boards. Hardwoods such as beech and oak form the basis, but are also more expensive than softwoods such as pine and spruce: The right mix between hardwood and low-cost softwood is therefore crucial for efficient chipboard production.

With hyperspectral imaging, the spectral information of the wood chips on the conveyor belt is recorded via a line scan in the near-infrared range between 1000 nm and 2500 nm wavelength – with up to 300 measurements per second! These images contain the complete spectral information at each pixel. Due to small but measurable differences in the response of the various woods, these are assigned to the wood types in real time after a one-time learning process. This works because the measurement data is assigned to individual classes after processing and data reduction. Various classifiers are available for this purpose in order to react flexibly to specific applications. In the example, the correct assignment succeeds in over 95 percent of cases.

Much more than just wood detection

The method is not only suitable for wood species identification, but can also detect foreign substances in piles, determine the degree of ripeness of fruits and vegetables, or be used for sorting different materials. Depending on the application, the measurement principle including hardware and software is adaptable for different scenarios.

More info at www.itwm.fraunhofer.de/optical-metrology

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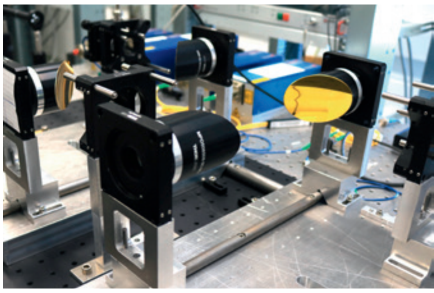
TeraSpect for Multispectral Measurements

Together with the industrial partner TOPTICA Photonics AG, Fraunhofer ITWM and Goethe University, Frankfurt am Main, have combined two successful technologies of terahertz measurement technology into a new measurement principle: the terahertz spectroscopy system TeraSpect.

Transistors from standard processes in the semiconductor industry can be used as highly sensitive terahertz detectors over a wide frequency range. If a series of these detectors is specifically optimized for several individual frequencies, which are then referred to as resonant detectors, these individual frequencies can be effectively filtered out from a broadband terahertz radiation source. So-called "spectral fingerprints" can then be measured. These are characteristic absorption lines that can be used to uniquely identify materials.

The system can be used, among other things, for authenticity testing in goods inspection.



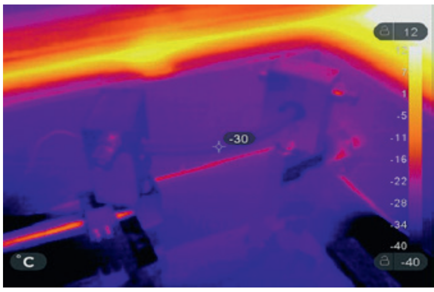
The TeraSpect system enables fast multispectral terahertz measurements.

More informations at www.itwm.fraunhofer.de/teraspect-pm

New Features for MeSOMICS®

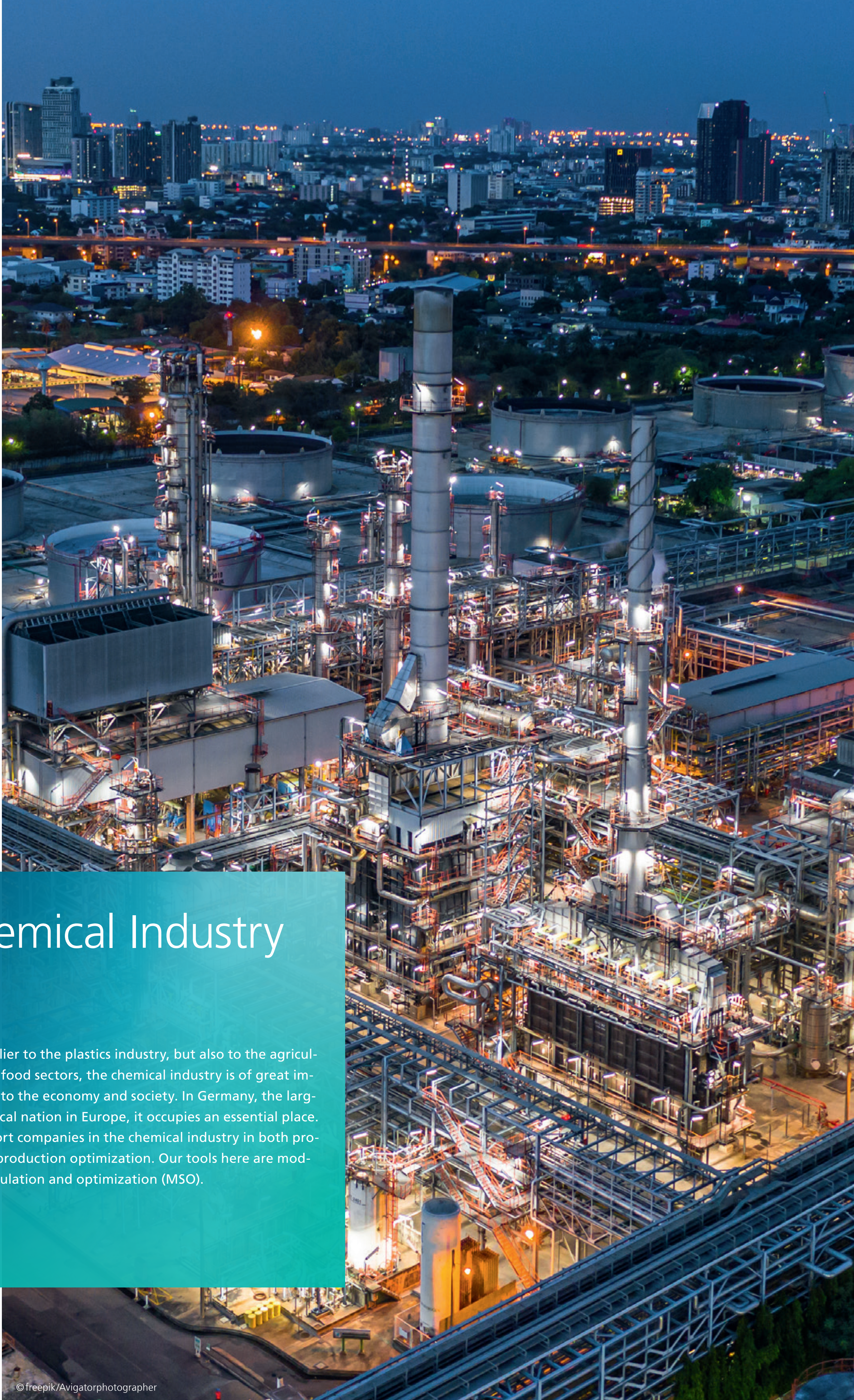
It looks simple, but it has what it takes: the highly automated MeSOMICS® measuring machine, designed and constructed in the division Mathematics for Vehicle Engineering. MeSOMICS® stands for "Measurement System for the Optically Monitored Identification of Cable Stiffnesses" and supports the IPS Cable Simulation product family. This software simulates and optimizes the routing of cables and hoses, especially in the confined installation spaces of modern vehicles. To ensure that the simulation is as realistic as possible, the mechanical properties of the individual cables must be determined. Especially important here are bending and torsional stiffnesses. With MeSOMICS® even the users of the IPS software can quickly and easily determine the required parameters themselves: The desired data sets are available in just three hours and are used for the numerical simulation in IPS Cable Simulation.

But MeSOMICS® can do even more: namely measure test specimens under pressure (up to 1000 bar) and ambient temperatures between -30 °C and 130 °C. "These options have been increasingly requested by our customers. Now we can offer them as a service in our Technical Center," says its head Dr.-Ing. Michael Kleer with great satisfaction.



A thermal imaging camera checks the temperature of the test specimen in the MeSOMICS climate chamber.

Further information at www.mesomics.eu



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Chemical Industry

As a supplier to the plastics industry, but also to the agricultural and food sectors, the chemical industry is of great importance to the economy and society. In Germany, the largest chemical nation in Europe, it occupies an essential place. We support companies in the chemical industry in both process and production optimization. Our tools here are modeling, simulation and optimization (MSO).

AI Meets 100 Years of Engineering Expertise

The innovation platform KEEN (Artificial Intelligence Incubator Labs in the Process Industry) aims to accelerate the use of AI technologies and AI methods in the process industry. Employees of the "Optimization" division contribute their know-how around the digitization of chemical production to the project.

The chemical industry has been considered a driver of progress in Germany for more than 100 years. The KEEN project brings together a total of 20 startups, corporations and research institutions. Together, the participants are working to take the experience of the traditionally knowledge-based industrial world in new directions with the possibilities of artificial intelligence. Because one thing is clear: "AI alone will not work. It is a matter of bringing knowledge and data together to unleash practical benefits," says Dr. Michael Bortz.

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What if ...

Fraunhofer ITWM runs two subprojects for this purpose: In the first step, together with TU Kaiserslautern, thermodynamic properties of mixtures are modelled so that AI can be used for the prediction of substance properties. In the second step, process simulations are carried out. "Only when we know how substances behave can we, for example, even design a process for separation," says Bortz.

Specifically, the team is working on a decision support system that can run "what if" scenarios in real time. By using AI, it is also possible to display the effects of changes in the process in real time, even in computationally intensive and time-consuming process simulations: "We set up AI models that we train with simulation data and that can then calculate considerably faster and even be capable of real-time," says Bortz, describing the vision.

Three major fields of research

The KEEN consortium is researching three major topics: the modeling of processes, product properties and plants, engineering, and the realization of self-optimizing plants. The research will run until 2023, with the first commercial AI products for the process industry expected to be available by 2025. The project is 60 percent funded by the German Federal Ministry for Economic Affairs and Energy and has total funding of 23 million euros.

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Further information is available on the website at www.itwm.fraunhofer.de/keen-en

Optimizing Chemical Formulations With Low Risk

Changing a successful product requires a certain amount of courage. Costs and benefits have to be weighed up against each other in order to make a sound decision. In the FORCE (Formulations and Computational Engineering) project, researchers at Fraunhofer ITWM are developing a system that supports such decisions.

> Good decision-making is the objective of FORCE.

People are creatures of habit. If their favorite shampoo suddenly feels different, many people find this annoying and may switch products the next time they buy. "Companies do not easily change chemical formulations of successful products, whether that is in the cosmetics sector or in other industries," says Dr. Peter Klein, a scientist in the "Optimization" field who is leading the FORCE project.

Assessing consequences – making decisions

The objective of FORCE is to develop a Business Decision Support System (BDSS) specifically tailored to the optimization of chemical formulations. The software-based optimization and decision support system will cover the business processes of product optimization,

The FORCE project started in January 2017 and ended in March 2021 after extension. It is funded under the Leadership in Enabling Industrial Technologies LEIT pillar of the EU H2020 program.

Left: Ten international project partners were involved in FORCE – the entire team came together for the launch. Right: New scent, different feel? Changes in the production process must be well considered.

development and quality control. In order to be as close as possible to the needs of the industry, case studies from three different companies with their specific products will be used: project partners are Dow Benelux (PU foams for thermal insulation), Megara Resins SA (PU-based liquids for paints, coatings or printer inks) and Unilever UK Central Resource Ltd. (shampoos).

"Production processes are complex. Anyone who intervenes in them has to take a great many parameters into account," says Klein. "Our platform is therefore designed to reveal to the user what which adjusting screws do and to show different options." "Ultimately," he says, "it is always a matter of finding the best possible compromises between goals that are in conflict with each other." The system shows its users the best possible compromises on the basis of Pareto fronts.

Interactive Decision-Making

For a decision strategy, you compare, for example, which substances can be changed in their concentration ratios and then receive results that need to be evaluated: "Then you have to weigh things up. For example, you compare production costs with quality," says Klein, describing a typical dilemma. "We can support this process with interactive decision- making, for example, by simulating that the consistency of a shampoo changes due to the modification of attributes from the chemical process. On this basis, it is possible to decide whether the product will continue to meet the expectations of its target group and whether the production costs saved should be accepted for the noticeable change to the product."

In addition, the BDSS also incorporates constraints, such as legislation or certain standard values that must also be changeable: If a regulation changes, the performance indicators in the formula must be renewed. For the software users, this means that they can repeatedly check an optimization problem including new constraints. "The same is true for price, when you match production and material costs with technical requirements: We can simulate different ingredients for the same result while checking the cost issue."

Further information is available on our website at www.itwm.fraunhofer.de/force_en

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Take a Seat – Simulation of PU Foam Expansion During Injection Molding of Car Seats

Car seats have a complex structure: frames, load-bearing structures, heating systems, back and seat cushions. The latter are composed of polyurethane foams (PU foam) – often in different degrees of hardness. The ITWM tool FOAM simulates the expansion process during the production of such PU foams – in arbitrary geometries and provides the possibility to digitally calculate foam formation and foam density in advance.

Simulation enables prediction: How does foam spread?

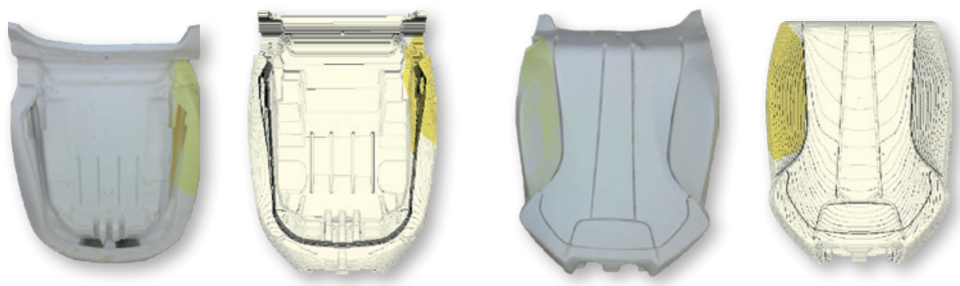
Optimal foaming as a complex process

The process is divided into the following steps: First, the material is injected into an open mold, during which the foam already starts to expand. Then the mold is closed and the foam continues to expand until it fills the entire cavity. It is also possible to influence the flow of the foam by tilting the mold in a certain direction. Injection paths, inclination of the mold as well as the amount of material are all important for the injection phase in order to obtain a uniform foam density at the end of the process.

It should also be noted that carbon dioxide is released during foaming. This excess gas is usually removed from the mold by vents. Here again, the arrangement of the vents is important, as incorrect placement can lead to gas bubbles or large cavities. We take all these aspects of the process into account in the simulation with our FOAM tool.

Project objective and collaboration: From experiment to simulation

The objective of the project between Fehrer Automotive, Audi and our institute is to validate these strengths of FOAM. Our main focus was on predicting the expansion of PU foam – also in a real car seat geometry. The latter was provided by Audi, while Fehrer Automotive was responsible for conducting the experiments. At the start of the project, the team selected two foam systems and conducted simplified foam expansion tests for each system supplied by Fehrer. These provided information on the volumetric expansion over time as well as the development of the foam temperature. A specific amount of foam material was injected into a cylindrical tube. The foam height during expansion was measured at the centerline and the foam temperature was measured at the sensor position five centimeters from the bottom. This data served as the basis for the identification step of the input parameters of the FOAM model. On this basis,



The simulations (each on the right) show the very good qualitative match with the experiments with regard to the position of a pouring path (yellow) in top/bottom view

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“The ITWM has a unique competence in the virtual representation of complex physical processes, from physical and mathematical modeling to efficient numerical computer-aided computation. The cooperation with ITWM is always pleasant and straightforward.”

Dr.-Ing. Johannes Spahn
Audi AG

we calibrated the input data of the model to match the experiments.

After successful model calibration, validation tests were performed in a box geometry under different configurations. In all cases, a certain amount of material was injected into the open box. After injection, the mold was closed with a transparent lid and the foam expansion was filmed with a camera. In this way, the development of the foam front could be closely observed and used to validate the simulation results. Very good qualitative agreement was found between such tests, including those with Audi’s real car seat geometry, and the simulation.

FOAM has demonstrated its value as a simulation tool for predicting foam expansion in complex molds. It enables testing of different injection paths and correct vent positioning in early development phases. By using FOAM, companies not only save a large number of experimental tests, but also time and money.

Further information and simulation videos are available on the website: www.itwm.fraunhofer.de/pu-simulation-car-seat

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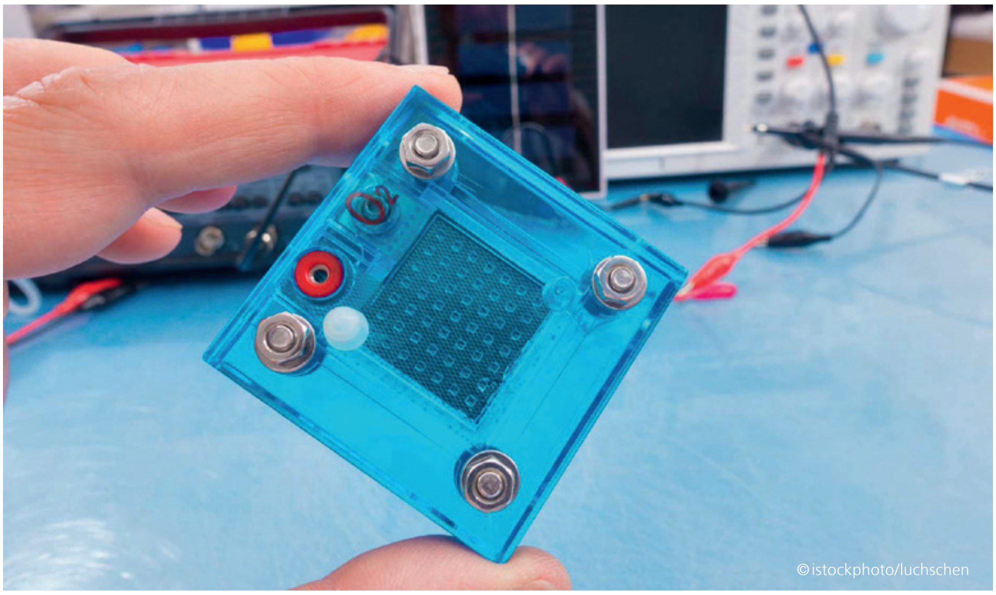
Understanding Hydrogen Electrolysis on a Small Scale – Achieving Big Things for Greener Energy



Hydrogen technologies are seen as paving the way for climate-neutral mobility and as holding out hope for the climate-neutral design of the energy industry and the chemical industry. But to achieve this, the chemical processes of the cells need to be better understood. A team from the "Transport Processes" department supports the design and optimization of the cells with novel shape optimization methods.

The fuel cell seems to be the ideal vehicle drive: quiet, clean and independent of oil. The hydrogen required for this can be obtained from green electricity via electrolysis. An electrolysis cell is similar to a fuel cell, except that the entire process is reversed: Using electrical energy, hydrogen is obtained by splitting water into hydrogen and oxygen. Among other things, a cell consists of two metallic plates (bipolar plates) and a membrane. "The flow dynamics of the bipolar plate are quite crucial for the performance of the cell ," says Dr. Christian Leithäuser from the "Transport Processes" department. "We want to design these in such a way that the oxygen produced is discharged sufficiently quickly to make the cell more efficient. To do this, we simulate a multiphysics problem and use shape optimization methods."

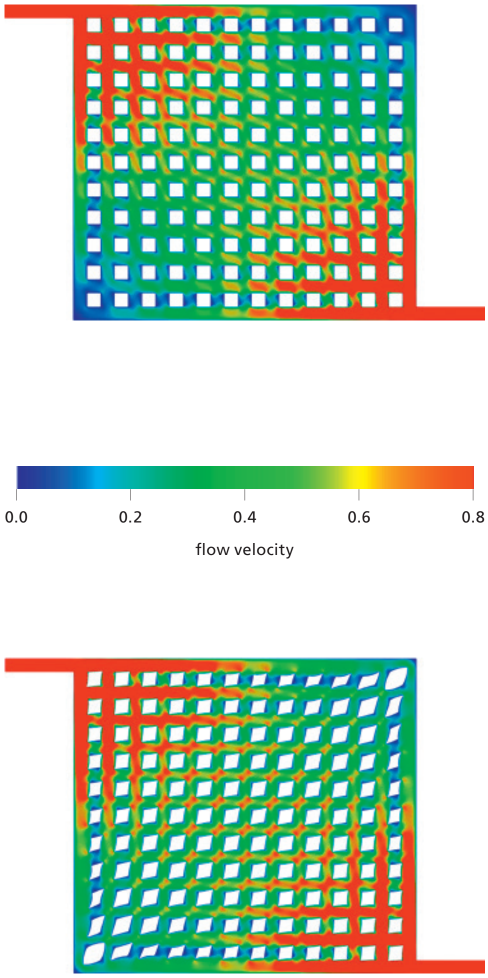
PhD thesis results in simulation tool CASHOCS for design

This topic of "designing bipolar plates for hydrogen electrolysis" was investigated in more detail by his colleague Sebastian Blauth in his doctoral thesis: "An open-source software package called CASHOCS was created based on my work," Blauth reports. This stands for "Computational, Adjoint-Based Shape Optimization and Optimal Control Software". "CASHOCS has since become a generic tool that we now use for the design of chemical reactor components." Similar issues arise in fluid dynamic stack design. Here, too, it is important that all cells are flowed to as uniformly as possible and without major pressure losses.

Example PEM electrolysis: Optimize free of dead zones

In Proton Exchange Membrane (PEM) electrolysis, water is supplied via the bipolar plate on the anode side. This is also split into hydrogen (H_2) and oxygen (O_2) by the supply of energy. The hydrogen migrates through the membrane and is collected on the cathode side. The resulting oxygen must be removed via the bipolar plate on the anode side so that the cell efficiency does not drop.

The bipolar plate should therefore always have an even flow – without so-called death zones from which the oxygen does not escape quickly enough. The graphic on the right illustrates the design with the CASHOCS tool. The reference design is shown above with the inlet in the upper left corner and the outlet in the lower right corner. The flow velocity is illustrated by the color scheme. In the lower left and upper right corners of the reference bipolar plate are death zones with poor flow. The bottom graph shows an already optimized bipolar plate. The tool's algorithm cleverly manipulates the reference geometry until the best possible uniform flow is achieved. The optimized bipolar plate is then free of dead zones.



Optimized stack design: Two bipolar plates before and after shape optimization. Blue areas are death zones with insufficient flow (reference above, optimization below).

In particular, such an approach with a digital twin opens up a detailed insight into the complex processes within the microstructures that would not be possible at all purely experimentally. Looking to the future: Implementation of the new design is now easily possible using additive manufacturing processes. The development results will thus flow into the next generation of electrolysis cells.

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More about the focus "Fluid Dynamics Process Design"
www.itwm.fraunhofer.de/tv-process-design

More about the CASHOCS tool: www.pypi.org/project/cashocs/

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Main Focus

- Surface and material characterization
- Quality assurance and optimization
- Virtual Image Processing
- Industrial Image Learning
- Condition Monitoring and Predictive Maintenance

Image Processing

Mathematical models and image analysis algorithms for industry

The department develops mathematical models and image analysis algorithms and converts them into software suitable for industrial use, primarily in production. The application areas include, in particular, sophisticated surface inspection and analysis of microstructures. We have been developing and distributing software for 2D and 3D image analysis for over 15 years and develop both new methods and domain-specific machine learning algorithms.

In recent years, one focus in machine learning has been on image processing for production and industry. Methods such as "Deep Learning" require a high volume of annotated data, for example of the defects to be found in a production plant. Now, however, in a well-functioning manufacturing plant, there are many images of defect-free products, but only a few of products with defects. We therefore often use hybrids of the "traditional" parameterizable methods (filters, morphology, edge detectors) and machine learning. In addition to solutions for production, we also offer "typical" machine learning solutions for image processing. These are often projects in which very large amounts of image data are processed manually and this process is to be automated by software.

Another focus is microstructure analysis. The microstructure of modern materials significantly determines their macroscopic material properties. We develop algorithms for characterization and stochastic modeling of such microstructures based on image data, e. g. from CT, FIB-REM, SEM. Our products serve the deeper understanding of the complex geometry and structure-property relationships in materials . This opens up new possibilities such as optimization of material properties by virtual material design. Based on the parameters obtained from image data, stochastic geometry models are fitted to the real microstructures, which reflect the geometric structure relationships well and thus simplify or enable numerical simulations in the first place.

The latest research field is virtual image processing. Here, the complete, physically correct simulation of inspection systems is planned. The objective is a software infrastructure that simulates the complete inspection environment. This includes not only the properties of the product/object to be inspected but also the properties of all hardware components (illumination, camera, optics, etc.).

Department topics in this report:

- Bending and observing concrete beams – quantum computing speeds up analysis of CT data, p. 21
- Better understanding lung damage caused by Covid-19, p. 34
- Tracking down fraud with algorithms and AI, p. 48
- Seeing better virtually: New approaches in image processing, p. 70

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Main Focus

- Billing audit
- Retirement and life insurance
- Flexible loads on the energy market
- Data Science

Financial Mathematics

Methodological competence in financial mathematics, stochastics and data

The department has its methodological foundations in Financial Mathematics and Data Science. Data Science refers to an interdisciplinary scientific field with the goal of gaining scientifically robust insights from data. This often involves the use of methods from Machine Learning, which are the basis for many applications in the field of Artificial Intelligence (AI). Financial mathematics includes stochastic modeling, simulation and optimization as well as statistical methods and time series analysis.

We use our methodological competencies to make sustainable contributions to current societal challenges in cross-sector business areas: demographic change, energy transition and digitization. We are convinced that collaboration generates more value than the sum of the individual parts, which is why we cooperate with partners from the institute, academia and industry at many points.

In the business area of retirement provision, we have a holistic view of retirement provision in Germany and Europe in close cooperation with the Product Information Office for Retirement Provision (PIA). For example, we use our stochastic simulation technology for retirement provision products to assess the risks and rewards of tariffs from the customer's point of view.

Flexible loads will become increasingly important in the energy system of the future. These will act price-sensitively in electricity trading; thus, a currently still existing basic assumption of many models is no longer valid. We are developing new solutions for this, because the integration of flexibility requires new mathematical algorithms, which we are developing together with energy industry expertise.

The digitization of processes is creating new opportunities to efficiently check billing processes. We have already developed audit methodology and software for several industries and are working closely with industry on new algorithms in ongoing projects. We are expanding our expertise in the direction of the healthcare industry and are working with public prosecutors and the police on methods for auditing nursing service billing.

Together with industry partners, we are active in quantum computing and are developing new approaches to solving problems.

Department topics in this report:

- Quantum computing: joint project "EnerQuant", p. 20
- Researchers in financial mathematics calculate smart solvency capital, p. 46
- Tracking down fraud with algorithms and AI, p. 48
- FlexEuro: Flexible and smart management wins in the energy market, p. 56

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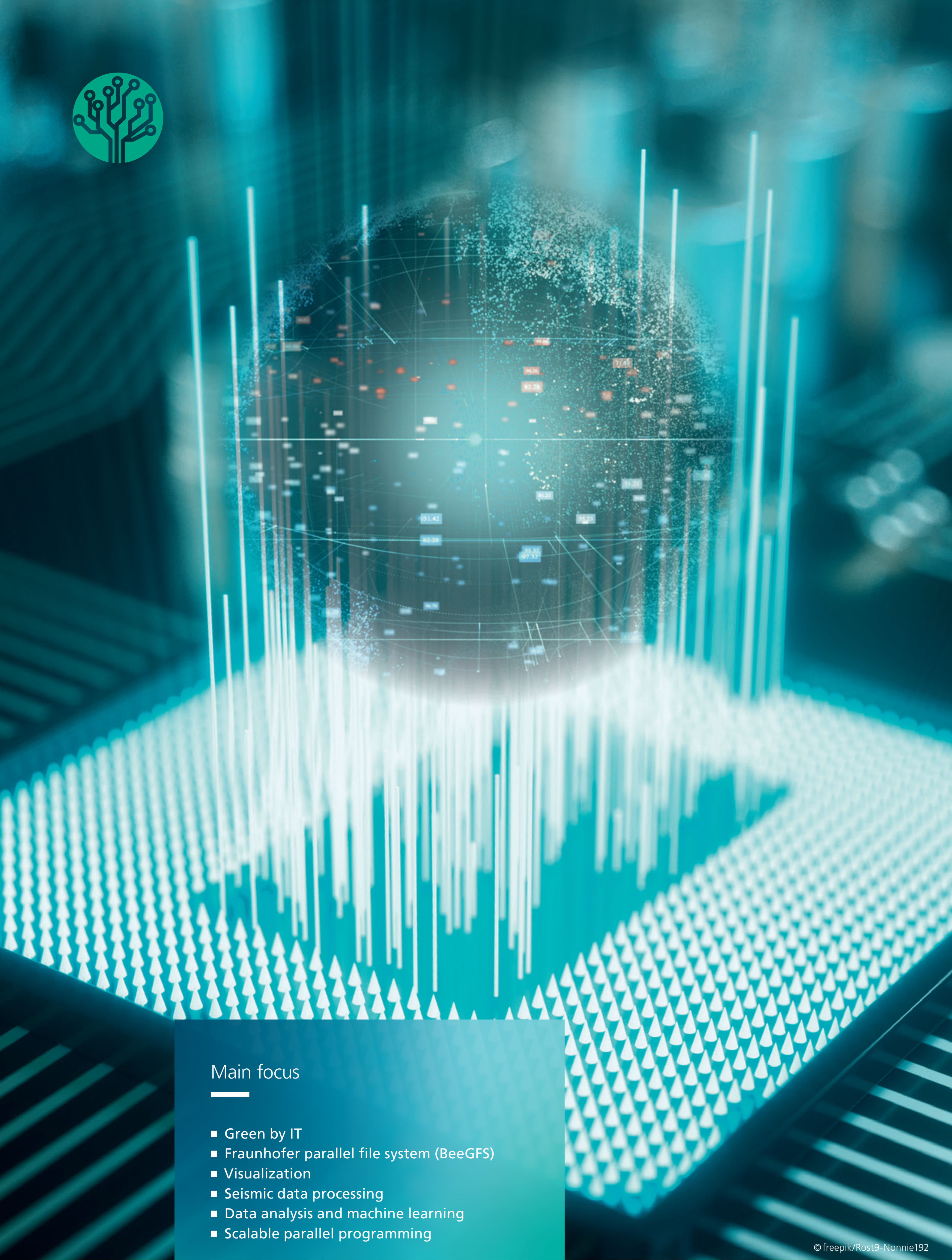

Main focus

- Green by IT
- Fraunhofer parallel file system (BeeGFS)
- Visualization
- Seismic data processing
- Data analysis and machine learning
- Scalable parallel programming

High Performance Computing

Innovation, disruption and holistic thinking in the world of distributed computing

Our IT systems are among the largest single energy consumers and CO2 emitters, with energy consumption continuing to rise. Currently, this accounts for five to ten percent of electricity consumption. However, this share will probably grow to twenty percent – this is in the order of a completely electrified private car traffic. Most of the time, the focus is on "green" data centers, which are powered by electricity from renewable sources, and on efficient cooling technology. However, the much greater potential lies in the software and how it is used on which processors, and thus in its effect on the majority of the remaining IT systems.

In high-performance computing, energy costs are already a crucial factor in hardware procurement. However, the efficiency of the software used is even more important. Software that does not take advantage of the parallelism of modern processors and their architecture quickly loses an order of magnitude in energy efficiency here as well. For us in the HPC department, High Performance Computing means the use and development of highly optimized software on suitable hardware. In 2008, the Pegasus system by ITWM was already among the TOP 500 of the fastest HPC systems and number one in the Green 500! Our software was orders of magnitude more efficient than the original customer software. Here, the saved energy costs of one year of operation alone would have financed the Pegasus computer and the development of the software. Our experience in many industrial projects shows that non-optimized software can often be improved by at least one order of magnitude. Today, we are the specialists in energy-efficient programming, i.e. green computing. However, it must become easier for everyone to write efficient software. The STX processor, which we developed in the EPI project, brings us a great deal closer to this goal. Its design makes it easy for a large class of algorithms to save energy and costs with the support of the compiler. Energy Efficient Computing today means the perfect utilization of parallelism, optimal data transport as well as suitable algorithms in combination with the right hardware. This holistic approach to Green Computing is the core of our self-image and motivation for the employees of the HPC department.

Department topics in this report:

www.itwm.fraunhofer.de/en/hpc

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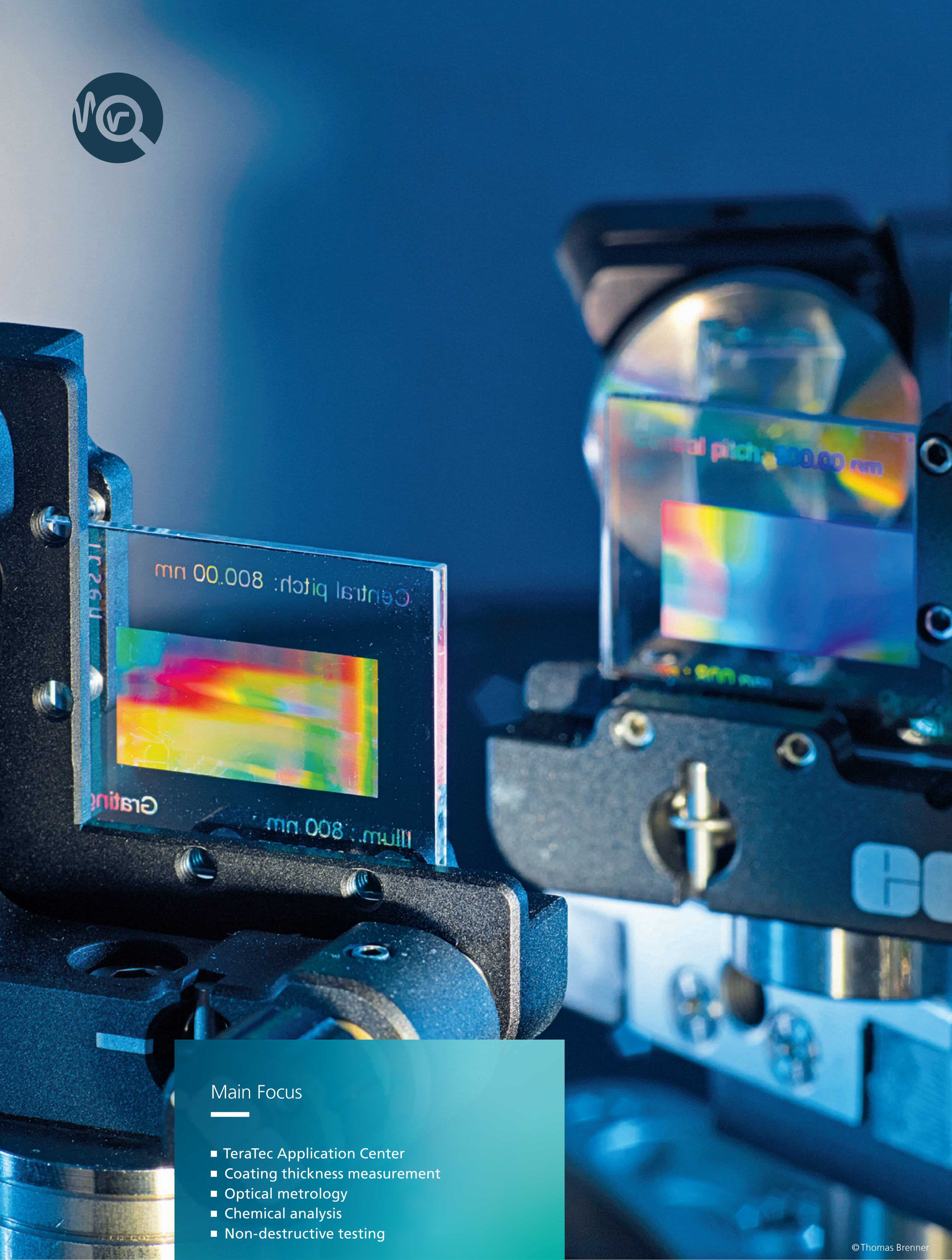

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Main Focus

- TeraTec Application Center
- Coating thickness measurement
- Optical metrology
- Chemical analysis
- Non-destructive testing

Material Characterization and Testing

Perspective with millimeter, terahertz and optical waves

Many things remain hidden from the human eye: Most materials are opaque, so we can usually only optically detect the surface of objects. This is not sufficient for checking whether components have been manufactured without defects: Adhesive joints in composite materials, for example rotor blades of wind turbines or also on window panes of vehicles, cannot be inspected in this way.

At the Center for Material Characterization and Testing, we develop non-destructive and non-contact testing methods that are optimized for use in the production line and enable reliable control of the production process. Our terahertz layer thickness gauges measure the thickness and material parameters of each individual layer. Our pipe inspection systems check wall thickness directly at the extruder. Defects in composite materials are detected by our radar-based FMCW inspection system. Bonds can also be inspected in this way. And sometimes we even check the paint layers of famous works of art.

Machine learning helps us recognize subtle material differences so that, for example, wood species can also be reliably distinguished in the chips for particleboard – the mixture is crucial here for the quality and durability of the particleboard.

Our scientists, engineers, and technicians use technologies ranging from optical coherence tomography (OCT) in the visible spectral range to time-domain spectroscopy in the terahertz frequency range and electronic system concepts in the millimeter-wave range for customized solutions. Initial successes in the use of quantum technology enable us to detect material properties in the terahertz frequency range using only visible light. The expertise of our employees includes a detailed understanding of processes. This enables us to transfer results from basic research to application – the latest technological developments can thus be identified and used as solutions for demanding applications.

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Department topics in this report:

- Quantum computing: Fraunhofer lead project "QUILT" (Quantum Methods for Advanced Imaging Solutions), p. 19.
- Keeping the Current Flowing: Non-destructive testing of power plant generator rods, p. 54
- From RGB to hyperspectral: Seeing more than the eye can see, p. 72
- TeraSpect for multispectral measurements, p. 73

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Main Focus

- Digital environmental data
- Load data and durability
- Dynamics and system simulation
- Human modelling and human-machine interaction
- Cables, hoses and flexible structures
- Tire models – CDTire
- Technical Center: Human Machine Interaction and driving simulators

Mathematics for Vehicle Engineering

Simulation-based engineering in the vehicle industry

The division is divided into the two departments, Dynamics, Loads and Environmental Data (DLU) and Mathematics for the Digital Factory (MDF), the project group Tire Simulation (CDTire), and the cross-sectional unit MF Technical Center, which operates the simulator laboratory with the interactive driving simulator RODOS and the measurement vehicle REDAR and takes care of all the division's testing and measurement related tasks.

In the Dynamics, Loads and Environmental Data department, we develop methods and tools for data analysis and system simulation. In doing so, we rely on a problem-adapted best possible combination of physics-based and data-based (AI, ML) modeling. The increasing availability of data from vehicle development, operation and production constantly leads to new opportunities and challenges here, which fit perfectly with our many years of experience in data-based mathematics and hybrid modeling. Special attention is paid to the inclusion of digital environment data and the simulation of usage variability. In this way, we address the vehicle development attributes of durability, reliability, energy efficiency, and the validation of assistance systems and automated driving functions. In line with this, we are focusing our system simulation activities on vehicle-environment-human interaction and developing tire simulation models (CDTire) as well as methods for interactive simulation.

Mathematics for the Digital Factory bundles the activities for the development of software tools for virtual product development and product creation. Our software product IPS Cable Simulation, developed jointly with the Fraunhofer Chalmers Research Center for Industrial Mathematics (FCC) in Gothenburg (S), supports virtual design, optimization and validation for assembly and operation of cables, harnesses and hoses. In addition, we have developed IPS IMMA, a digital biomechanical human model to virtually optimize assembly processes. Efficient and fast algorithms enable an efficient evaluation and optimization of the ergonomics of assembly processes.

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Division topics in this report:

- Scattershot: Statistics blog and podcast, p. 29
- The Technical Center – tests and simulations under one roof, p. 37
- CDTire – reinventing the tire with simulation, p. 38
- Making better use of data – AI and ML in vehicle development, p. 40
- EMMA learns to drive – dynamic human model for autonomous vehicles, p. 68
- New features for MeSOMICS®, p. 73

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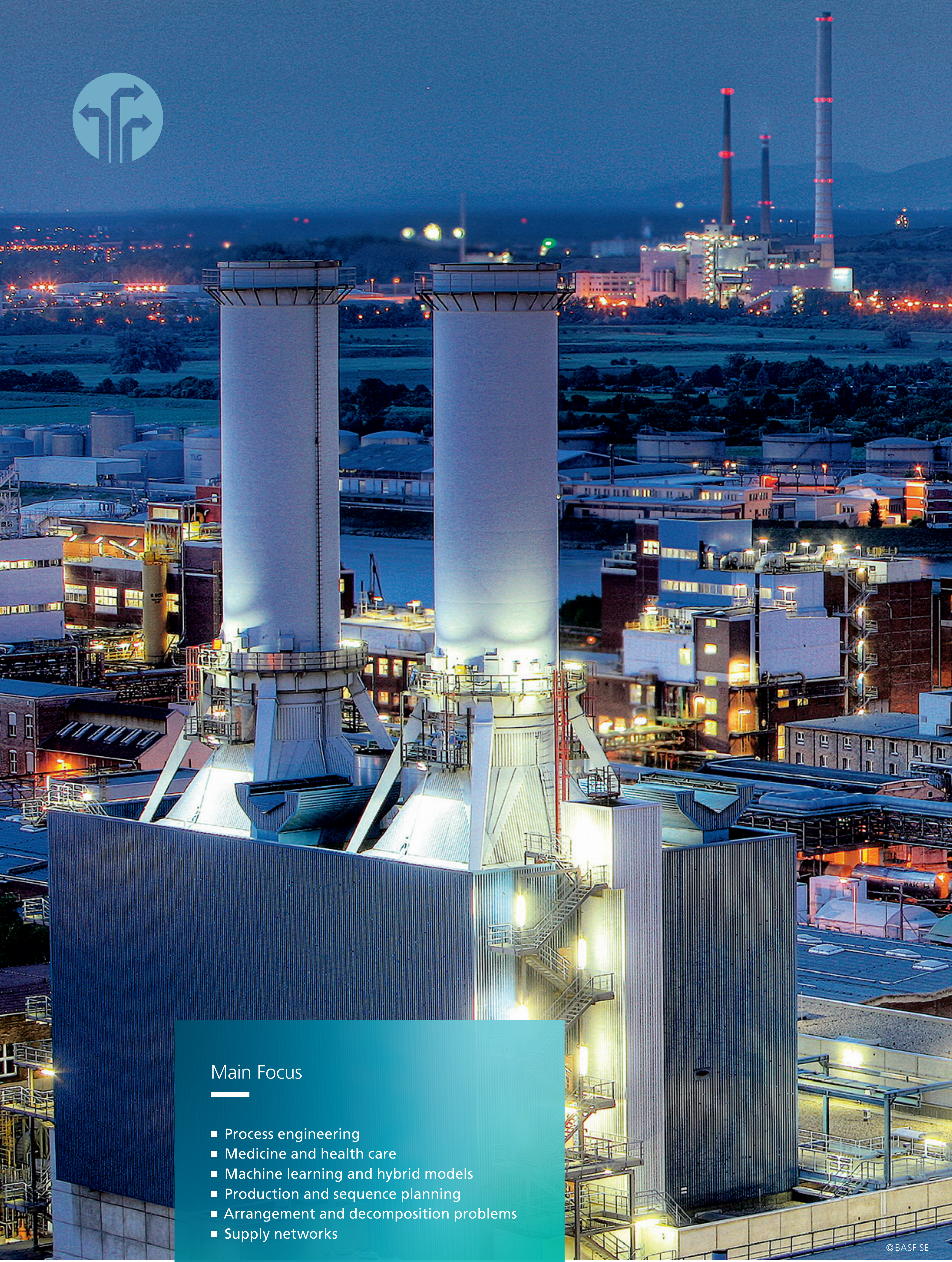

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Main Focus

- Process engineering
- Medicine and health care
- Machine learning and hybrid models
- Production and sequence planning
- Arrangement and decomposition problems
- Supply networks

Optimization

Simulation-based engineering in the vehicle industry

The central task of the department is the development of individual solutions for planning and decision-making problems in logistics, engineering and life sciences, always in cooperation with partners from research and industry.

Methodologically, the work of the department is characterized by an interplay of data analysis, simulation, optimization and decision-making support. By simulation we mean the knowledge and data-based creation of mathematical models, taking into account design parameters, restrictions and quality measures to be optimized as well as costs.

Core competencies of the department are the development and implementation of application and customer-specific optimization methods. These compute the best possible solutions for the design of processes and products. Unique selling points are the integration of data analysis, simulation and optimization algorithms, the special consideration of multi-objective approaches, as well as the development and implementation of interactive tools for decision support in customized user stories.

Overall, optimization is understood less as a mathematical task, but rather as a continuous process, which we support by developing suitable interactive tools. Special attention is paid to the adequate choice of the model with respect to the quantity and quality of the available data. We draw on machine learning methods to process the data and calibrate models, but also to augment models and explain phenomena that cannot be explicitly modeled. Important application domains are:

Production planning: The challenge is to achieve a good balance of on-time delivery, inventory levels and utilization of production resources against a background of fluctuating demand and growth prospects, in good connection with the supply chain.

Chemical process engineering: Process planning to manage the conflicting demands of product quality, production speed and energy consumption (CO_2 footprint) in the face of fluctuating raw material prices

Medical therapy planning: Individual therapy plans in balancing chances of healing and probabilities of complications

Renewable energy: Use of renewable energy and storage technology for robust and cost-efficient supply

Division topics in this report:

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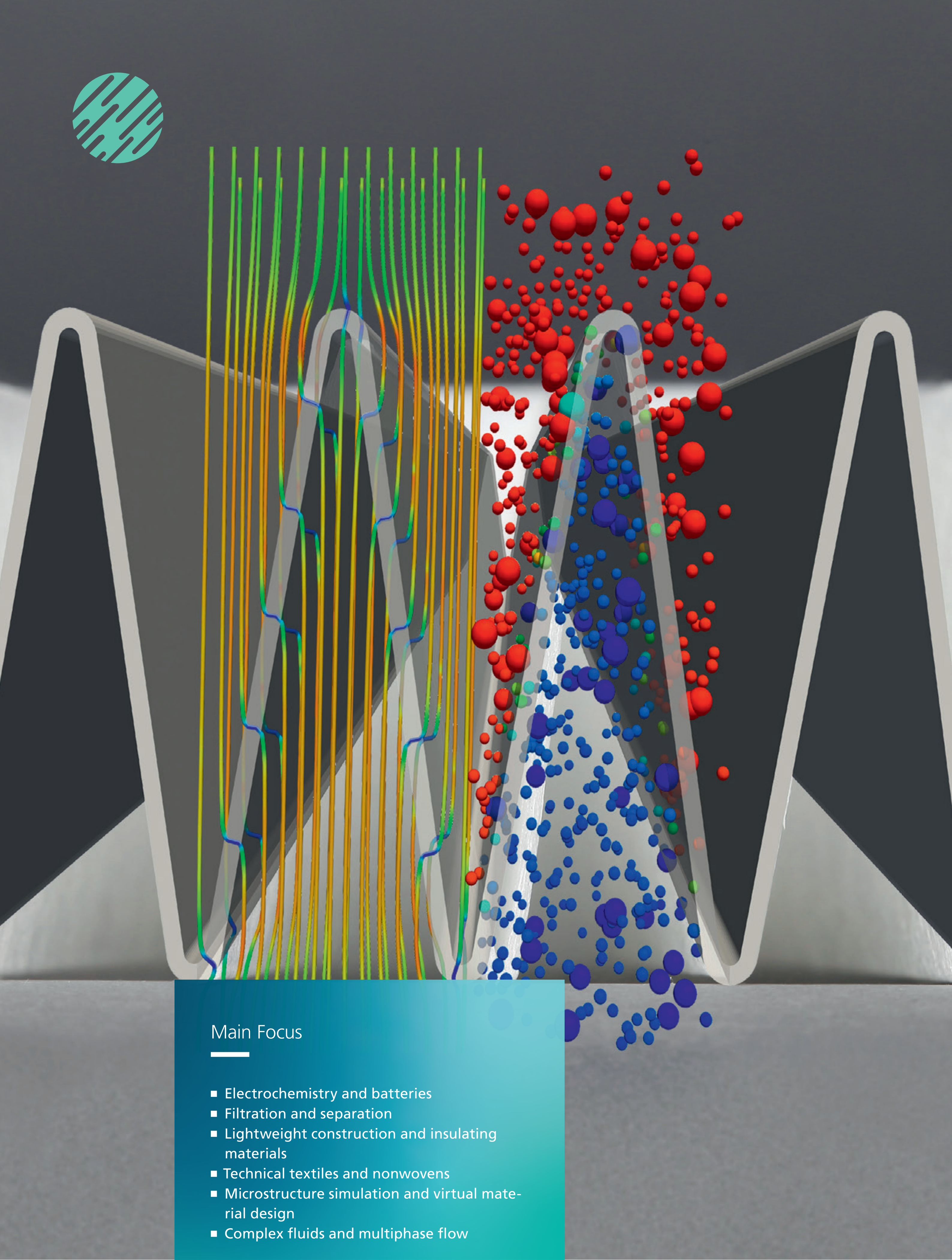

Main Focus

- Electrochemistry and batteries
- Filtration and separation
- Lightweight construction and insulating materials
- Technical textiles and nonwovens
- Microstructure simulation and virtual mate-rial design
- Complex fluids and multiphase flow

Flow and Material Simulation

Industrially applicable multi-scale simulation and customized software solutions

The department “Flow and Material Simulation”” offers competent research and development support in modeling, simulating and optimizing the production, functionalization and use of porous materials and composite materials for a wide range of applications. Inquiries concern, for example, the production and functionalization of filter materials and technical filter systems, battery or fuel cells, technical textiles for hygiene products or sports textiles, foams for insulation and damping and fiber- and particle-reinforced lightweight components.

Our unique position is characterized by the development, provision and specific application of industrially suitable multiscale and multiphysics methods, the development of digital material and product twins and company-specific software solutions. Our simulation tools use the latest research results such as model order reduction techniques, automatic parameter identification, machine learning, modern software and database concepts to increase efficiency.

Microstructure simulation and virtual material design enable numerical simulation and optimization of functional properties of porous materials and composites. Our highly efficient micromechanical methods for material design of fiber-reinforced composites, foams and technical textiles are in great demand. The efficient integration of micromechanics and dynamics as a multiscale material model for CAE software enables the detailed prediction of local crash, damage or even creep behavior. To complete digital material twins, we combine our simulation methods with suitable data space descriptions and database concepts.

The simulation-based design of complex flow processes deals with the associated manufacturing processes such as coating, mixing, foaming, injection, filtration and separation. The main focus of industrial applications is on filtration and separation processes and, in addition, the product design of filtration plants. Reactive processes such as catalytic filtration, polyurethane foaming or the electrochemical processes in battery and fuel cells are correctly represented in our simulation programs.

In combination with the corresponding digital material data spaces, we create multi-scale digital twins for filter elements, battery cells, textile products and lightweight components, among others, which enable virtually supported product design, production and operational control.

Department topics in this report:

- AVATOR – How do aerosols spread indoors?, p. 30.
- Meltblown: Fewer clouds in the simulation sky, p. 32
- DEFACTO – Simulation of batteries, p. 42
- Simulation of PU foam expansion, p. 78

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Main Focus

- Power generation and distribution
- Real-time plant operation and drive technology
- Biosensors and medical devices
- Machine learning
- Control of complex systems
- Model identification and state estimation

System Analysis, Prognosis and Control

Analysis and prediction of complex system and process behavior

The focus of the department is on real-time plant operation and drive technology in production and power generation by means of digitization. To model dynamic, multi-physical systems, we combine physical knowledge with (deep) machine learning methods based on measurement data. We create digitized representations of complex plants, individual machines and components, also taking into account possible disturbance overlays of the measured data. Together with our customers, we integrate these as digital twins in versatile applications and innovative business models.

Applications include quality analysis and prognosis (e.g. electric motors, extruders) or condition monitoring (CM) as well as predictive maintenance (PM) for production plants and energy producers (e.g. combined heat and power plants or wind turbines). Targeted, agile project implementation creates a deep understanding of the system among project partners. In close exchange with operators, operating states of production plants are monitored and predicted to ensure production quality, avoid failures, and optimize maintenance procedures.

We perform energy efficiency and flexibility analyses of production processes for distributed predictive energetic process control as demand-side management and create the design for innovative controls for production optimization. The system integration in electronic control units is validated by means of hardware-in-the-loop (HiL) methods to test the application even in extreme situations. For this purpose, we use a HiL simulator with extensive I/O interfaces to test the electronic control units through system simulations.

We create turnkey CM or PM systems or control units and test their real-world use without resource-intensive experiments. Our projects support customers from idea to operation in the development and integration of analysis, prognosis or control systems. We implement new concepts, e.g. 5G communication for data transmission between sensors, controllers and actuators. Here, we develop problem-driven solutions based on methods of systems and control theory and machine learning. We also apply this in biological-medical systems for the analysis of biosignals, e.g. EEGs, medication or diagnostic support.

Department topics in this report:

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Main Focus

- Flexible structures
- Fluid dynamical process design
- Grid-free methods
- Energy transport networks and model reduction

Transport Processes

Mathematical modeling, simulation and optimization of transport processes

The department models complex industrial problems and develops efficient algorithms for the numerical simulation and optimization of these problems. The problems are in the technical-scientific context (fluid dynamics, structural mechanics, radiative transfer, optics, etc.) and lead in the modeling to partial differential equations, which are mostly to be characterized as transport equations.

From the point of view of customers, this typically involves the design of production processes and the optimization of products. Our range of services extends from cooperation projects with the engineering-oriented research and development departments of partner companies, to studies with design and optimization proposals, to software solutions – from building blocks to complete tools.

The department is structured according to four research fields. The "Flexible Structures" field focuses on mathematical modeling, simulation and optimization of the dynamics of threads, fibers and filaments with a focus on the design of production processes of technical textiles. The "Fluid Dynamical Process Design" team covers the manifold fields of fluid dynamics with its competencies. One scientific focus is the development of tools for optimal shape design. The "Grid-free methods" team researches a simulation approach based on a particle method, from which the MESHFREE software is being developed for a wide range of industrial applications. One focus in the "Energy Transport Networks and Model Reduction" research field is the modeling and simulation of energy transport in networks. Accompanying this, model reduction methods are applied to industrial tasks.

We were able to compensate for the Corona-related decline in industrial contract research by acquiring additional public research projects and concluded the year with a positive overall result. Various participations in anti-Corona projects played a special role. We were able to contribute our know-how in the production of nonwovens (protective masks), our expertise in fluid dynamics (aerosol dispersion) and new ideas on retarded differential equations (epidemiological models).

Department topics in this report:

- AVATOR – How do aerosols spread indoors?, p. 30.
- Meltblown: Fewer clouds in the simulation sky, p. 32
- MESHFREE – Process simulation to the point, p. 63
- Understanding hydrogen electrolysis on a small scale – Achieving big things for greener energy, p. 80

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