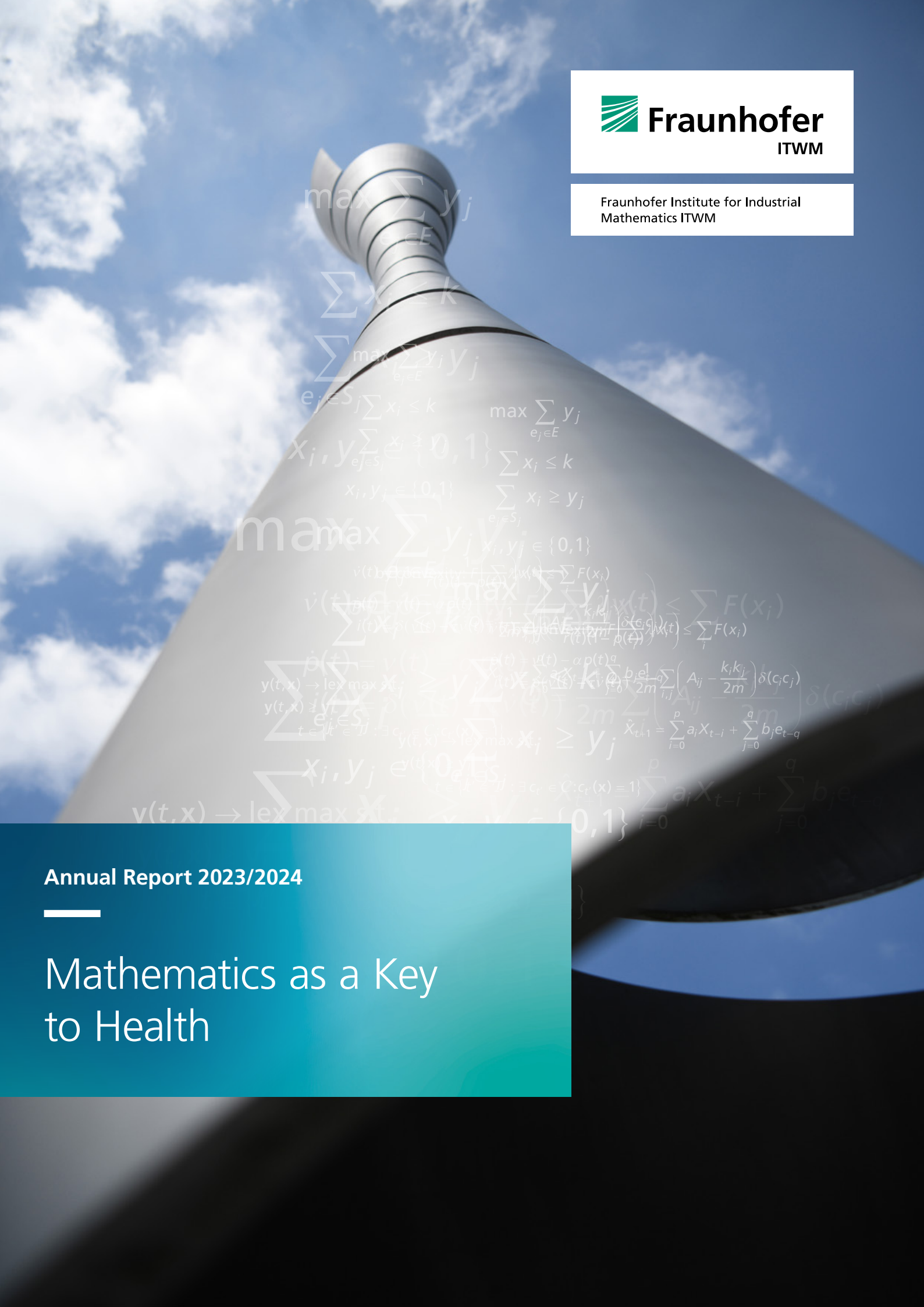


Fraunhofer ITWM

Fraunhofer Institute for Industrial Mathematics ITWM

**Annual Report 2023/2024**

# Mathematics as a Key to Health

**Cover**

The hyperbola in front of the Fraunhofer Center is a significant landmark of our institute. The official title of the artist Martin Willing from Cologne is „Hyperboloid“.

The artwork can also be interpreted as a DNA helix and thus symbolizes a key that provides essential access to health.

**Annual Report 2023/2024**

# Mathematics as a Key to Health

# Mathematics as a Key to Health

Dear readers,

"Health" is the main topic of our annual report this year. Health is said to be the greatest good. Hardly a day goes by without us thinking or talking about our own health or the physical and mental health of people close to our hearts – or reflexively wishing someone "Good health!".

## Mathematics as a Key to Health

Mathematics can improve health: our research has been helping to improve medical care for many years. We have used mathematics to initiate major advances in radiotherapy, played a key role in planning vaccine production against COVID-19, optimized the production of personalized pharmaceuticals and recently contributed to the development of an app for assessing one's own mental resilience and an energy-efficient chip for detecting atrial fibrillation.

At our institute we are working on exciting health-related research projects, particularly many of them in our division "Optimization", which is why we have created a separate department there. Optimization in the Life Sciences" focuses on projects in medicine, healthcare and social sector and medical technology. Our mathematics supports decision-making and helps to optimize processes. You can find out more about this new department in the cover story of this annual report.

## Carrying out Socially Relevant Research Work

Working as a mathematician is versatile! This is demonstrated by the numerous projects we present in our annual report: We look at energy, digitalization, process engineering, mobility and quantum computing – all important topics of our time and relevant to society. This aspect is very important to many of our employees and they choose to work for us for precisely this reason. This is one of the insights we gained from our employee survey in 2023.

## Leading the Way in Transfer to Industrial Application

A lot has happened since we were founded in 1996. We have grown from just about 60 employees back then to over 550 employees today. We look back with pride on what has been achieved here in Kaiserslautern. We have succeeded in developing our scientific discipline – mathematics – into an "enabling technology" for almost all economically relevant fields of technology. Our annual report reflects this to some extent. And this is also confirmed by the auditors who accompanied us through our strategy process last year. In their report, they write: "The Fraunhofer ITWM is a pioneer and role model for numerous initiatives in Germany and Europe. In the unanimous opinion of all auditors, it is the world's leading institute for the transfer

**We research important topics of our time.«**

**Prof. Dr. Anita Schöbel,**
Director of the Fraunhofer ITWM

of mathematical research into industrial applications." We are all proud of this and I am delighted to give you an insight into our research and project work in the 2023/24 annual report.

I hope you enjoy reading it and invite you to get in touch with the contacts listed for further information!

Kind regards

Anita Schöbel

Prof. Dr. Anita Schöbel
Director of the Fraunhofer ITWM

A comprehensive overview of our other research activities on medicine and health can be found online.

**www.itwm.fraunhofer.de/healthcare**

# Content

# The Institute in Profile

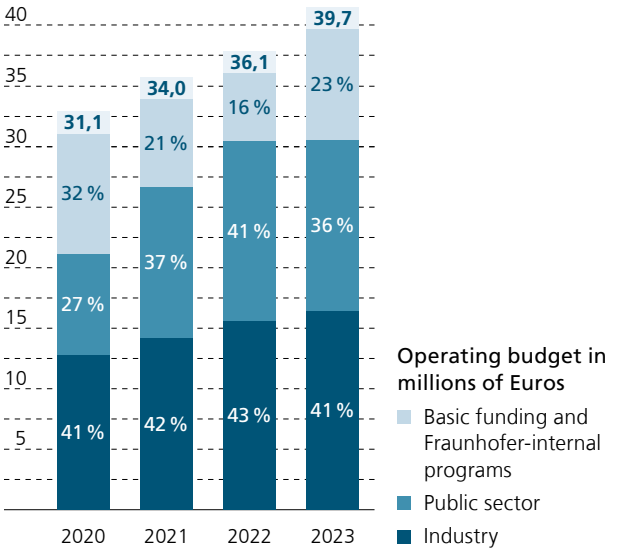
**Computer simulations are indispensable when designing and optimizing products and processes. Mathematics plays a fundamental role in the development of this digital world. After all, it is the technology with which these images are generated and efficiently converted into software, the raw material of the models and the core of every computer simulation. We have succeeded in developing our scientific discipline mathematics into an "enabling technology" for almost all economically relevant fields of technology.**

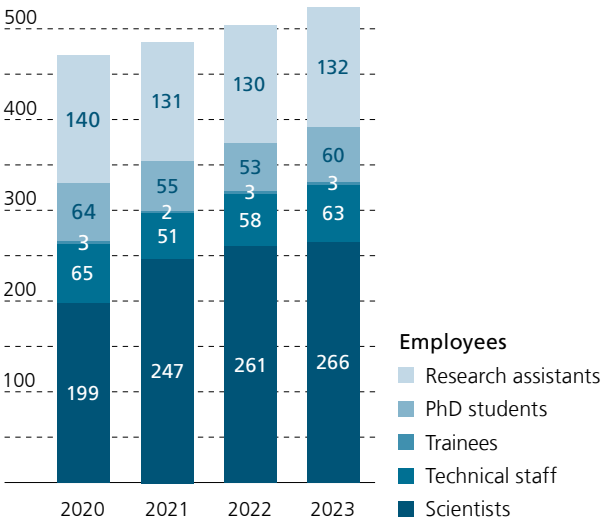
At the Fraunhofer ITWM we do not only want to build the bridge between the real and virtual world ourselves, but also to be the link between university mathematics and its practical implementation. Therefore, the close connection to the Department of Mathematics at the University of Kaiserslautern-Landau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

## Industries – Who Do We Work For?

The expertise of our departments and the broad spectrum of their fields of application are used in numerous industries. The following applies to all of them: our modeling and simulation expertise generates real competitive advantages on the market.

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



## Board of Trustees

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(as at 2023)

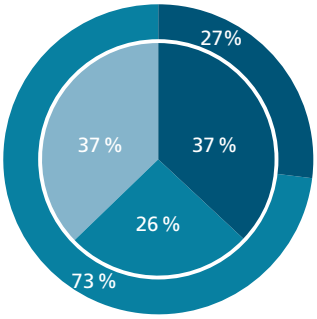
# The Institute in Figures

## Research

16.4 million in industrial revenue, 175 industrial clients, 339 industrial projects

## Industrial Yields

- Regional companies (closer than 150 km))
- Other German companies
- International companies
- Small and medium-sized enterprises
- Other




## Qualifying and Publishing

21 dissertations, 26 master's theses, and 169 publications

Complete list under:
**https://s.fhg.de/publica2023-itwm**

## Teaching

At 9 universities and colleges, 16 employees – including 4 professors – worked a total of 137 semester hours per week.

## Networking

2 Fraunhofer Groups

and 12 alliances and research areas

## International

The Fraunhofer ITWM employs people from all over the world:

39 from Europe (except Germany), 66 from Asia, 7 from Africa, 9 from America, 1 from Australia

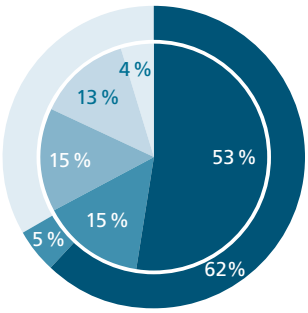
## Presenting

We participated in 214 trade fairs and events as exhibitors, with presentations and posters or as providers of workshops

## Fields and Doctoral Degrees

- Mathematics
- Computer science
- Physics
- Engineering
- Other

- Doctorate
- Habilitated




## Computing

More than 7,500 computer cores provide the necessary computing power.

# Cooperations and Spin-Offs

## Networking within the Fraunhofer-Gesellschaft

A large network and bright minds are crucial for the success of projects. Our specific mathematical expertise makes us a sought-after and valued cooperation partner within the Fraunhofer-Gesellschaft. We are a member of the Information and Communication Technology Group IUK, have guest status with the MATERIALS Group and are represented in various leading market-oriented alliances:

- Plant, machinery and vehicle construction
- Chemical industry
- Digital economy
- Energy industry
  Healthcare industry
- Mobility industry
- Food industry


## Fraunhofer-Chalmers Research Center for Industrial Mathematics

One of our most important international partners is the Fraunhofer-Chalmers Research Center for Industrial Mathematics, or FCC for short, which was founded in 2001 by Fraunhofer and Chalmers University in Gothenburg. In 2023, 56 employees were working there on topics such as fast algorithms, multiphysics and real-time simulation, robot path planning, bioinformatics and statistics as well as data mining. Areas of application include virtual product and process development. The budget amounted to around 6.3 million euros.

**www.fcc.chalmers.se**

## Center of Excellence Simulation and Software-Based Innovation

Transferring new results and ideas into practice as quickly as possible is the mission of the Center of Excellence Simulation and Software-Based Innovation in Kaiserslautern. The Center transforms scientific results into innovations and thus meet the requirements of industry and society. In the Fraunhofer internal ranking of 21 High-Performance Centers, it took first place in 2023!

**www.leistungszentrum-simulation-software.de/en**

## Felix Klein Center for Mathematics

The Felix Klein Center for Mathematics (FKZM) is an institutional link between the Department of Mathematics at RPTU Kaiserslautern-Landau and the Fraunhofer ITWM.

The focus is on promoting young talent. This takes the form of modeling weeks for schools or scholarships and a mentoring program for mathematics students.

**www.felix-klein-zentrum.de**

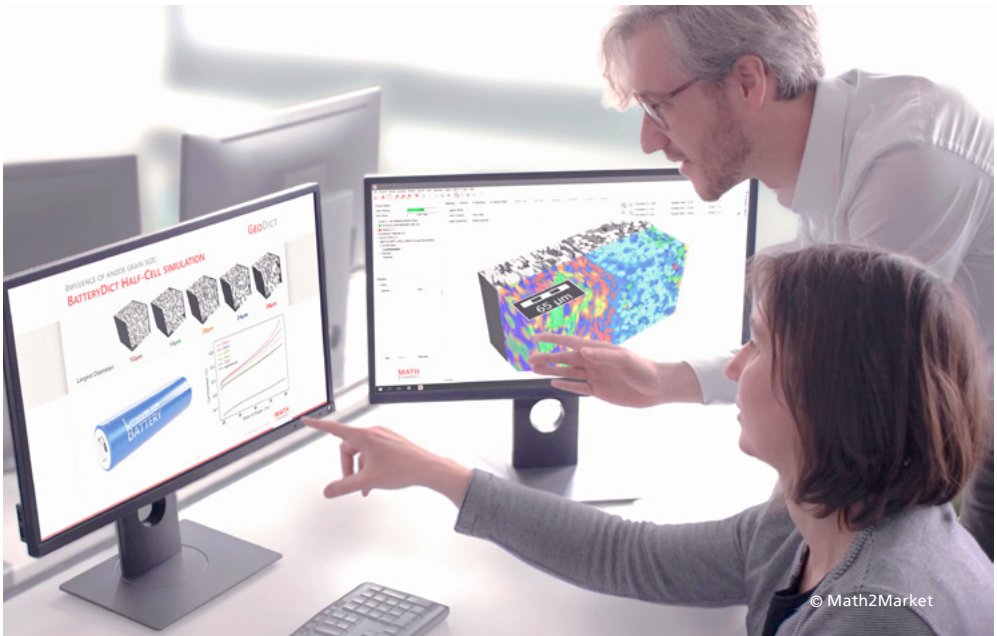
Many young people benefit from our scholarship.

## Spin-Offs

The successful transfer of research at our institute is also reflected in the seven spin-offs that we have launched since 2009. They continue to be important partners of our institute for new developments.

- **fleXstructures** – Specific engineering projects and services for the simulation of flexible components
- **Math2Market** – Comprehensive software service, such as GeoDict®, an innovative simulation software for digital materials research and development
- **Produktinformationsstelle Altersvorsorge PIA** – Risk/reward classification of subsidized pension products
- **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
- **Wendeware AG** – Software ecosystem for the energy transition
- **UNEEC Systems** – Distribution of the highly efficient STX processor technology (stencil and tensor accelerator)

**www.itwm.fraunhofer.de/networks**




© Math2Market

# Highlights 2023/2024 – Awards

A year at Fraunhofer ITWM is filled with numerous events related to our research work. Our employees took part in over 200 events in 2023. It is difficult to choose which of these is a "highlight", because the researchers put their heart and soul into each of our projects. We have picked out a few special moments from the past year to give you an impression of how work, research and sometimes even celebrations take place at our institute.

## Science Award for Anita Schöbel

At the annual conference of the Society for Operations Research (GOR), Prof. Dr. Anita Schöbel received the GOR Science Prize, endowed with 8,000 euros, for her entire body of work. Every two years, the society awards this prize to researchers for exceptional achievements in the development of the focus area "Operations Research". In her acceptance speech, Schöbel emphasized how relevant OR has been for her research and her career to date. "It is wonderful to advance the field in dedicated teams on so many levels. The award confirms to me that this is perceived in the same way in the community. Even though the award actually honors a lifetime achievement, my work here is of course far from over!"

**www.itwm.fraunhofer.de//gorprize_anita_schoebel**

## Special Award for Our Institute Director

© Gesellschaft für Operations Research e.V.


## ICT Dissertation Award for Sebastian Blauth

Dr. Sebastian Blauth from our "Transport Processes" department has been awarded first place in the ICT Dissertation Award of the Fraunhofer ICT Group for his outstanding dissertation. The prize is endowed with 5,000 euros. The Group awards the prize annually for research work that deals with innovative developments and technologies in the fields of computer science, mathematics or natural sciences. Read more about Blauth's research on page 61.

**s.fhg.de/ICT-Dissertation-S-Blauth-en**

## Award of the Sparkassenstiftung for Tania Jacob

The Foundation honored Tania Jacob (department "Financial Mathematics") for her outstanding achievement with an award for her Master's thesis on the detection of anomalies in component manufacturing processes. It is not only her research work that is impressive, but also Jacob's career: after several years as a software developer in Australia, the 41-year-old decided to change career direction and embark on a new Master's degree program. In 2020, she came to the Fraunhofer ITWM and while studying at RPTU.

**www.itwm.fraunhofer.de/interview_tania_jacob_en**

# Highlights 2023/2024 – Events

## International and Interdisciplinary: ISOLDE 2023

Together with the "Optimization" working group of the University of Kaiserslautern-Landau (RPTU), the Fraunhofer ITWM hosted the ISOLDE ("International Symposium on Locational Decisions") conference in 2023. Prof. Dr. Anita Schöbel was the main organizer of the conference. Around 80 scientists from the operations research community from 18 countries came together for five days in Kaiserslautern and at the second conference venue in Baden-Baden. The participants from the disciplines of mathematics, economics, engineering and geography experienced compact days with a balanced mix of conference and networking opportunities.

**www.itwm.fraunhofer.de/pm-isolde-en**

## Honor to Whom Honor Is Due

The department "Financial Mathematics" and the RPTU Kaiserslautern celebrated Prof. Dr. Ralf Korn's 60th birthday with a special workshop. Many mathematicians whose professional careers are closely linked to him came to our institute for the event. Korn founded the "Financial Mathematics" department and continues to be involved in research as a consultant to the Fraunhofer ITWM. Impressive figures are a must when honoring a mathematician: Korn has supervised 84 diploma theses, 109 master's theses, 22 bachelor's theses and 60 doctorates up to the time of the event and has taken around 1200 oral examinations at RPTU.

**www.itwm.fraunhofer.de/workshop-korn-en**


## KLAIM 2023: Mathematics in Application

The "Kaiserslautern Applied and Industrial Mathematics Days" (KLAIM), initiated by Fraunhofer ITWM and RPTU, took place for the second time in September 2023. They offer a platform for mathematicians from academia, research laboratories and industry to exchange ideas and present current results. Around 60 presentations were submitted and offered a varied program. The second edition of KLAIM focused on the synthesis of models and data.

**www.itwm.fraunhofer.de/klaim2023-en**

More than
**100**
people took
part in KLAIM.

## Promoting Talents

More than 300 students were guests at the Fraunhofer ITWM in 2023. Whether at events for advanced courses or school classes, two Math Talent Schools and a ceremony for the participants of the Mathematical Olympiad – the Fraunhofer ITWM is happy to host young math enthusiasts and offers them insights into a varied professional environment.

# Highlights 2023/2024 – Projects

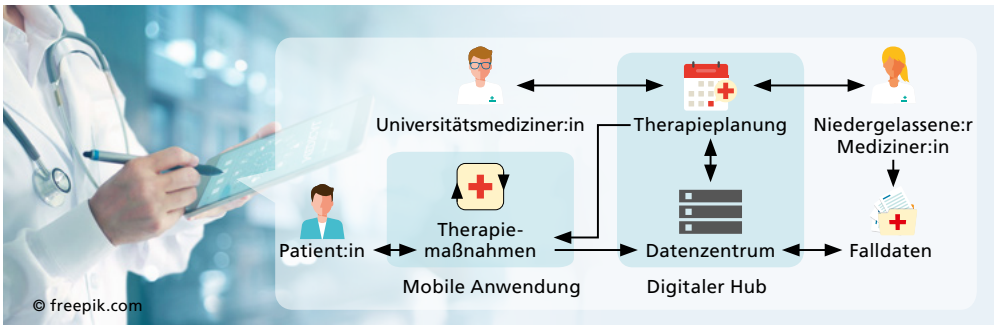

© View, Rainer Voss


© View, Rainer Voss

## State Government Funds Preliminary Research

Biotechnology and quantum computing are two important research priorities for the state of Rhineland-Palatinate, which is why Science Minister Clemens Hoch brought two funding decisions to Kaiserslautern in March 2023. The Rhineland-Palatinate Quantum Initiative (QUIP) and the MaTBiZ project (microstructure design and additive manufacturing of a chromatography column for separating biological cells), which is based at the Fraunhofer ITWM, are being supported.

**www.itwm.fraunhofer.de/PR_matbiz-quip**




## "Decide" Project Wins Nationwide Competition

In the "Digital Places in the Land of Ideas 2023" competition, the project "DECIDE: Digital Counseling, Data Integration, Decision Making and Empowerment" wins in the "Health" category. The project, which is coordinated by the Institute of Medical Biometry, Epidemiology and Informatics (IMBEI) at the Mainz University Medical Center, aims to use digital solutions to provide the best possible healthcare regardless of where people live. Patient data transmitted via an app is analyzed by a system developed at the Fraunhofer ITWM using artificial intelligence.

**www.itwm.fraunhofer.de/decide-en**

## Study: How Realistic Are Pension Products?

A study commissioned by MLP Finanzberatung SE analyzes how high the effective costs of typical old-age provision products are under realistic cost parameters. It shows that the costs resulting from calculations based on the specifications of the Federal Ministry of Finance significantly exceed the realistic costs. Calculations according to the existing legal requirements and calculations of realistic cost rates were compared.

**www.itwm.fraunhofer.de/study-pension-insurance**

## Insights into life with mathematics

Between strong coffee, dedicated project work, exciting online meetings and new algorithms – ARD alpha Uni accompanied our colleague Dr. Tobias Seidel every step of the way in his everyday life at the Fraunhofer ITWM. The video was viewed almost 500,000 times within a year. The Fraunhofer ITWM communications team and the Department of Mathematics at the University of Kaiserslautern-Landau have also captured exciting insights in their own video series "Lautrer Mathe Stories". More on our Youtube channel.

**www.itwm.fraunhofer.de/lautrer-math-story**

# Health and Life Sciences

Improving healthcare, increasing the chances of recovery, supporting diagnoses – these are the goals that the Fraunhofer-Gesellschaft wants to achieve in the lead market "healthcare industry". We are contributing to this, particularly with a focus on smart tools for decision-making and the optimal use of digitalization. This year, our cover story is dedicated to this major topic, highlights projects and presents the extensive work we are doing at the Fraunhofer ITWM. More ITWM projects on medicine and health can be found online.

**www.itwm.fraunhofer.de/healthcare**

# Socially Relevant, Wide-Ranging, Individual

**In this interview, Prof. Dr. Karl-Heinz Küfer, Head of the "Optimization in the Life Sciences" department, and his deputy Dr. Alexander Scherrer report on developments in our research in the healthcare sector.**

**The "Optimization in the Life Sciences" department has been in existence for around two years. What makes working in this focus area different from the other departments in the division?**

**Küfer:** The topics of health and medicine have always met with greater interest in external communication and also appeal to many people emotionally, because unlike technical topics, they actually affect everyone. Our research aims to support decision-making – for those treating and caring for patients, but also for the sick and those in need of help. The results of our work often lead to changes in behavior. This requires a great deal of sensitivity, because at the core, people don't want any changes at first.

The life sciences are not new territory for us. Although the department has only been around since 2022, we previously had the major flagship project for radiotherapy planning for many years. We have been cooperating with internationally renowned medical research companies such as the German Cancer Research Center, Heidelberg University Medical Center and Massachusetts General Hospital as well as the global market leader Siemens Healthineers – Varian Medical Systems for a long time, and we now have a much broader thematic and methodological base, which is why it made sense to establish a separate department for focused communication of our activities.

**Scherrer:** In the healthcare sector, the "Optimization" division began shortly after the company was founded in the 1990s with projects for clinical patient transport. In 2001, we started with the planning of radiotherapy, which for me personally meant starting as a doctoral student at the Fraunhofer ITWM. These many years of industry experience in the life sciences have paid off particularly in the past six years, during which we have succeeded in entering many new fields of application thanks to intensive networking and acquisition work. We have never had so many research and industry projects on topics from medicine, healthcare and social services as we have recently, and we cooperate with numerous partners from Germany, Europe and beyond. The strong strategic "regional axis" between Mainz as a healthcare location and Kaiserslautern as a technology location is important for us.

**Küfer:** The target group for our solutions has become much broader. Even in radiotherapy, we had to respond to the needs of the doctors planning the treatment. Above all, they want intuitive software tools with well-communicated and balanced treatment plans and were very open to new approaches to improve their work in the interests of seriously ill patients. The discussion of mathematical methods in the background is less important in the life sciences than in technical issues, which we often discuss with well-trained research engineers, for example.

**Contact**

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**Contact**

Dr. Alexander Scherrer
Deputy Head of Department
"Optimization in Life Sciences"
Phone +49 631 31600-4609
alexander.scherrer@itwm.fraunhofer.de

## Methodological Focus of the "Optimization in the Life Sciences" Department

- In the healthcare sector, we use operations research methods to improve organizational structures and processes.
- Doctors use our optimization methods to create the best possible individual treatment plans.
- We develop methods for decision support for the effective solution of complex planning tasks.
- Extensive databases are analyzed and evaluated in a targeted manner using artificial intelligence.
- Mathematical simulation is used to efficiently run through medical technology design processes.

### What does this mean in practice for the composition of the project teams?

**Küfer:** All project teams in the "Optimization" division are put together according to methodological expertise for the respective issue under consideration. Projects are assigned to departments and employees work freely across departmental boundaries. However, it is important to speak the language of the respective industry and to present a less methodical approach. In the life sciences in particular, we use mathematics and computer science to fill gaps that – when approached in an interdisciplinary manner – offer great opportunities for innovation and improvements in the field.

An important field of application for our projects for many years has been oncology, where individualized therapy design is a major topic. For decades, cancer patients were always treated in the same way, e. g. with the same radiation doses. New approaches are now being taken to both radiation and medication, as people respond differently to therapies. Individually designed decisions take tumor markers, blood values and other parameters into account. Our mathematics helps us do this. For example, we are part of a working group of the German Research Foundation under the heading "Optimal Stopping Radiotherapy". (For information on how our mathematics also supports the production of personalized pharmaceuticals, see page 26). We have also been sought-after experts on infection and pandemic prevention since the coronavirus era. (more on this on page 28).

### Where do you think the journey will take us?

**Scherrer:** In recent years, projects have been added that focus on digitalization and the use of artificial intelligence in geriatric diseases, care and mental health. Overall, advancing digitalization is opening up new possibilities in many fields. All available information can be brought together and used jointly in order to adapt the procedure to the individual circumstances in the best possible way. This applies to care through the use of artificial intelligence, for example, to support care planners in making complex decisions. In general, AI can create major improvements in many areas of the life sciences, but the responsible use of AI for and on people is a key challenge.

**Küfer:** In terms of content, there is still a lot to be done, particularly in care. Currently, only 25 percent of people are cared for in a nursing home, but this will not remain the case for much longer due to demographic change and the shortage of skilled workers. How can better use be made of decentralized care in the area? The complex organization and the distribution of the few resources in the form of skilled staff are also major challenges. These offer a huge opportunity for our mathematics – whether in cancer research, heart disease or other areas of focus.

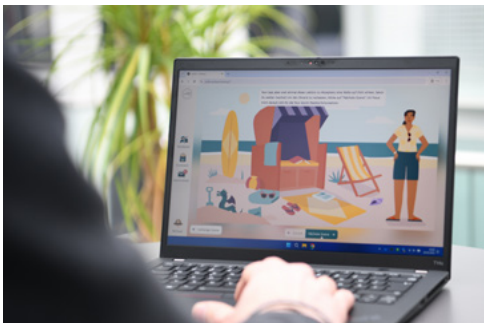
**www.itwm.fraunhofer.de/life-sciences_en**

# Optimized Health Strategies With Artificial Intelligence

## More Resilience – Training Mental Resilience

Incisive events and challenging life circumstances place an enormous burden on mental health. People with a high level of resilience are better prepared for stress and strokes of fate. But can this mental resilience be learned? In the "APPWAG" project, researchers from the "Optimization in the Life Sciences" department and the Leibniz Institute for Resilience Research LIR have developed the freely accessible web application "www.resilir.eu", which users can use to assess and train their personal resilience online. The abbreviation "APPWAG" stands for "Expansion of resilience promotion programs into a platform with target group-specific health promotion offers". The project was funded by the Ministry of Science and Health of the State of Rhineland-Palatinate with funding from the European Regional Development Fund (ERDF).

**www.itwm.fraunhofer.de/appwag-en**




## Preventing Age-Related Diseases With AI

Demographic change is leading to an increased incidence of age-related diseases such as dementia and frailty. Early diagnosis and targeted treatment of these diseases ensure a much better quality of life. However, neither the medical expertise nor comprehensive data on individuals is generally available to a sufficient extent. In the "COMFORTAGE" project, we are working together with numerous European partners from research, healthcare and industry on methods and software tools for dealing with dementia and frailty.

The project is funded by the Horizon Europe Framework Program "Computational Models for New Patient Stratification Strategies".

**www.itwm.fraunhofer.de/comfortage-en**

# Digitization in the Care Sector

## Support for Care Staff: Long-Term Care With AI

Inpatient care for people in need of care is facing major challenges. According to Statista, the number of people in need of care will increase by 50 percent by 2030. At the same time, the labor supply will continue to decrease. AI-based digital systems offer one option to counteract these developments: In the project "Care-integrated artificial intelligence in the professional care process" (ViKI pro), we are working with partners to support care professionals in identifying individual care needs and planning suitable measures with the help of AI. "To do this, we are pursuing a model-based approach and using existing specialist knowledge, digitizing it and making it usable for AI," says Dr Alexander Scherrer.

**www.itwm.fraunhofer.de/vikipro-en**


© istockphoto


## Mathematics Optimizes Tours in Outpatient Care

If the routes are well planned, there is more time for care. A study carried out by our researchers at the Fraunhofer ITWM together with the billing service provider ARZ Haan shows just how much potential there is for improvement in route planning. The results of the two-year project "Conception of data-driven business models in the healthcare sector", or KoGGe for short, are impressive: Tours are on average twenty percent shorter, the use of highly qualified nursing staff for comparatively simple tasks has been reduced by more than ten percent and the desired time periods in which those in need of care want to be cared for have almost all been met – significant improvements overall.

**www.itwm.fraunhofer.de/kogge-en**

## Artificial Intelligence and Robotics in Hospitals

In hospital, providing patients with a balanced supply of food and drink is important for their recovery. If too little is eaten or drunk, the need for medical action can be identified at an early stage. Systematically documenting and analyzing food and fluid intake and reacting to situations of malnutrition is difficult in the hectic day-to-day running of a hospital. In the "KoniuS" project, we are supporting the IT company CONET Solutions GmbH in designing a robotic system for intelligent food and drink distribution at Bonn University Hospital. In future, the system will automatically record people's food consumption and compare it with medical recommendations. By digitizing the process, the aim is to reduce the workload of nursing staff and provide optimal care for the people requiring it.

**www.itwm.fraunhofer.de/konius-en**

# Oncology – Mathematics to Fight Cancer



## Cancer Treatment With Proton Therapy

Compared to conventional radiotherapy, proton therapy allows for more targeted radiation, which means that the organs and surrounding tissue are better protected. However, these advantages can only be used effectively if uncertainties regarding the range of the radiation and its biological effectiveness are reduced during the planning stage. We are working on a project with the Ludwig-Maximilians University in Munich to incorporate additional information into the planning process and thus be able to suggest optimized treatment plans to medical professionals. The project is funded by the German Research Foundation (DFG).

**www.itwm.fraunhofer.de/proton-therapy**

## Aftercare in Oncology

The successful treatment of cancer not only includes therapy but also detailed aftercare. To date, this has largely been carried out according to medical aspects in direct dialog. In contrast, improving the quality of life of patients by involving their social environment plays a subordinate role. The aim of the "ONCORELIEF" project is to develop a digital assistance system that supports patients in improving their state of health after treatment. This system assesses quality of life and recognizes the need for intervention at an early stage. Suitable measures are then proposed on this basis. 13 partners from seven countries are working together on the EU project.

**www.itwm.fraunhofer.de/oncorelief-en**

# Fighting Cancer With Algorithms and Digitalization

## Optimal Treatment Paths for Lung Diseases

Lung diseases form a very heterogeneous group of serious illnesses. Targeted and successful treatment requires an early and precise diagnosis of the disease in question. Carrying out complex examinations and planning the best possible individual therapies is a major challenge in everyday clinical practice. In the "AI4Lungs" project, digital tools, methods and models for the optimal selection of clinical treatment paths for lung patients are being developed in cooperation with international partners from research, development and medicine – with a particular focus on the treatment of cancer.

**www.itwm.fraunhofer.de/AI4Lungs-en**

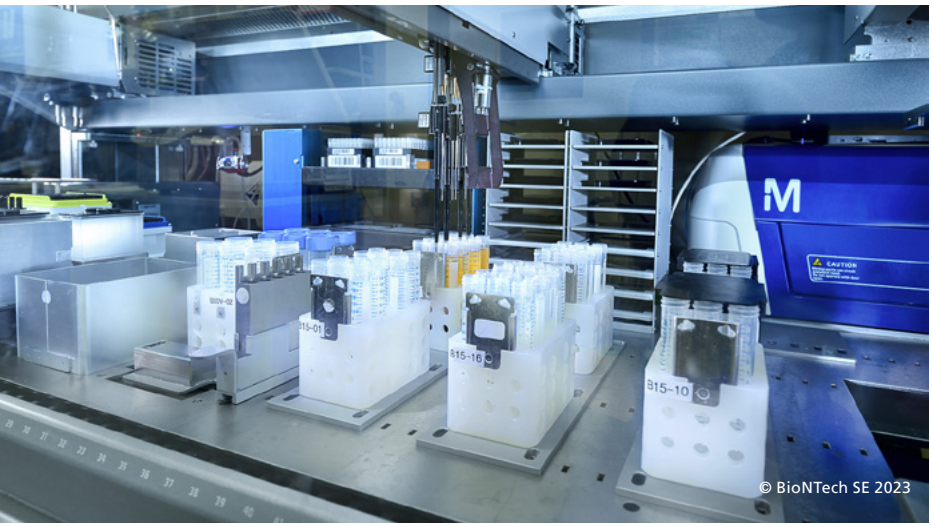
## Lifestyle Optimization for Pancreatic Cancer

Pancreatic cancer is a common cancer that is often associated with a very painful course of the disease and a low survival rate. By changing lifestyle in parallel with treatment – such as nutritional programs, physical activity or pain therapy – the quality of life of patients can be improved. In the "RELEVIUM" project, we are working in an interdisciplinary consortium on digital solutions for independent self-management, optimized communication with the doctor and targeted planning of life with pancreatic cancer.

**www.itwm.fraunhofer.de/relevium-en**

# Personalized Pharmaceuticals – New Technologies and Universal Mathematics

**Production planning with the company BioNTech is the focus of the work of the team led by Dr. Heiner Ackermann, Head of the "Optimization – Operations Research" department in the "Optimization" division. Not only do the researchers grow with their tasks, but mathematics also benefits from the collaboration.**



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## Research Transfer in Pharmaceutical Technology Since 2016

Many people have heard of mRNA at least since the COVID-19 vaccinations. In a therapeutic context, messenger RNA is used as an information carrier to train the immune system. The first ever approved mRNA vaccine was developed in the laboratories of BioNTech. The Mainz-based company has been a partner of the Fraunhofer ITWM since 2016 and is developing mRNA-based therapeutics against cancer and prophylactic vaccines against infectious diseases. These new possibilities go hand in hand with opportunities in personalized medicine.

In practice, the pharmaceutical company faces particularly great challenges in production – because unlike a mass vaccine, for example, individualized pharmaceuticals take into account a person's specific characteristics. In contrast to established production processes in the pharmaceutical industry, this not only requires a considerably more complex process organization from the clinics to production and back again, but also solutions for handling samples in production.

### Software Optimizes Productionn

In collaboration with BioNTech, the Fraunhofer ITWM team led by Ackermann is therefore developing software that not only enables these processes to be carried out, but can also be adapted to ever new requirements. "The production of individualized medicines differs significantly from established processes. All steps have to be carried out individually for each patient with great care, and batches are considerably smaller," says Ackermann, who is responsible for the development of the software platforms as project manager.

"There are several aspects to consider: Not only does it have to be produced individually, safely and as cheaply as possible, but quality fluctuations in the source material are also uncertainties that are proactively factored into capacity planning." What does material mean? In the case of cancer, healthy tissue is compared with diseased tissue. Put simply, you look for specific changes in the tumor material to decide what to use.


*Production and laboratories at BioNTech for individualized cancer medicine.*

"Production in the industry is very different from others. In the automotive industry, for example, there is a clock cycle, work steps are always structured in the same way and the workplace is defined. In the production of individual pharmaceuticals, on the other hand, the times are not arbitrary and the machinery is very specialized. This makes it particularly difficult in terms of organization." The infrastructure is also expensive because you need clean rooms and complex technology. Fluctuating process times make adjustments to the plan necessary.

"At the same time, people are very hopeful that they will quickly receive an individual remedy that helps," says the computer scientist. In the beginning, a spreadsheet was sufficient to control production for the organization with only a few patients. This is no longer the case. "We support the structuring and digitalization of processes. Our software and algorithms help computers to take over routines," emphasizes the head of department. People continue to make the critical decisions, and the mathematical models help them to do so.

## New Scheduling Model Brings Success

The team took a familiar mathematical approach to this major task and expanded it to include the specific features: The solution is called "scheduling theory", supplemented by so-called "due dates" – planning with different due dates. It is particularly popular in the area of operations research and logistics. "It's always nice to see how universal mathematics is. We have developed a new model from the core theory that fits the circumstances exactly."

A detailed paper entitled "Scheduling a Single Machine with Multiple Due Dates per Job" was published at the beginning of 2024. It focuses on the scheduling of single machines with multiple due dates per job – a key area in which there has been little research to date. As a result, not only does the industrial company benefit from the results, but applied mathematics also makes progress in the world of science.

**www.itwm.fraunhofer.de/personalized-medicine**

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# What Wastewater Tells Us About Infections

**A team from our "Optimization" department and the "Transport Processes" department is investigating the incidence of infection in Rhineland-Palatinate based on wastewater analyses relating to coronavirus and the representative "SentiSurv" cohort study. Always in view: How can the results help us to be better prepared?**

"The Data Situation Is a Real Stroke of Luck"

Wastewater is a rich source of information that was already being used occasionally to identify pathogens before the COVID-19 pandemic. However, wastewater monitoring has only been the subject of intensive research since the coronavirus years. Back in March 2021, the EU Commission called on the member states to introduce systematic monitoring of SARS-CoV-2 in wastewater under the project name "ESI-CorA". In February 2022, a nationwide pilot operation for coronavirus wastewater monitoring was therefore launched at a total of 56 locations. The Rhineland-Palatinate Ministry of Science and Health has also included a total of 16 wastewater treatment plants that provide samples every two weeks.

## Wastewater Monitoring Combined With Cohort Study Results in Optimal Data Situation

"Germany initially lagged somewhat behind in European comparison, but Rhineland-Palatinate is now a pioneer in this type of study," says Dr. Neele Leithäuser. Our researchers have also contributed to this, as they have repeatedly supported the state politicians with their expertise on various issues with figures and tools for making decisions. "In late summer 2022, it was clear that the mass tests would be phased out and that there would no longer be any reliable figures. Prevalence in particular is what you need to be able to assess the situation," explains Dr. Jan Mohring.

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*Monitoring viral load in wastewater is now considered an important source of information for research. But what does the evidence tell us?*


*It is crucial to derive the prevalence from data. It describes the total number of cases of illness in the population under consideration during a certain period of time.*

This refers to the total number of cases of the disease in the population under consideration. "But it was not possible to determine this on the basis of wastewater data alone. It was unclear: What do the wastewater values even mean? How many people are infected?" says the mathematician. The values are subject to many fluctuations and uncertainties – for example due to measurement inaccuracies or dilution.

## "SentiSurv RLP" – Representative Cohort Study Clarifies Wastewater Figures

It was a real stroke of luck that the "SentiSurv" project was launched at the same time as the new wastewater data on behalf of the Ministry. Under this name, the Mainz University Medical Center is monitoring the incidence of SARS-CoV-2 in the population of Rhineland-Palatinate. A representative population cohort took part in three phases from December 2022. Depending on the phase, this involved up to 12,000 people who tested themselves for coronavirus once or twice a week and passed on the results as a photo including a questionnaire via an app. The last phase took place from January to March 2024.

"In order to put the wastewater results in better perspective, it was particularly important that the locations of the wastewater treatment plants also have a large overlap with the "SentiSurv" cohorts. We were involved in the discussions with the state government and were able to put this forward as a proposal. This is certainly not something that happens very often anywhere in the world, such an optimal data situation that has brought us really great results," says a delighted Neele Leithäuser. "To put it bluntly, we have found the magic conversion factor for prevalence, at least for this period, which nobody believed in at the beginning." Researchers are learning from the "SentiSurv" and wastewater data. The detailed results are recorded, for example, in the paper "Estimating the COVID-19 Prevalence from Wastewater". "However, we also know that the calibration can no longer take place if the cohort data is no longer available, then the wastewater data can be more off the mark again, especially with new variants, but we have the reference points," summarizes Mohring.

## Early Warning System for the Future and Expertise Required at Many Levels

The aim of the study is to establish app-based monitoring to protect against future threats to public health, not just those caused by the pandemic. This can also make it easier to monitor other pathogens via wastewater. Elsewhere, new studies and projects are already underway to detect influenza, smallpox and polio pathogens.

**www.itwm.fraunhofer.de/itwm-vs-corona**

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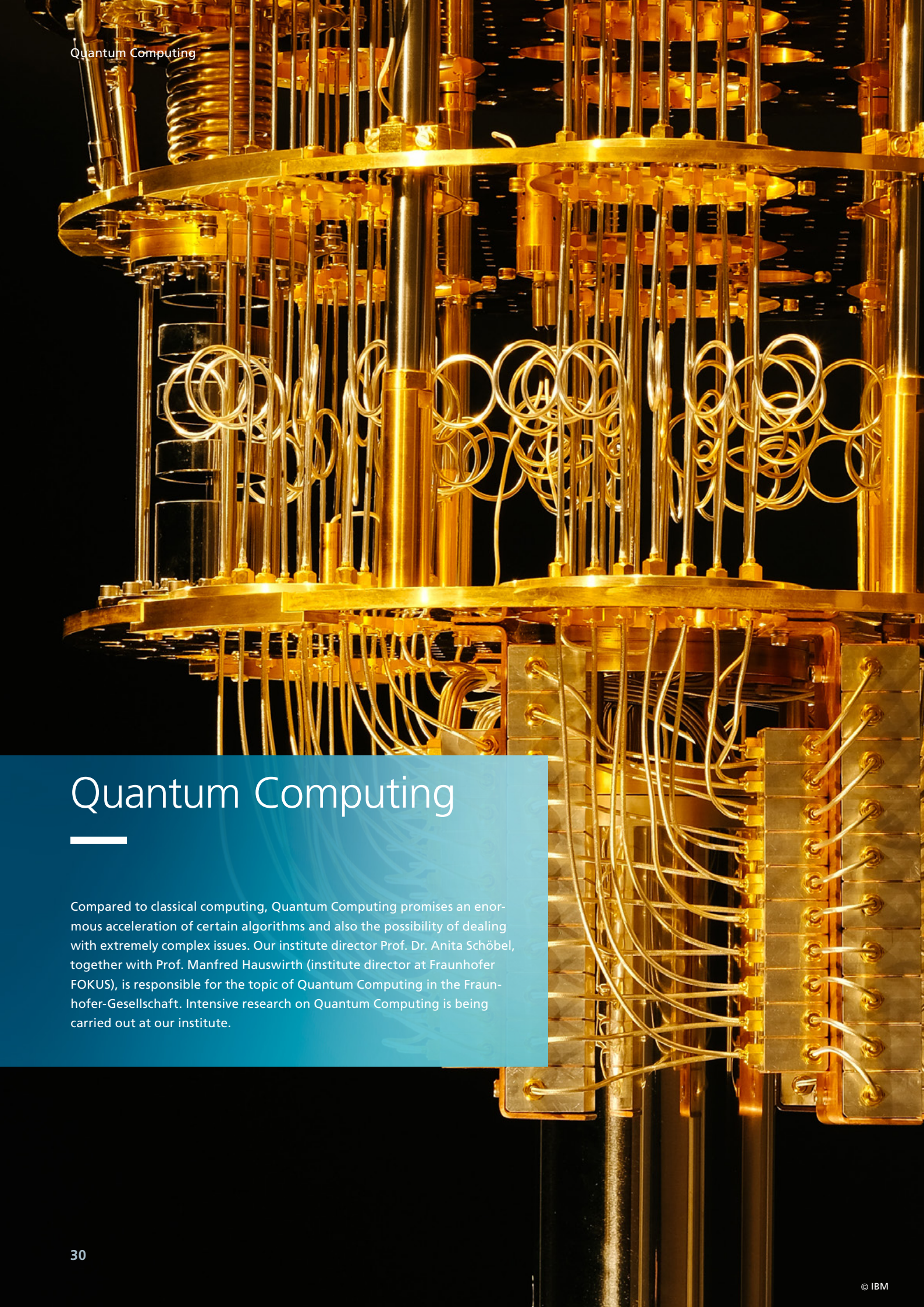


# Quantum Computing

Compared to classical computing, Quantum Computing promises an enormous acceleration of certain algorithms and also the possibility of dealing with extremely complex issues. Our institute director Prof. Dr. Anita Schöbel, together with Prof. Manfred Hauswirth (institute director at Fraunhofer FOKUS), is responsible for the topic of Quantum Computing in the Fraunhofer-Gesellschaft. Intensive research on Quantum Computing is being carried out at our institute.

# Quantum Computing: Gold-Rush Fever in Research

Quantum Computers are currently expected to bring nothing less than a paradigm shift: the significantly increased amount of information that can be processed is raising high expectations. Researchers see the opportunity to carry out completely new computing operations to solve mathematical problems that have so far prevented conventional computers from working. Eva Fröhlich from our "Communication" team talks to our Institute Director Prof. Dr. Anita Schöbel and Dr. Pascal Halffmann, Research Coordinator Quantum Computing at the Fraunhofer ITWM, about the current state of research.

"We have found our niche."

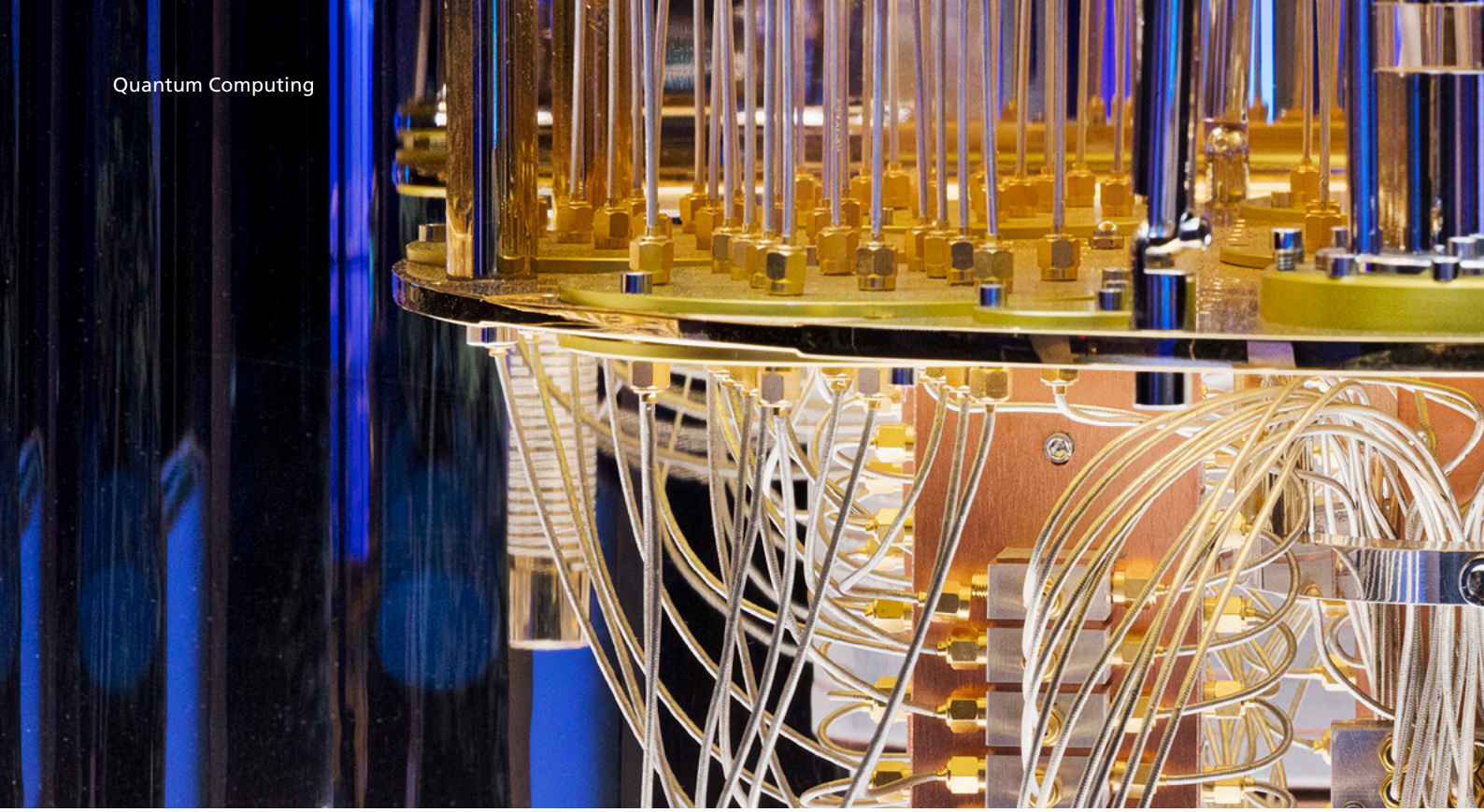
**The Fraunhofer-Gesellschaft has defined quantum technology as a strategic field of research and is thus pooling the expertise of the various Fraunhofer Institutes. What are the most important findings from Fraunhofer series so far?**

**Schöbel:** First of all, I realized that it is incredibly exciting to talk about and research Quantum Computing. Since I have immersed myself in this field, I have found many open research questions and that is fun. But I've also noticed that: Quantum Computing is very collaborative, especially in the Fraunhofer context – I don't know of any other area where Fraunhofer collaborates so intensively. It's not just our departments or the institutes themselves, we even work with universities and the Leibniz and Max Planck Institutes across research institutions. I think it's remarkable that Quantum Computing brings so many people together.

**Halffmann:** Quantum Computing is a very broad, interdisciplinary field, which means we need different skills. In the beginning, we had a very broad approach here at the Fraunhofer ITWM. I think that we have now found our niche in which we can best transfer the strengths that we already have in the departments to the quantum world. And that is in the field of applied Quantum Computing. Improving classical algorithms and hybrid algorithms is where we are strong and where we have achieved good results in recent times. Be it in financial mathematics, image processing or high performance computing – we are seeing progress. Our investment in these areas in the last three to four years are paying off scientifically.

**Since 2021, Fraunhofer has been able to test application-related quantum software and expand its expertise on the "IBM Quantum System One" in Ehningen, the most powerful quantum computer in Europe to date. It is now known that this cooperation will not be continued in its current form. What will happen with practical research?**

**Schöbel:** The experience from Ehningen really helped us to take the first steps. We calculated a lot in the IBM Cloud and we saw a lot: To be honest, most of all what is not yet possible, but definitely progress. The collaboration will continue in a different form, Fraunhofer will continue to have computing time at IBM. But this also offers us the opportunity to look at other hardware platforms. There are very different types of hardware that are perhaps better or less suitable for certain algorithms. It is therefore important that we also explore other platforms.



"Expectations are becoming more realistic."

**Halffmann:** At IBM in particular, we have been able to see very clearly how hardware has developed. This is very important for us because we are partly involved in building hardware ourselves. And I agree that we are clearly hardware agnostic, because we can't predict at this point in time which hardware technology will develop and how, and which will really become established. We are testing a broad selection. But it's definitely important for us to have some form of access to hardware so that we can see: How is the progress? Do the algorithms we are developing work? We want practice, we want application-oriented research and so we also have to look at: how well do our methods work in application? And this is particularly important for our young scientists, so that they get a feeling for how to work with a quantum computer.

**Almost all departments at the Fraunhofer ITWM have gained initial experience with Quantum Computing. Where do you see the greatest potential? Are there any projects that stand out?**

**Schöbel:** With image processing, you can literally see how the recognition of images is getting better and better. For the simulation, we put a lot of work into the fast Fourier transformation, so we can assess both the potential and the pitfalls. And in the Rymax project, I find it impressive that we are involved in the construction of a real quantum computer in Kaiserslautern. Not in the construction itself, but we are trying to contribute the algorithms and also those that mediate between software and hardware. That is exciting to experience.

**Halffmann:** In financial mathematics and optimization, we focus on algorithms, in particular algorithms from Quantum Machine Learning and quantum optimization, which we really – and this is the exciting thing here – try out with specific use cases. In the energy sector, for example, we have solved a power plant scheduling problem. This has definitely brought significant improvements in the performance of Quantum Machine Learning.

**The public has high expectations of quantum technologies and there is a great deal of interest. What do you think is realistic in the near future?**

**Schöbel:** Unfortunately, it's still a bit of a guess as to what will be ready for industrial use and when. We have identified a few areas where we believe progress is realistic. What I find interesting is that the areas where we can prove mathematically that it really is better than anything we've seen before still seem to be further away from application than other

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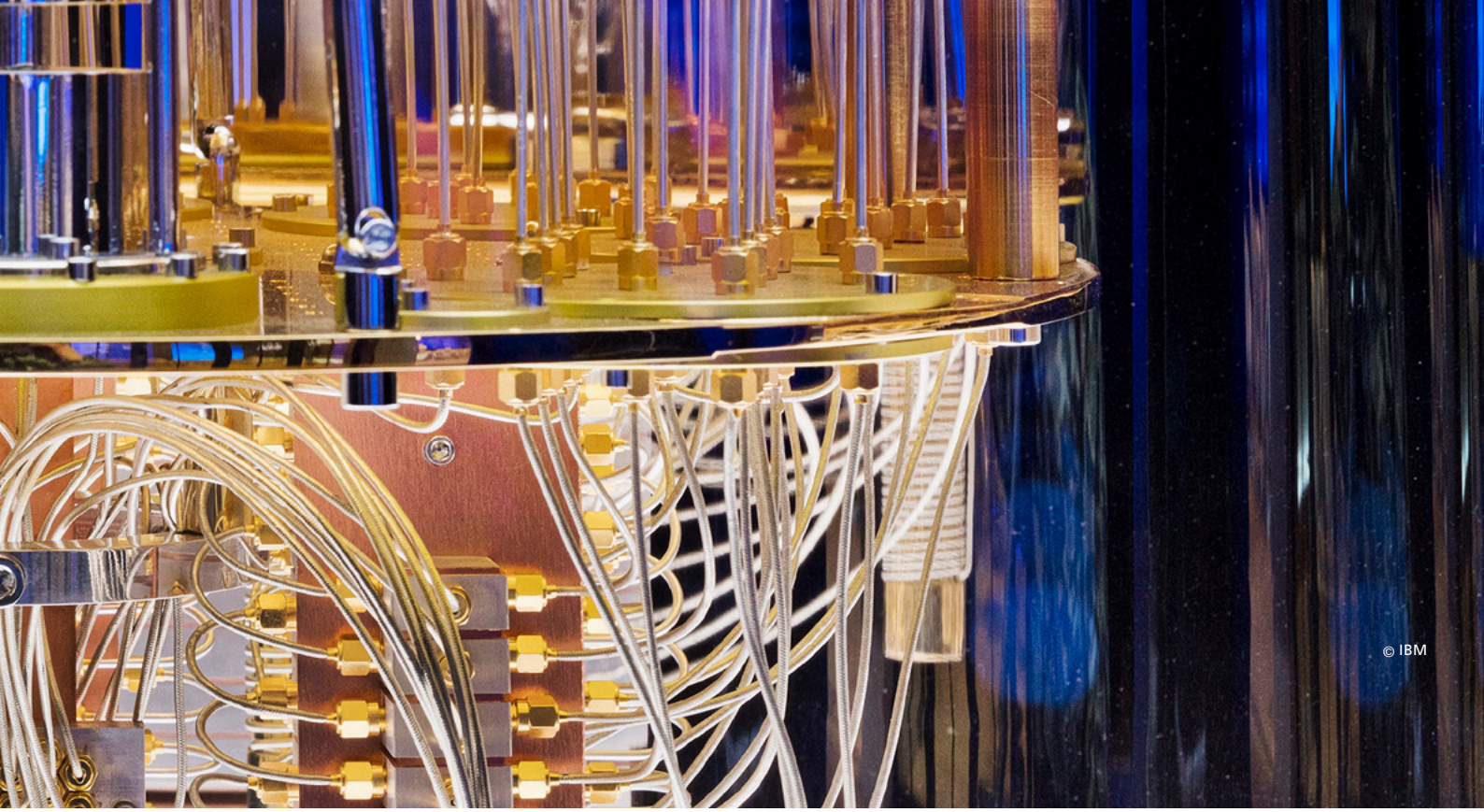


areas, such as optimization, where quantum annealing technology, for example, is already working quite well. Quantum annealing is not an exact procedure that leads to a provably good solution, but a heuristic. However, it is becoming apparent that this may be better than other methods that are currently available.

**Halffmann:** In my view, public expectations have changed over the past year and a half. People have become a little more realistic after the first two years of quantum hype – we surfed along on this wave. We have taken advantage of this, but we have always remained realistic.

**Anita Schöbel:** I agree with you! My very first application for AnQuC already states that we are starting with the aim of seeing what works and what doesn't work. And I also agree with you that expectations are becoming more realistic.

**Halffmann:** We can't promise that we will have quantum superiority in five years' time. Even if some people postulate this, we have not yet seen any reliable arguments for this. Nevertheless, we are optimistic that the use of (hybrid) quantum algorithms will provide advantages in certain areas, some of which include our areas of application. Until then, however, there is still plenty of work to be done, especially in order to achieve sustainable practical benefits from these algorithms.

### In conclusion: From a scientific point of view, what fascinates you about the topic of quantum?

**Halffmann:** I jumped in at the deep end when I joined the Fraunhofer ITWM. I had no background in Quantum Computing when I came here and started straight away with my first project. For me, the exciting thing is simply that we have to completely rethink things, a big difference to classical methods. It's fascinating to be involved in a young topic at an early stage. There's a kind of gold-rush fever in research.

**Schöbel:** I feel the same way. New paradigms are emerging. There are many things that are turning around a bit and that makes it particularly exciting from a scientific point of view. Quantum Computers offer potential and maybe we need another spark, a brilliant idea, and then something completely new could emerge. The whole time you have the feeling that the last word has not yet been spoken.

"The last word has not yet been spoken."

**www.itwm.fraunhofer.de/quantum-computing**

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# Quantum Technology: Our Experience

Almost all of our departments and divisions have already carried out projects with the support of quantum technologies. An overview of the research activities in the "Application-oriented Quantum Computing" (AnQuC-3) project funded by the state of Rhineland-Palatinate.

## Image Processing

In the field of Machine Learning (ML) with Quantum Computers (QC), researchers have developed their own algorithm for recognizing edges in images using QC. The algorithm delivers very robust results – not only on a quantum simulator, but also on a currently still error-prone superconducting QC. Our team has thus developed what is probably the first quantum edge detection algorithm that can also be used for larger image sizes. Compared to existing methods, the method developed at the Fraunhofer ITWM requires only a few measurements of the quantum states.

## Financial Mathematics

The department's research activities focus on identifying use cases in financial mathematics, transferring classical financial mathematics methods to QC applications and further developing QC algorithms. The researchers investigate and evaluate the use of quantum algorithms and computers for financial mathematics issues.

In addition, quantum algorithms are further developed, for example by automatically finding QC circuits, e.g. for the simulation of financial mathematical processes. Artificial Intelligence methods are used to enable the most efficient possible calculation of a wide range of simulation problems. Existing, so-called variational QC algorithms are adapted accordingly to the department's use cases.

## High Performance Computing

Our "High Performance Computing" (HPC) division focuses on the interplay between HPC and QC. In the AnQuC project, researchers are looking at the benchmarking of Quantum Computers and other quantum chemistry simulations.

Comparing different systems with each other is important in order to quantify the advantages of Quantum Computing. Various parameters are considered. The focus is on the runtime of quantum circuits. In addition to specific measurements, the department is also working on the German industry standard (DIN) SPEC 91480 "Benchmarking of Quantum Computers" in order to identify suitable metrics and methods.

## Materials Characterization and Testing

Optical technology is playing an increasingly important role in production. Quantum technology is revolutionizing the way we deal with light and can be used in many industries in the future. The department conducts research into quantum measurement technology, spectroscopy and tomography in particular.

## Mathematics for Vehicle Engineering

The "Mathematics for Vehicle Engineering" division looks at various ways of using QC for traffic control. In particular, the researchers are investigating whether the use of hybrid quantum algorithms, such as the "Quantum Approximate Optimization Algorithm" (QAOA) or "Quantum Annealing", can already achieve performance gains compared to classic optimization methods.

## Optimization

The "Optimization" division sees the potential of QC mainly in specialized optimization algorithms and for quantum-based Machine Learning (ML) methods. Hybrid quantum algorithms are methods in which both conventional digital computers and Quantum Computers are used. They can be used, for example, to solve combinatorial optimization tasks.

The randomness of measurement results is an intrinsic property of quantum systems. Random numbers are also an essential component of numerous Machine Learning methods, especially in the field of deep learning. It therefore makes sense to combine these two topics. An empirical study by the research team refutes earlier hypotheses that predicted a clear quantum advantage.

## Flow and Material Simulation

Numerical simulation is an important tool for characterizing composite materials. The researchers are focusing on the potential of Quantum Computers to resolve complex material models quickly and efficiently. To this end, they are investigating both methods that promise a long-term advantage – such as the Quantum Fourier Transform (QFT) – and heuristic methods that could be used in the short to medium term – such as variational hybrid methods.

The QFT makes it possible to accelerate the classical Fourier transform exponentially. The latter is the bottleneck in the creation of replacement models for the multiscale simulations of composites. It has been possible to carry out small material simulations on IBM Quantum Computers.

**www.itwm.fraunhofer.de/anquc-3-en**

# Quantum Technology: We Train the Next Generation

**The Quantum Initiative Rhineland-Palatinate (QUIP) focuses on young scientists: young researchers are given the opportunity to familiarize themselves with the topics of Quantum Computing (QC) or quantum technologies (QT) at the Fraunhofer ITWM or at our project partners in Rhineland-Palatinate. The Rhineland-Palatinate Ministry of Science and Health is funding the project.**

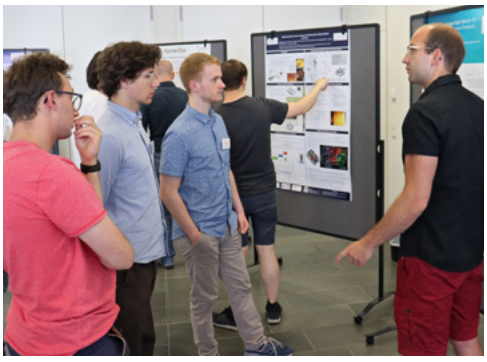
At "QUIP", young quantum scientists receive a detailed, broad research program for training, further education and networking. "It's really great that the ferderal state is supporting us in this way, both in terms of funding and networking," emphasizes Institute Director Prof. Dr. Anita Schöbel. Quantum technologies and QC research are well established in Rhineland-Palatinate, both in projects at universities and institutions as well as in companies.

QUIP is already successfully training and developing experts, bringing them to Rhineland-Palatinate and networking them in a targeted manner. The first "Summer Schools" and "Winter Schools" have already taken place. "The skills are still rare, there are few offers but a high demand for experienced researchers," says Quantum Research Coordinator Dr. Pascal Halffmann.

"It is important that we have established our own program. For the 'Winter School' in February, we were able to attract speakers from the major Quantum Computing players. This event led to internships with people from the USA and Europe, which was the only way we could get them to come to Rhineland-Palatinate."

## Structured Qualification Concept at the Quantum Graduate Center

The Quantum Graduate Center (QGC) is another central element of QUIP. All doctoral students with topics in the field of "Quantum Computing and Quantum Technologies" can apply for the QGC and thus benefit from a wide range of scientific programs and individual training courses.



**www.itwm.fraunhofer.de/quip-en**

## Dr. Alexander Geng, Image Processing

In my doctoral thesis, I investigated the potential of Quantum Computers in the field of image processing. The focus was not only on the theoretical advantages, but especially on the practical benefits and limitations of Quantum Computers in the current NISQ era, where the hardware still has comparatively large errors.

In addition to loading an image onto a quantum computer and improving the algorithm, I developed a robust algorithm for detecting object edges after recognizing the limitations of current Quantum Computers. Finally, I combined the topics of Quantum Computing and Machine Learning to develop a hybrid algorithm to solve a classification problem in an industrial setting.

## Tom Ewen, Financial Mathematics

Since the EU introduced the Solvency II Directive in 2016, insurers in Europe have had to calculate their solvency capital requirements. The Monte Carlo simulations required for this – even if highly parallelizable – are particularly time-consuming, so that they are usually only carried out once a year.

In my PhD, I am investigating how methods from Quantum Computing, such as Quantum Machine Learning or the Quantum Fourier Transform, can help to accelerate these calculations. In particular, I am looking at the problem of pricing options as an important building block in the calculation of the solvency capital requirement.

## Thomas Cheng, High Performance Computing

My thesis covers different aspects of state-of-the-art quantum algorithms in order to improve the performance in the simulation of fermionic systems, e. g., those found quantum chemistry.

A particularly relevant problem is that of the encoding to the qubit space. The standard here is the Jordan-Wigner transformation, which requires M qubits for M fermionic states, however, this can be reduced to Nlog M qubits for an N electron system. Using techniques from error correction, we have developed a classical scalable quantum data compression method with optimal qubit count and measuring costs. This scheme can be encoded and decoded in polynomial time and reduces the number of qubits required as well as noise. This scheme can be generalized to address quantum error correction and theoretic bounds for quantum information in physical systems.

# Higher, Faster and Further

Computers are expected to be able to do more and more – which increases the performance requirements for hardware and software. Conventional computer technologies are reaching their limits. "Next generation computing" is a strategic field of research at the Fraunhofer-Gesellschaft. Our researchers are looking for new solutions to significantly increase the efficiency of data processing. Three streams are particularly promising: specialized energy-efficient supercomputing, neuromorphic computing and Quantum Computing.

## Newly Founded: UNEEC Systems GmbH

August 2023 saw the launch of the latest Fraunhofer ITWM spin-off to date – UNEEC Systems GmbH. Its goal: to market energy-efficient supercomputers based on European technologies. At the heart of the spin-off is the stencil and tensor accelerator (STX), which is being developed using a consistent hardware-software co-design approach. The team of researchers at the Fraunhofer ITWM led by Dr. Jens Krüger is working on optimizing the hardware.

## Simulate Instead of Destroy

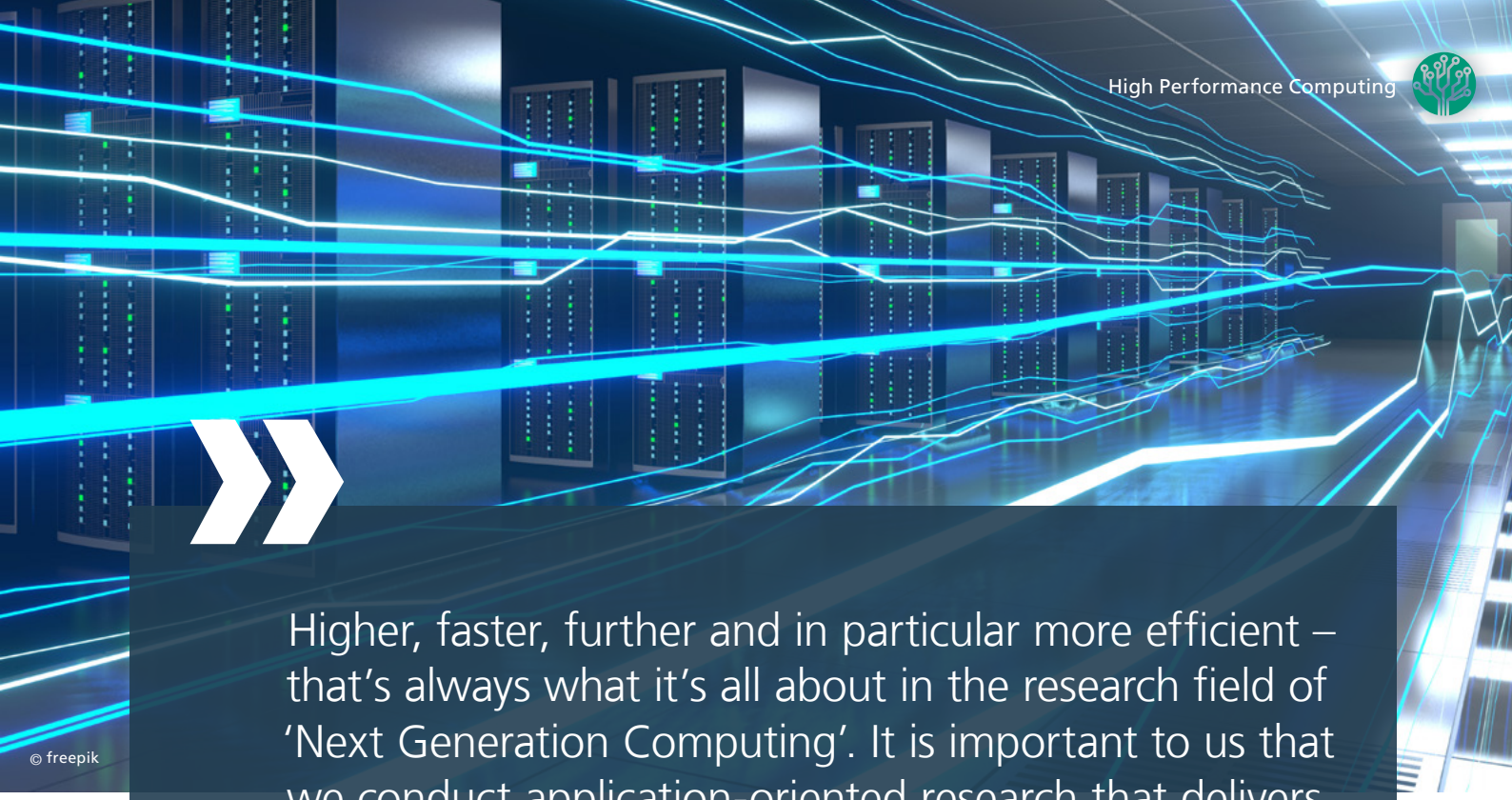
The aim is to create optimal conditions for improved simulations in particular. "Simulations are now an integral part of science and industry, but they also consume energy. Model-based simulation is now replacing many experiments, such as crash tests in the automotive industry," explains Dr. Jens Krüger. "Digitalization is therefore the key to increasing efficiency, but ever larger amounts of data and more complex algorithms mean that IT is expected to account for around ten percent of total energy requirements. It is important for us to use our research to help ensure that high-performance, energy-efficient systems are part of the solution and not the problem."

UNEEC Systems GmbH's approach includes its own system-on-chip architecture – from a plug-in card to a complete HPC rack. The company is thus picking up on the trend of offering application class-specific solutions: If you know what the user expects, you design the hardware accordingly. Thanks to the co-design approach, the STX system concept combines an innovative architecture, maximum energy efficiency and simple programmability for highly parallel simulation applications.

## Neuromorphic Computing: NASE Extended

A bird's brain is small, but extremely powerful: The organ manages to navigate the bird, enables communication with conspecifics and all other functions that ensure its survival – to put it simply: a small brain with enormous output. Neuromorphic chips aim to mimic this efficiency. The AI product NASE (Neural Architecture Search Engine) has now been developed on the basis of an energy-efficient AI chip, for which researchers at Fraunhofer ITWM received the 2021 Pilot Innovation Award from the German Federal Ministry of Education and Research.

With NASE, a team from the "High Performance Computing" department is helping companies to design neural networks tailored to their needs



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Higher, faster, further and in particular more efficient – that's always what it's all about in the research field of 'Next Generation Computing'. It is important to us that we conduct application-oriented research that delivers real added value for our clients. But we also see it as our responsibility to develop energy-efficient solutions."

**Dr. Jens Krüger**
Team Lead "Next Generation Computing – New Architectures"

and integrate them into their own networks. NASE brings together several technologies for this purpose. "We at Fraunhofer ITWM are developing a hardware-aware neural architecture search with NASE," explains project manager Dominik Loroch. "This type of search also takes into account the limitations of the hardware platform, and we find solutions that run optimally. Anyone who wants to use NASE only provides the data and needs little to no knowledge of DNN (Deep Neural Networks). Since both the search and the training are automatic, this is a very scalable method for quickly obtaining solutions for the hardware." NASE acts as a productivity booster that identifies complex DNNs very quickly and thus significantly reduces development costs.

## Quantum Computing

The researchers from the "Next Generation Computing" department are naturally also looking very closely at the topic of "Quantum Computing". "It's exciting for us to see how two worlds – the classical and the quantum world – are developing," says Krüger. "We see a lot of potential, especially for using quanta in a hybrid system as an accelerator unit. An exciting question for us is how to optimally distribute parts of applications in a system consisting of classical and Quantum Computers. We are researching this in an application-oriented way with realistic applications from industry, while many others focus primarily on the hardware."

**www.itwm.fraunhofer.de/nextgenerationcomputing-en**

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# Energy

We need a lot of energy to maintain our standard of living. This makes it all the more important to use it efficiently. Renewable energies and efficiency technologies, smart grids and the digitalization of the energy industry are the focus topics of our institute. The focus is always on the secure and sustainable supply of heat and electricity – including for e-mobility.

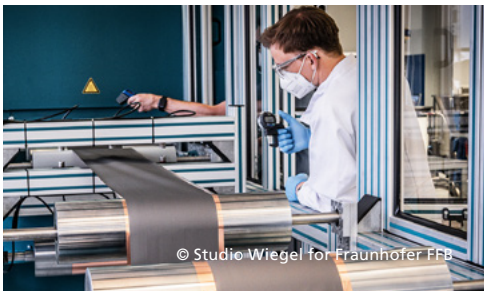
# Terahertz Measurement Technology for Checking the Coating of Battery Foils

**In the coming years, 1,000 production lines for electrode foils are to be built in Europe; similar figures apply to Asia and North America. Only non-contact systems can be used to monitor quality inline during production. This is why researchers in the "Material Characterization and Testing" department have expanded their expertise in terahertz measurement technology for inline coating control of battery foils.**

The production line here refers to the equipment for coating the electrodes. The coating is usually applied as a liquid – called slurry – to copper or aluminum foils. For optimum battery performance, the coating must meet high requirements in terms of layer thickness and homogeneity. Until now, the industry has used beta and X-ray radiation to determine the layer thickness. These have the disadvantage that they only measure the total thickness, i. e. the film including the coating, and therefore require differential measurements before and after coating. If measurements are not always taken at the same strip position, the measurement errors add up drastically.

## New Sensor Technology Makes You Flexible

Terahertz radiation can be used to measure faster and more accurately. "This technology measures in reflection and thus directly records the coating thickness; it takes less than five milliseconds for a measurement," explains project manager Dr. Joachim Jonuscheit. The new sensor technology can be flexibly adapted to the respective task in terms of the number and position of the measuring heads as well as the measuring frequency. The optimization to frequencies between 50 GHz and 1 THz, frequency stabilization through improved driver electronics and adapted signal processing enables precise thickness measurements on thin,




highly absorbent and electrically conductive layers.

## Coating Thickness Measurement With Terahertz

"We measure the cathode coating with terahertz TDS, as we use it to measure paint coatings in the automotive industry." This allows 1,000 measurements per second. The conductivity of the anode is higher than that of the cathode. Their coating can be measured using photonic terahertz FMCW – a new measuring principle. Several manufacturers are already working on the dry coating of battery foils, which significantly reduces $CO_2$ emissions by shortening the drying process and thus improves the environmental balance of the manufacturing process. The use of terahertz measurement technology is particularly advantageous here, as beta and X-ray radiation cannot be used for process-related reasons.

*The cathode carrier material consists of aluminum, with a layer thickness of between 30 µm and 300 µm. Copper is used as the carrier material for the anode.*

**www.itwm.fraunhofer.de/layer-thickness-measurement**

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# A Look Inside the Battery Cell

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**The heart of electromobility is the battery. It powers cars as well as trucks and therefore has to meet a wide range of requirements. Electromobility has been booming over the past five years thanks to political engagement and support. This has only been possible because research into this topic has been going on for a long time – also at our institute. Dr. Jochen Zausch, Team Leader "Electrochemistry and Batteries" and Dr. Falco Schneider explain where the beginnings lie and what level of research has been achieved. Both work in the "Flow and Material Simulation" department.**


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### How long has the Fraunhofer ITWM been doing battery simulation? What was the trigger?

**Zausch:** It's been around since I've been here, i.e. since 2009, and was triggered on the one hand by the cooperation with Opel and on the other by the Fraunhofer System Research for Electromobility: this research initiative began in the same period, funded by the German government. So battery cell research has been going on for a long time, but most models neglect the microscopic details. We can describe these well with our multi-scale approach.

### What does that mean in detail?

**Zausch:** An electrode consists of porous material, i.e. a powder with particles of the order of five to ten micrometers, and these particles together form the complex structure of the electrode.

Clearly, this microscopic structure naturally has an influence on the macroscopic battery behavior. With a simulation that takes the three-dimensional microstructure into account, it is now possible to draw conclusions about the macroscopic battery behavior. And this is our unique selling point, manifested in the Battery and Electrochemistry Simulation Tool BEST. It allows us to simulate how the battery behaves during charging and discharging and, of course, to optimize it.

Now there is additional aspect to this, namely battery production. Here, for instance, we profit from our expertise in complex flow simulation as electrodes are cast on metal foil in the form of a viscous slurry. In the next step, calendering, i.e. pressing the foil between two rollers,

we also apply our knowledge in the simulation of mechanical properties and use our FeelMath tool. Going down the production line, we use FLUID to simulate the electrode wetting, i. e.the absorption of the electrolyte liquid into the pores of the porous layers of the cell. With our FOAM software, we can simulate the expansion and curing of a foam in the spaces between the cells, which is intended to ensure mechanical stability and thermal insulation between the cells.

### Falco Schneider is working on the new research area of battery ageing. Why has this topic come into focus alongside calendering, wetting and foaming?

**Schneider:** Like many other products, batteries only have a limited product life. We want to describe what happens at the microstructure level when both charging capacity and battery performance decrease. The underlying electrochemical processes can be investigated only to a limited extend by experiments, which is why simulation is useful here.

### What exactly happens during battery cell ageing?

**Schneider:** Battery cells age both during active use and during storage. There are many factors that influence the ageing behavior. For example, mechanical stress during operation can cause parts of the cell to become inactive so that they no longer contribute to charge exchange. On the other hand, chemical side reactions take place which reduce the cyclable lithium inventory of the cell by binding it in various reaction products. The observed symptoms of these effects are a loss of capacity and an increased internal resistance, which leads to a loss of performance.

We focus on describing the individual effects in order to gain a better understanding of the cells and to investigate how to slow down these special ageing processes in order to save resources and energy in battery production in the long term.

### Several departments at our institute deal with batteries; where are the points of contact?

**Zausch:** Our internal cooperation is best illustrated by the DiBaZ project funded by the federal state government. Together with three other departments, we are working on a digital twin for all process steps in battery production. At the end of the project, we will be able to offer our industrial partners methods and models that not only simulate battery production, but also enable non-destructive quality control and include energy management with predictive control.

### Let's venture a prediction: can electric vehicles guarantee the mobility that is desired in Germany?

**Zausch:** I think so, especially in passenger transportation. The range of current electric vehicles is certainly sufficient for the majority of journeys. What is still being worked on, however, is improving the fast-charging capability of the batteries. This is intended to counter customers' reservations about electric vehicles. In this context, another challenge for the acceptance of electromobility is the sufficient availability of suitable charging points: e. g. on long-distance roads, where high charging capacities are required for fast charging, or in urban areas, where residents do not have the opportunity to charge their vehicles overnight at their own homes. Another obstacle is the relatively high purchase price. It is hoped that costs can be reduced in the medium term through mass production. In addition, new, cheaper cell chemistries, such as those used in sodium-ion batteries, could also help to reduce costs in the long term and become even more sustainable and independent.

**www.itwm.fraunhofer.de/electrochemistry-batteries**

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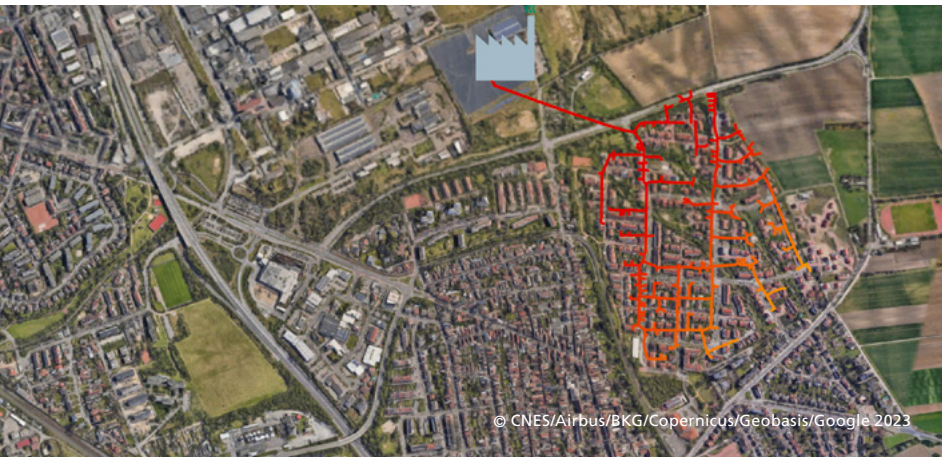
# AD-Net – Intelligent Control of District Heating Networks

District heating is considered a central component of future energy supply. The optimal control of networks is currently a lively area of research in which researchers from the "Transport Processes" department are also involved. Their software tool "AD-Net District Heating" dynamically simulates and optimizes the operation of heating networks in real time. The software has been developed since 2015 in close collaboration with Technische Werke Ludwigshafen AG and GEF Ingenieur AG.




*Heating network with temperature distribution*

District heating suppliers often operate their systems at a constant temperature of around 90° C. In this operating mode, the feed-in power follows consumption, which fluctuates greatly throughout the day. In order to cushion the consumption peaks in the morning and evening, an additional gas boiler often has to be started up, which results in high costs and additional fuel consumption. The researchers therefore looked into the question of whether this additional firing could be avoided, at least during the transitional periods, by feeding water at a variable temperature into the pipe system.

## Cut Load Peaks by Preheating

Like the drinking water supply, the district heating network also works via pressure equalization; this means that what is withdrawn by end consumers must be added at the plant at such a pressure that the heat exchangers in the households can work properly – but certainly at different temperatures. "In our model, the producer sends water at a high temperature but low speed into the grid before the consumption peak, which keeps the feed-in rate moderate. When the hot water reaches the customers, the plant feeds in a lot of water, but at a low temperature. This allows a high extraction rate while maintaining a moderate feed-in rate," explains project manager Dr. Jan Mohring. This principle of pre-heating is well known, but can now be systematically optimized.

## AD-Net Plans Two Days in Advance

AD-Net's data is based not only on empirical values for consumption and temperature curves in the district heating network, but also on weather forecasts. This allows providers to plan even better, usually for two days. This facilitates the reliable supply of heat when large heat pumps or solar parks are also included in the energy mix in the near future.

**www.itwm.fraunhofer.de/ad-net-district-heating**

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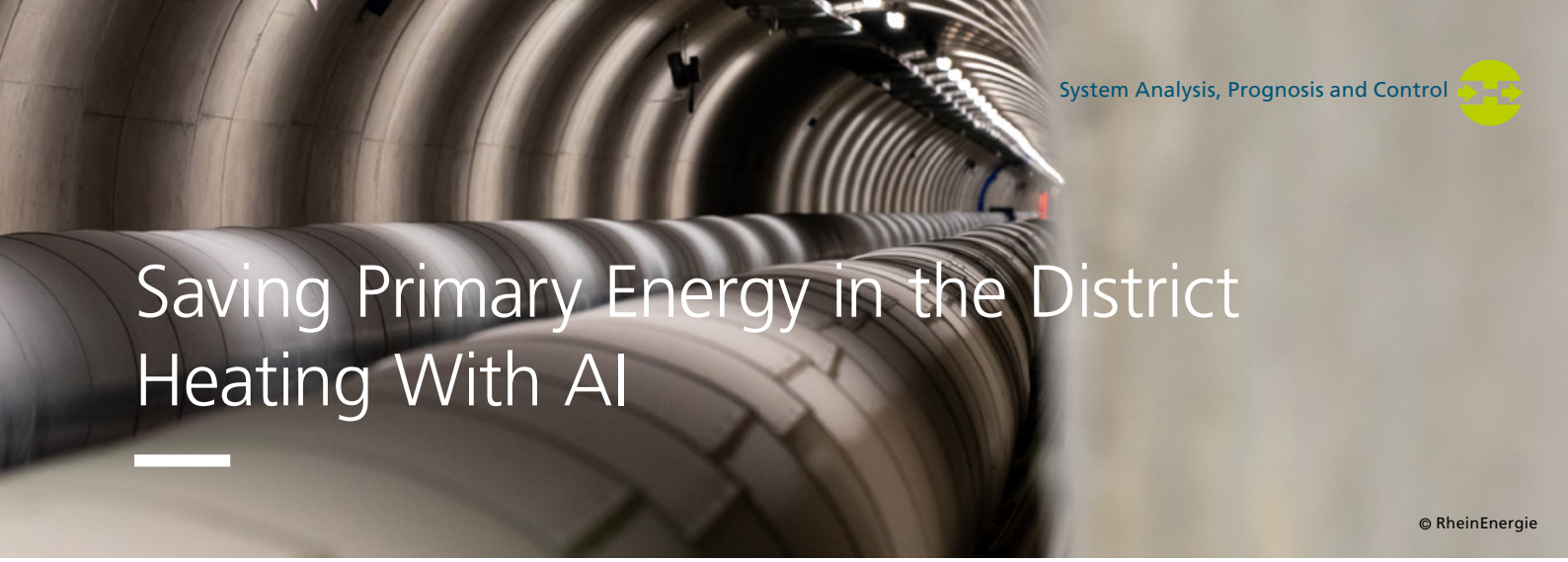

# Saving Primary Energy in the District Heating With AI



*The temperature must be right in the heat tunnel.*

**AI methods can be used not only to optimize consumption in the extensive district heating network, but also to save primary energy at the Fraunhofer ITWM. In a pilot project with the energy service provider RheinEnergie AG, a team from the "System Analysis, Prognosis and Control" department has succeeded in improving the processes around boilers and thus saving a significant amount of primary energy – especially gas.**

In general, heating networks are divided into a primary and a secondary side: the boilers are located on the primary side and generate the heat, which is pushed into the secondary side, i. e. into the grid, at a transfer point. "Our task was to control heat generators in such a way that the current demand in the network is covered, but at the same time as little surplus energy as possible is fed into the network," says project manager Dr. Christian Salzig. "The demand at the transfer point is interesting, i. e. where the heat passes from the primary to the secondary circuit. To determine this, we use machine learning methods to create individual, weather-related load profiles." Based on these load profiles, the developed prediction models can forecast the heat demand for the coming hours very precisely and controle the generators accordingly.

## Keep Mains Temperature Stable

In addition to demand-based control, another problem with the heat supply was resolved in the project: Measuring points on the grid side report current temperatures, but due to the length of the grid there are runtime delays. It can therefore happen that too little energy is detected in the network and the machines heat up even though the heat currently produced will already cover the demand. This leads to significant temperature oscillations in the grid. For this reason, predictive controllers have been developed that take transport delays into account and almost completely eliminate these oscillations. This allows the energy supplier to controle heat generation precisely to the predicted demand. This allows the temperature in the grid to be lowered without jeopardizing the security of supply, which leads to significant savings in primary energy.

## Ensuring Security of Supply

Furthermore, the researchers can use their method to predict whether it is worth starting up an additional heat generator or whether it is better to run the lead boiler at its output limit for a short time in order to compensate for spontaneous fluctuations. External sources, such as electricity-driven CHP units or waste heat from connected businesses, present a particular challenge here. The intelligent control system therefore ensures that the heating plant has a control reserve that can always compensate for unplanned failures of external heat sources.

The ongoing evaluation shows: Depending on the outside temperature, the implemented AI controllers save between six and thirteen percent natural gas. The controllers are currently being implemented in other local heating systems at RheinEnergie AG.

**www.itwm.fraunhofer.de/heating-ai-en**

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# ENERDIG – Digitalization and Artificial Intelligence for Energy Management 2.0

**ENERDIG stands for "ENERGY MANAGEMENT 2.0, DIGITALIZATION, AI, OPTIMIZED PROCESSES" and aims to achieve holistic energy management. Four departments contributed their expertise to the project and worked together to develop new digitalization and AI-based strategies. The focus was on residential and industrial buildings, plastics production, chemical production and nonwovens production.**


For example, the research teams developed AI methods to charge electricity storage units based on weather forecasts, which in turn supply heat pumps and electric cars with as much renewable energy as possible. This is a further step towards energy self-sufficiency, both for private households and companies.

## SME Benefit From Research

In the industrial sector, the researchers focused on nonwoven production, which is aerodynamically optimized using software solutions. This leads to more stable product quality and significant energy savings.

This is also possible in plastics production. In order to support SMEs in particular on their way to Energy Management 2.0, the Fraunhofer ITWM is developing algorithms for identifying and evaluating energy consumption and flexibility based on digital twins of machines and production systems.

A similar approach applies in the energy-intensive chemical industry: making energy consumption more flexible means that companies can adapt their processes to changing energy costs at short notice. Thanks to ENERDIG, the availability of raw materials is now also taken into account in plant optimization.

**www.itwm.fraunhofer.de/enerdig-en**

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# Other Projects With a Focus on Energy

### Hytwin – Hybrid Digital Twin for the Optimization of Plastics Processing Processes

Computer simulations and digital twins offer the possibility of optimizing almost the entire extrusion process. The project team from the "System Analysis, Prognosis and Control" department took a hybrid approach: they developed a digital twin that is both data-based and model-based, which predicts and optimizes using AI. The result is an easy-to-use software platform for quality forecasting that also helps small and medium-sized enterprises (SMEs) to achieve higher production speeds, greater flexibility and higher product quality at the lowest possible cost.

**www.itwm.fraunhofer.de/hytwin-en**

### OpenMeter – Data and Analysis Platform to Increase Energy Efficiency

The availability of consumption data is important for increasing and evaluating energy efficiency, for smart grid planning and for the interdisciplinary development of innovative services and business models. The OpenMeter project created the high-performance digital open data platform "Open Energy Meter Data" – visualization, analysis and comparison of energy consumption data. A team from the "System Analysis, Prognosis and Control" department researched and evaluated mathematical methods of artificial intelligence to derive energy baselines and parametric forecasts of future energy consumption.

**www.itwm.fraunhofer.de/OpenMeter_EN**

### DYNEFF and DingFESt – Efficient Operation of District Heating Plants

In the "DYNEEF" project, researchers from the "Transport Processes" department are working together with GEF Ingenieur AG and Technische Werke Ludwigshafen on "Dynamic network simulation to increase efficiency in district heating generation". The successful collaboration led to the follow-up project DingFESt "Digital twin for flexible and efficiency-optimized control of decentralized district heating networks". With the results, the research team is helping supply companies to ensure highly efficient network operation in the long term without jeopardizing their stability, resilience and security of supply – even under increasingly complex and varying operating conditions.

**www.itwm.fraunhofer.de/DingFESt-EN**

# Digitization

The amount of data in many companies is growing rapidly; processing and analyzing it is becoming a key competitive skill. Our researchers support companies in building up know-how and developing solutions in business processes, production and logistics. We attach great importance to feasibility, cost-effectiveness, data protection and security.

# EU Project OPTIMA Accelerates Industrial HPC Applications

**The main goal of the completed EU project OPTIMA was to optimize and test industrial applications and open source libraries on HPC systems with FPGA chips. These special chip technologies, known as field-programmable gate arrays (FPGAs), accelerate certain applications that are executed on a supercomputer. Research work from the MESHFREE and CARME groups has been incorporated into the project.**

FPGA chip technologies are known for their lower power consumption compared to CPUs and GPUs. It therefore makes sense to use them for energy-intensive calculations such as simulations. "OPTIMA gave us the opportunity to test whether FPGA-controlled approaches are generally suitable for our simulation software MESHFREE and how we need to adapt them so that our simulations run faster on FPGA chips," says Sebastian Fett, who worked on the project for the Transport Processes department.

## Challenge: Complex Algorithms From MESHFREE

The researchers use MESHFREE to simulate complex flow processes such as the passage of a car through water. "Due to the wide variety of applications and the complexity of our algorithms, very large amounts of data are generated that have to be transferred to the FPGA environment. This led to a bottleneck," explains the computer scientist. In addition, MESHFREE is based on code that has grown over a long period of time and had to be restructured before the data could be ported to FPGAs. Nevertheless, he and his team believe that speed increases using FPGAs in an adapted version of MESHFREE are realistic.

## Carme Framework Extended

Researchers from the HPC department were also involved in OPTIMA. With the help of their open-source framework Carme, multiple users are able to manage available computing resources without prior knowledge of workload management tools such as Slurm. The graphical user interface enables interactive access to hardware resources.

"We have provided support for GPUs in Carme right from the start; the integration of FPGAs was previously missing from the Carme framework," says Dr. Matthias Balzer, describing his department's motivation for participating in OPTIMA. "During the course of the project, we integrated the essential components for FPGA support into the framework. The available accelerators, i.e. both GPUs and FPGAs, can be conveniently selected via the Carme web frontend." In addition, a simple prototype of an FPGA kernel library for machine learning was implemented.

**www.itwm.fraunhofer.de/meshfree_en**

**www.itwm.fraunhofer.de/carme-en**

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# From Excel to the App: Data Science in Real Estate Financing

**Real estate financing is a key area of business for many insurance companies. The financing of both commercial and private real estate involves a flood of sometimes manual processes, from the initiation of business to risk management. Intelligent digitalization and automation can save immense costs. This is demonstrated by researchers from the Financial Mathematics department in a project with R+V Versicherung.**

R+V Versicherung is active as a lender in the construction sector; on the one hand, it grants loans for private residential property, but also finances commercial real estate such as shopping centers or office buildings. In risk controlling, suitable forecasting methods help to estimate the probability of loan default. To do this, the insurer wants to know how repayments will be made. "Fixed repayment installments are relatively easy to predict. Statistical methods can be used to include unscheduled repayments, terminations or deferrals in the forecast. If sufficient data is available, machine learning methods can also provide a better prediction," explains Dr. Jörg Wenzel, Head of the Financial Mathematics department.


## Dashboards for Commercial Real Estate Financing and Individual Transactions

The basis of every good forecast is as much data as possible. Until now, banks and insurance companies have often recorded and processed this data in Excel. In the new app, which is being developed together with the Fraunhofer ITWM, all relevant data on real estate financing is brought together in a database and made usable via a dashboard. R+V Versicherung employees now have a tool with which they can quickly create, process, evaluate and analyze business transactions.

The entire financing portfolio can be viewed at the click of a mouse and the app can support the creation of annual reports and management reports. Users are also positive about the app's much more user-friendly interface.

"Furthermore, we support the development of an app that includes a variety of visualizations in the form of graphs or tables," says Wenzel. These help to provide a compact overview of large volumes of complex data and ultimately support important business decisions. For example, the visualizations enable a comparison of competitors over time or a customer overview with regard to various criteria.

**www.itwm.fraunhofer.de/asset-allocation-portfolio-optimization-en**

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# Effective Procurement Strategies for Energy Trading

**Trading and procuring electricity and gas are key areas for energy suppliers. Many of these companies rely on digitalization, automation and artificial intelligence to meet the increasingly complex requirements of politics and business. In collaboration with SWK Stadtwerke Kaiserslautern GmbH, our "Financial Mathematics" department has analyzed and optimized procurement strategies in the "Dynamic Optimization of Trading Strategies" project. With complete success – because the researchers developed a prototype and want to continue working together.**


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With the increasing expansion of renewable energies, it is essential for suppliers to be flexible. They must be able to react dynamically to market movements and change their procurement strategies at short notice. However, this requires reliable systems that effectively support and profitably assist strategic decision-making.

This is where the work of our researchers begins. Their expertise includes mathematical modelling of energy markets, risk management, the optimization of trading strategies and the associated software development. They combine mathematical analysis and modeling with concrete implementation in software in order to offer practical solutions for various challenges. This combination makes the Fraunhofer ITWM a strong partner for a wide variety of problems.

## Successful Cooperation on Site

This was also the case in the project with the Kaiserslautern-based energy supplier. "Here, we worked on the analysis and validation of procurement strategies and carried out various optimizations of the strategy using different evaluation criteria," explains project manager Christoph Gärtner. The result is a software prototype that presents the results of our research in a user-friendly way and at the same time allows users to carry out their own optimizations. However, the prototype also shows potential for further research in both energy trading and energy procurement. "We want to work on this together with our partner in a subsequent project. In this way, we are not only securing the future viability of energy suppliers, but also meeting the challenges of the energy transition. We look forward to continuing our cooperation," concluded Gärtner.

**www.itwm.fraunhofer.de/flexible_loads**

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# Mobility

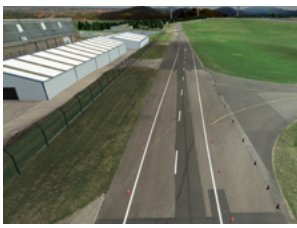
The topic of “mobility” is a constant companion for us at the Fraunhofer ITWM – be it for the automotive industry, in construction and agriculture or even for aerospace. Our focus is on our simulation methods, which optimize products, often before a costly prototype is built. However, we also test components with our terahertz research. We can boast a large number of projects in this area and are constantly adding new ones that improve mobility for suppliers and users.

# Virtual Worlds for Vehicle Engineering

**Autonomous driving functions and driver assistance systems such as parking or lane departure warning systems are considered pioneering technologies in the automotive industry and are already an integral part of modern vehicles. However, before they can be put on the road, they need to be tested and validated. Our "Dynamics, Loads and Environmental Data" department has developed a new module in the VMC® (Virtual Measurement Campaign) tool suite for this purpose: The VMC® Road & Scene Generator.**

Current methods often fail to reflect the diversity and complexity of the real world. For example, in manually created simulation models, there are often only simple basic intersections that rarely occur in the real world. However, modern assistance systems must ensure safety at all times – even in complex traffic situations. This requires realistic models of the environment.





*Left: Real scene (photo)*
*Center: 3D scan*
*Right: Virtual 3D scene*

## Multi-Level Generation of Environment Models

The VMC® Road & Scene Generator focuses on the creation of virtual worlds that depict public roads or test sites as required. The generation can be based on high-precision measurement data, such as measurements from the department's own "REDAR" measurement vehicle. However, the software package also offers another special feature: the module delivers valuable results even without detailed measurement data. "Thanks to the VMC® database, which contains worldwide, georeferenced data on roads, topography, land use and traffic, we can create digital 3D maps without having to carry out measurements on site. If required, we merge this data with other available information, such as that provided by surveying offices," says expert Tim Rothmann. If individual attributes are missing from the process, such as the number of lanes or width of a road, our researchers supplement these with customized prediction models based on regional or typical road conditions. Although this does not result in an exact representation of reality, it produces sufficiently realistic approximations for many applications. Thanks to the efficiency of the approach and its global availability and diversity, the Fraunhofer ITWM makes a significant contribution to the effectiveness and feasibility of scenario-based safeguarding concepts.

## One Module, Many Applications

The VMC® Road & Scene Generator always offers the right solution depending on the requirements: for simulations based on simple abstract information such as road network descriptions, as well as for more complex applications that require detailed and photorealistic 3D models or an exact replication of the real environment. "We offer the optimum balance of variability, degree of realism and effort," explains Rothmann.

**www.itwm.fraunhofer.de/vmc-road-scene-generator_EN**

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# VMC® Web Services – Cloud-Based Analysis of Vehicle Data

**The collection of usage data plays an important role in many areas. In the automotive industry, for example, it helps to determine relevant driving conditions or to record energy consumption. The VMC® Web Services developed at the Fraunhofer ITWM are available to interested vehicle manufacturers and fleet operators in order to utilize the data in a meaningful way. Thanks to highly automated, data-driven analysis options, they provide an important additional building block in the value chain of vehicle development.**

One focus of our "Dynamics, Loads and Environmental Data" department is on modeling the usage variability of vehicles while taking environmental data into account. They developed the versatile software and service package VMC® ("Virtual Measurement Campaign"). It supports vehicle manufacturers in gaining deeper insights into vehicle stress and use and extrapolating measurement data to the entire life of the vehicle.

Every vehicle collects data, every kilometer driven is recorded in real time – whether for cars or heavy trucks. This is information on how we use the vehicles, which routes we travel and much more. Vehicle manufacturers and fleet operators typically transfer this data to a cloud-based filing system, where it is available for comprehensive analysis. As the availability of vehicle data from ongoing operations increases, so do the possibilities for analysis.

## Another Building Block in Vehicle Engineering

"This is where our new tool – VMC® Web Services – comes in. It combines the collection of real usage data with the derivation of specific customer models and supports vehicle manufacturers in integrating this information into their product development," explains expert Thorsten Weyh. The web services correspond to the modules of the VMC® desktop software. However, the modules can be individually combined to realize highly automated, statistical evaluations for specific usage groups.

## Extensive Functions

The new web services offer several advantages. It is now possible to create specific routes including potential stopovers, project routes on VMC® map material, evaluate routes according to road type, curvature or mountainousness and combine and simulate speed profiles for different vehicle, driver and traffic models. As a cloud-based online service, no costly and resource-intensive local IT infrastructure is required. The hardware requirements on the customer side are reduced to a minimum, thus enabling low-threshold access to the web services. In addition to the geo-referenced analysis options already mentioned, the services also provide information on consumption and emissions over the selected route.

**www.itwm.fraunhofer.de/vmc-services_en**

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# Particle Simulation for Construction and Agricultural Machinery

The Demify® module is part of the IPS software family and offers, with the "Demify® for Heavy Machinery and Vehicles" toolbox, a particle simulation for various applications at the interface between granular materials and tools. The particle solver enables force prediction in the interaction between the ground and the tool of a construction and agricultural machine. Through Machine Learning, in particular recurrent neural networks (RNN), our researchers significantly accelerate the simulations.

Real-time tests in the RODOS® driving simulator are now also possible. Further research is being funded by the Fraunhofer-Gesellschaft as part of a PACT project. "Over the next two years, we want to develop further features, implement our ideas and establish Demify® on the market," says Dr. Sebastian Emmerich. In addition to AI models to increase efficiency, new methods for coupling particle systems and multi-body models as well as the co-simulation of flexible components are planned.

**www.itwm.fraunhofer.de/ips-demify**

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# Realistic Tire Model for Precise Rolling Resistance Prediction

The rolling resistance of tires is the result of energy losses. It is part of the EU tire label, which divides them into efficiency classes from A to E. It allows new tires to be compared under laboratory conditions. Lower rolling resistance improves fuel consumption and therefore also energy efficiency. In practice, however, the situation is quite different, which means that the efficiency classes cannot be achieved in everyday life due to many short journeys with "cold" tires. However, this is particularly important for electric vehicles, as it affects the range. Researchers in the "Mathematics for Vehicle Engineering" division are tackling this problem. The tire simulation software "CDTire", which enables physical modelling of all elements of a tire such as a steel belt – including temperature and pressure variations – has been further developed so that it now also takes internal friction losses into account. By coupling the internal friction with the temperature model, a realistic simulation of the rolling resistance is possible.

**www.itwm.fraunhofer.de/en/cdtire**

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# Terahertz for Space Travel

**Our modern terahertz systems measure non-destructively and precisely layer by layer– even with complex structures such as foams and their adhesions – thereby preserving the integrity of the materials. The terahertz technology we use is completely non-contact and non-destructive and does not use any harmful radiation. In a new project, we are now supporting "MT Aerospace" in examining the new tank for the "Ariane 6" launch vehicle.**


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The aerospace company "MT Aerospace" specializes in the production of lightweight constructions, particularly those made of metal and fibre composites. They are currently investigating the potential further development of the cryogenic liquid tanks of Ariane 6 for ArianeGroup in the PHOEBUS project. This latest European launcher currently uses classic metallic tanks and is currently in the final preparations for its first launch.

The aim of "PHOEBUS" is now to reduce the overall weight and costs of the rocket by switching the tank material by replacing the aluminum tank material by carbon fiber-reinforced plastics (CFRP). In a specialized process, hard foam panels are bonded to the CFRP tanks to provide mechanical damping and thermal insulation during flight. This process must not result in any defective glued joints or air pockets, as otherwise the stability of the entire structure is at risk.

## Between Infrared and Microwave Radiation

Terahertz refers to the range of electromagnetic radiation between infrared and microwave radiation with frequencies of around 0.1 to 10 THz. This radiation enables non-destructive penetration of objects, on the one hand for investigations using 3D imaging and on the other for material characterization.

## Optimized Material Bonding Through Terahertz Measurements

This is where the experts in our "Material Characterization and Testing" department come into play. With their terahertz technology, they examine complex components for internal, structural damage or production defects. This is because the measurement techniques they have developed are ideally suited to examining many non-electrically conductive materials – including the foams used in the PHOEBUS project. As soon as our robot-controlled terahertz scanners are integrated into the production system, they analyze the entire surface of the tank, including the glued-on rigid foam, and detect irregularities in the glued surface.

"We use our sensor to check the entire foam layer and observe the reflected terahertz signal on the CFRP surface," explains project manager Dr. Maris Bauer. "This allows us to record the interface between the two materials in great detail. In the terahertz images generated in this way, differences in contrast indicate faulty bonding. Based on these findings, we provide our project partner with precise information on how successful the bonding is and which areas may require further attention."


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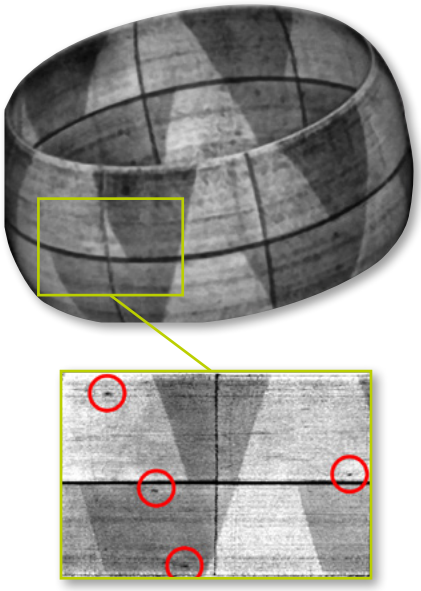

*Top left: Concept study of a potential upper stage with CFRP liquid fuel tanks*
*Top right: Terahertz image of the bonding surface of foam sheathing and cylindrical CFRP tank*

## Line by Line for Quality Assurance

The department's researchers are not only responsible for the actual measurement technology. They are also developing the system integration into a complete testing system. During the measurement process, a robot positions the terahertz sensor at a single point on the fuel tank, while the tank itself rotates on a rotary axis. This results in the analysis of exactly one measurement line along the surface of the foam-covered tank. Once a line has been completely scanned, the robot then moves the sensor a few millimetres further to capture the next line. The result is a 3D image of the entire structure of the foam and tank. The structure is thus analyzed systematically, layer by layer and millimetre by millimetre, over a period of several hours. The rotational speed of the tank is the decisive factor that defines the total measurement time of a complete tank. At present, this is still a few hours. However, improved mechanics are being planned to significantly reduce the recording time of the terahertz measurements.

"As the rocket tanks are just a few individual pieces, the measurement time is not the only decisive factor. With these extremely safety-relevant constructions, it is much more important that the bonding surfaces are inspected precisely and, above all, without gaps. This is where we differ from other point-by-point testing techniques, such as manual ultrasonic testing. Our method enables us to detect problems in production in good time and therefore offers reliable and guaranteed measurement technology," explains Bauer. "Through this thorough analysis, we not only ensure the quality of the end product itself, but also identify potential weak points in the manufacturing process, allowing corrective action to be taken at an early stage."

**www.itwm.fraunhofer.de/terahertz-testing**

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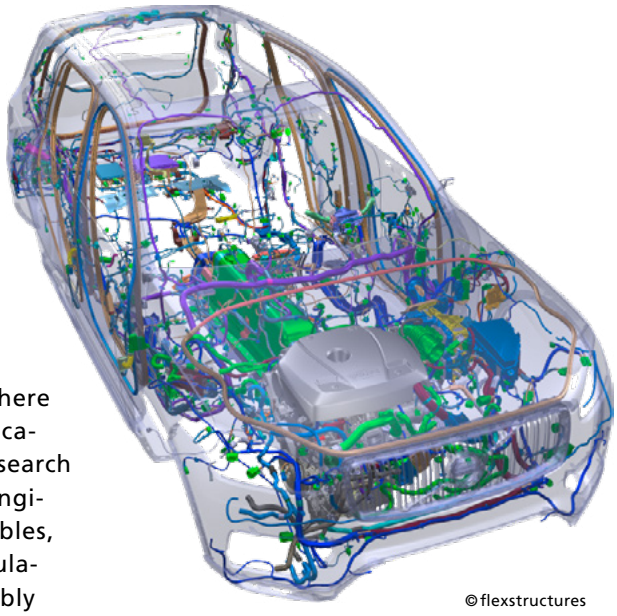
# How Long Does a Cable Last?



© flexstructures

*A look inside a vehicle: cables and hoses are everywhere.*

**They can be found almost everywhere in vehicles – we are talking about cables. This is why a core topic of research in our "Mathematics for Vehicle Engineering" division is the field of cables, hoses and flexible structures. Simulations help to optimize their assembly position long before hardware comes into play. But the ultimate question is: how long will the cable last?**

Our "IPS Cable Simulation" software package allows the simulation of cables and hoses in real time. This means that users can interactively carry out, modify and validate the 3D mechanical design of cables and hoses in the vehicle. This allows them to find the optimum design even before the first hardware assemblies are created. This saves time and costs and reduces prototypes and further iterations.

## We Continuously Enhance the Software

Although "IPS Cable Simulation" is already successful and is distributed by our spin-off "fleXstructures", our researchers are striving for continuous improvements and new functions. In current projects, for example, they are looking at the question: How long will the cable last?

The simulation already provides information about the locally occurring loads. But what do these loads mean for the cable lifetime? "A suitable cable SN Curve, which represents the relationship between local load amplitudes and the number of load cycles until failure, is crucial to the answer," explains expert Dr. Fabio Schneider-Jung.

## Comparative and Absolute Lifetime Predictions

Comparative statements are already possible with a generic SN curve. This means that although users do not know the absolute lifetime, they can compare different variants of an installation in terms of their lifetime. To additionally predict the actual lifetime, a specific cable SN curve is required.

However, determining this is no easy task. The researchers require a number of test specimens in various tests – whereby the test effort must always remain proportionate. Another hurdle is the almost impossible measurement of local loads along the cable. Here, they enrich the experimental data with simulations. Using the maximum likelihood method, they then search for the SN Curve that best matches the collected lifetime data.

"We have already determined cable SN Curves for some cables – with promising results, as the predicted lifetime was confirmed in further experiments," concludes the researcher.

**www.itwm.fraunhofer.de/IPS-Cable**

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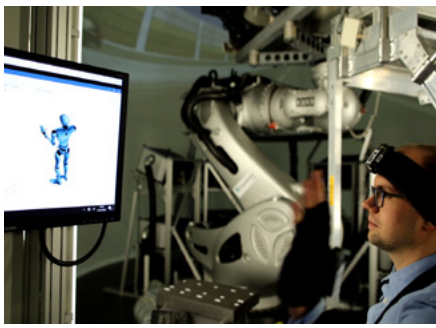
# Autonomous Driving: Safe and Comfortable Thanks to Our Innovative Human Model

**In the EMMA4Drive project, the "Mathematics for Vehicle Engineering" division is investigating the effects of various driving maneuvers on people, including their reaction behaviour and seat load, in order to calculate new body postures and movement sequences. A digital twin of vehicle occupants helps to investigate scenarios in the simulation and to analyze new seating concepts in terms of safety and ergonomics. Various studies are currently underway.**

If a person does not drive themselves and does not pay attention to the traffic, it is hardly possible for them to prepare for driving maneuvers – they merely react to perceived accelerations and forces. In order to reproduce such reactive behavior in a simulation, our researchers use optimal control. This provides realistic movements, with the human optimally compensating for the driving maneuver. However, they are also testing approaches such as nonlinear model predictive control.



*The RODOS® driving simulator in use – investigations during autonomous driving*

## Safe in Autonomous Buses

There are strict regulations for autonomous buses and shuttles with regard to starting and braking. "In order not to endanger standing passengers and still comply with the time-to-collision, we use simulations to determine the optimum load on the occupants. We calculate their compensatory movements in different standing directions and braking accelerations and determine optimum braking profiles for different TTC values. We also take into account the reaction time of the occupants," explains Dr. Monika Harant.

## Validate Simulations

Our researchers are also using the RODOS® driving simulator. They examine the seating position and attention of a driver during a sudden lane change. At different speeds, attention levels and positioning, they test the feeling of comfort and safety during the driving maneuvers. In addition, they record the seat pressure distribution via pressure measurement mats in order to obtain information about the mechanical driver-seat interaction.

"In order to compare our EMMA simulations with the observations from the RODOS® experiments and thus also validate the simulation, we then transfer the movements of the vehicle cabin into the simulations," says Harant. To do this, they measure the movements of the vehicle cabin using an IMU (inertial measurement unit) and enter the data into the simulation as a reference movement. Using the optimal control approach, they determine a compensatory movement for the driving maneuver and also take a reaction time into account.

**www.itwm.fraunhofer.de/emma4drive_en**

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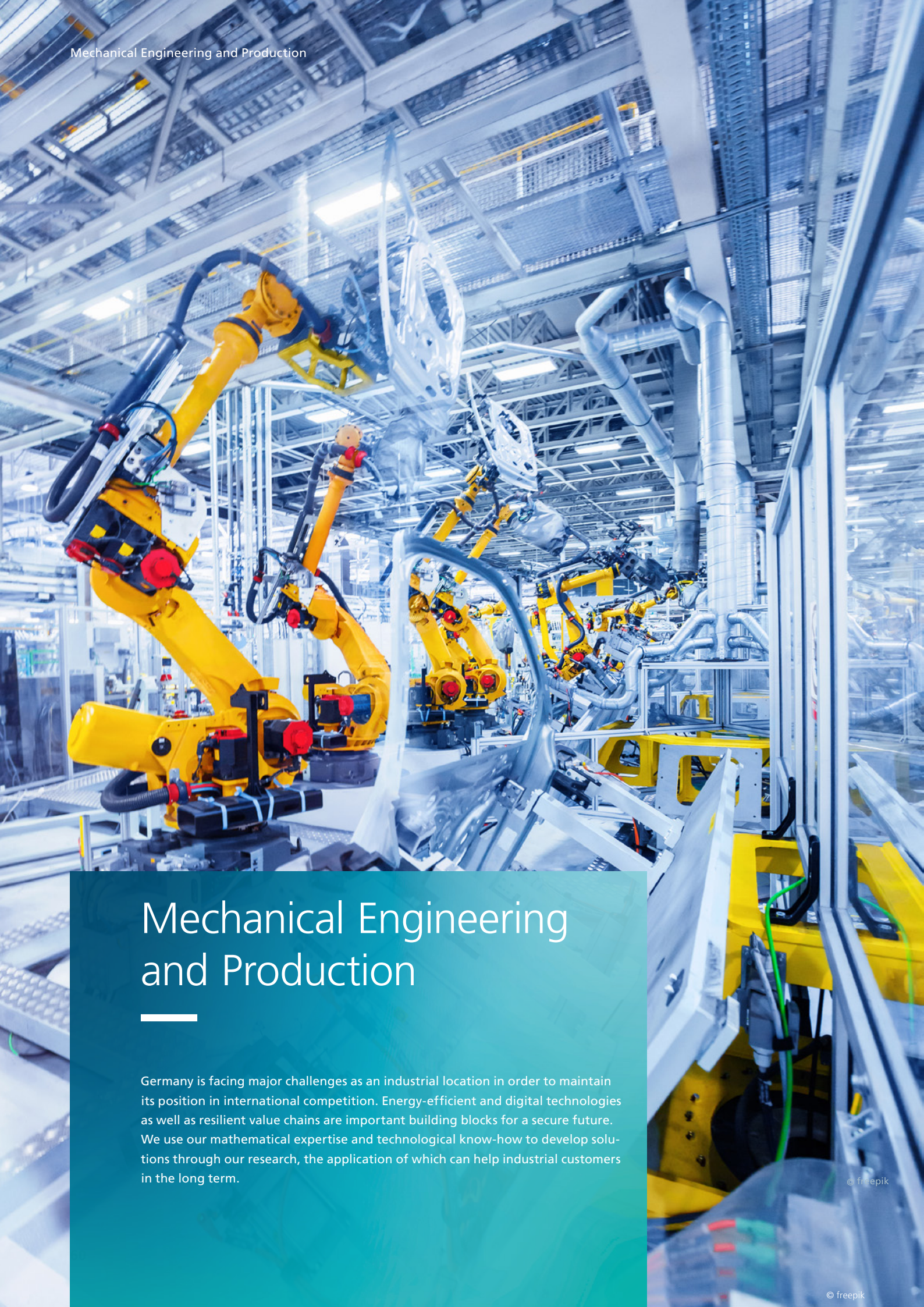
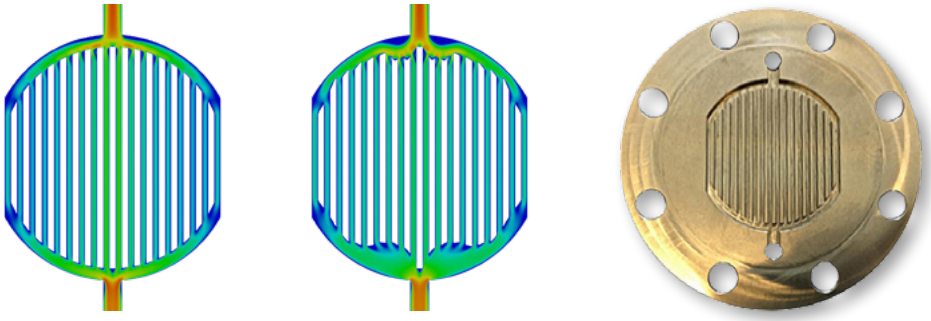


# Mechanical Engineering and Production

Germany is facing major challenges as an industrial location in order to maintain its position in international competition. Energy-efficient and digital technologies as well as resilient value chains are important building blocks for a secure future. We use our mathematical expertise and technological know-how to develop solutions through our research, the application of which can help industrial customers in the long term.

# Shape Optimization: From Research to Practice

**Dr. Sebastian Blauth received the ICT Dissertation Award 2022 for his dissertation, which resulted in the software package cashocs that can improve industrial processes through shape optimization.**



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*cashocs in use: The design of the flow field of an electrolysis cell is optimized. The flow is much more uniform and the design now combines uniform flow distribution and mechanical stability.*

Developing and applying the software cashocs as part of his doctoral thesis was an eye-opening experience for Sebastian Blauth, as the software automates tedious and error-prone manual calculations. "In my thesis, I looked at chemical reactors, or more precisely, distribution structures in electrolysis cells that break down water molecules to produce hydrogen," he explains. "My task was to improve the water distribution to increase the efficiency of the cell."

## Software Tool Provides Design Suggestions

Blauth investigated how to change the shape of the reactor in order to improve the process. The decisive factor here is often that special conditions must be present in the flow components, such as a uniform flow distribution or a low pressure loss. The software cashocs enables the shape optimization of such components and systems for industrially relevant problems. Thanks to automation with cashocs, even complex problems can be solved in a very short development time and new designs can be generated.

## Leap From Science to Application

The software is currently primarily used in fluid dynamics, where the focus is on improving flow components. "Until now, this type of optimization was primarily an academic issue," says Blauth. With the development of a software solution, the leap into specific applications is now taking place: "Using manual calculations was enormously time-consuming and error-prone. Until now, it simply wasn't practicable for industry to go to this immense effort." His research results are now helping to change this and herald the transfer into practice.

**www.itwm.fraunhofer.de/cashocs-en**

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# Customized Inspection Solutions for the Industry

**Industrial inspection systems must be designed for increasingly versatile, rapidly changing products. At the same time, the complexity of surfaces and materials is increasing. The "Image Processing" department develops individual systems and also relies on artificial intelligence (AI). An interview with department head Markus Rauhut.**

### Industrial inspection has been the focus of the "Image Processing" department for many years. What do you offer companies?

**Rauhut:** We build customized optical surface inspection systems that we integrate directly into production systems. In doing so, we do not see ourselves as competitors to the industry, but complement it where no solution is yet available on the market.

In cooperation with the "System Analysis, Prognosis and Control" department of our institute, we can go one step further and determine the causes of quality deviations directly at the customer's premises. For example, why a particular defect occurs particularly frequently and what measures can be taken in production to prevent or mitigate this.

### Why do you develop individual solutions and not rely on existing ones?

**Rauhut:** There are a large number of inspection systems that can be used directly for specific applications. In Germany in particular, however, the variation in production facilities is so great that customized systems often make more sense. Depending on the type of production and product, the potential defects that can occur vary greatly. In addition, many of our customers want to know why and how a fault has occurred so that they can make any necessary adjustments to production.

### "Image Processing" was one of the first departments at the Fraunhofer ITWM to use AI. How has work changed as a result of AI?

**Rauhut:** The project process for the development of industrial optical inspection systems in particular has changed significantly. Before the use of AI, our team used relatively little data to develop algorithms that find or classify defects. The difference to an AI process is that the developer specifies which properties describe a typical defect. For example, that a scratch is an elongated structure in the image. These properties are explicitly programmed.

In contrast, an AI process requires a great deal of data with which the AI is trained. For projects, this means that the first step must be to collect and curate as much data as possible directly from production using the sensors provided for this purpose. This is why a pure recording system is installed directly in production as quickly as possible.

**The use of AI therefore appears to be quite complex. Do you think the advantages outweigh the disadvantages?**

**Rauhut:** The short answer is: AI processes simply work better than any tools we have had to date. Technically, this means that the detection rate is much higher and the false positive rate is much lower. Furthermore, we can now inspect surfaces that are very difficult or impossible to inspect using conventional image processing. These are primarily highly textured surfaces such as wood veneers or cast parts.

**What other changes do you expect the use of AI to bring to your field of research and therefore also to your department?**

**Rauhut:** AI processes have already replaced many older algorithms and will continue to do so. However, due to the black box nature of AI systems, even more algorithms will be needed in the future to ensure the safety of AI. Especially in safety-relevant applications, such as in the rail or aviation industry, it is crucial to reliably detect defects. We are currently working on new algorithms, particularly in the field of data analysis, to meet these requirements. For us as mathematicians, this means that we have to continuously develop new algorithms and models in order to really use AI reliably in production.

**Is there a success story that shows why this approach is effective?**

**Rauhut:** Yes, we implemented an inspection system for a customer who had previously installed a standard system. The standard system was very good, but completely unsuitable for the company's requirements. In the end, they chose us because we are not only familiar with AI processes, but also master traditional image processing.

**www.itwm.fraunhofer.de/en/bv**

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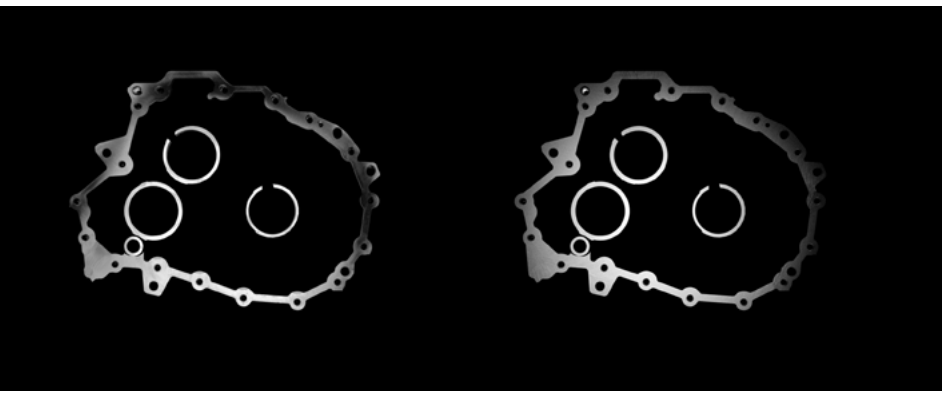
# Synthetic Data: How Realistic Would You Like It to Be?

**"Artificial intelligence (AI) offers solutions for demanding image processing tasks such as virtual inspection. To train an AI, you need data with ground truth, in this case images in 2D and 3D – and these are often in short supply. A team from our Image Processing department has developed its own mathematical models to create an optimal and reliable data basis.**



*A real image from a production inspection system and a synthetic image generated using ITWM technology.*

There are numerous challenges in image processing where the necessary training data for an AI is not available: In optical quality control in production, every type of defect must be detected. However, the less frequently a defect occurs, the more difficult it is to collect images containing this defect. Typical AI models must have seen each defect thousands of times in order to recognize it reliably.

## Create the Data You Need

"Many people generate synthetic data, but most of them recreate what they need," explains Dr. Petra Gospodnetić. "We use mathematical models for this. This makes everything controllable: we create exactly what we need and can adapt it to different industries." The data is generated on the basis of stochastic geometry models, allowing variable structures to be generated in almost any size and quantity.

A team from various disciplines – mathematics, physics and computer science – contributed their respective expertise. "Our methodology for generating synthetic data is unique," emphasizes Dr. Katja Schladitz. "Many people also use one AI to train another. This can be dangerous, especially in production." Another advantage of AI trained using the generated data is that it is more objective and reliable than humans when it comes to quality control. "An AI doesn't get tired, it doesn't get distracted or blink at the crucial moment."

## Scalable Degree of Reality

Another advantage of synthetic data: Their degree of realism can be adapted to the needs of the respective production. The scientists and their team are conducting intensive research into how realistic the structures and images need to be in order to be representative and which properties of the synthetic data are crucial for the success of AI training.

**www.itwm.fraunhofer.de/pr-bmw-detection-en**

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# New Software Solution for the Chemical Industry

**A team from the "Optimization – Technical Processes" and "Transport Processes" departments has jointly developed a software package for the simulation and optimization of batch distillation processes at industrial companies – inspired by district heating simulation. This benefits the production of highly specialized chemicals or medicines.**


© freepik

"Batch distillation makes it possible, for example, to produce special pharmaceuticals in small quantities relatively quickly or to carry out tests within a manageable period of time," says Prof. Dr. Michael Bortz. "In sectors such as the pharmaceutical industry or fine chemicals, there are substances that have to be produced continuously in the same quality. A batch is more of a special edition: specific properties are required for special cases."

Batch distillation processes are therefore very dynamic. This means that the material compositions, temperatures, pressures and flows in the distillation column are time-dependent and the process is inherently non-stationary. A dynamic simulation model is required to adequately support this dynamic operational management.

## Software Simulates Various Use Cases

The tool, which is already in use at companies, can weigh up costs and benefits in particular, for example how long it will take and how expensive it will be if a chemical is to be particularly pure. The underlying model consists of a set of non-linear algebraic and differential equations. These represent the degrees of freedom and quality criteria that exist in reality in order to optimize the batch reactions: How must substances be added? What happens if other additives are used? What does an optimal reflux trajectory look like? "We think backwards and define the path starting from the target," says Bortz. "Our software products make it possible to interactively discover potential for improvement and help to find the optimum solution."

## Bringing Together Expertise From Our Own Ranks

The impetus for the software package is also exciting: discussions with the "Transport Processes" department about their solutions for district heating simulation gave rise to the idea of adapting their algorithms for batch distillation. "Both departments actively worked on the project result and shared their expertise for the project," reports Bortz.

**www.itwm.fraunhofer.de/csdistillation**

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# We Are the Fraunhofer ITWM

## Department “Image Processing”

### Mathematical Models and Image Analysis Algorithms for Industry

The “Image Processing” department develops mathematical models and image analysis algorithms and converts these into industrial software, primarily for demanding surface inspections in production and for the analysis of microstructures.

The software required for image processing and analysis and system integration is developed in-house. Some software products have been maintained and marketed for more than 15 years. The available range of methods is constantly being expanded and improved.

Since 2016, domain-specific machine learning algorithms have also been developed, as well as methods for training them in a comprehensible, efficient and consistent manner. Optical and light microscopic images are generated in our own laboratory, 3D images and time series of 3D images using the department’s computer tomograph.

The scientific foundations include mathematical morphology, discrete geometry and topology, stochastic geometry, computer graphics and quantum computing.

**www.itwm.fraunhofer.de/en/bv**

# Department “Financial Mathematics”

### Methodological Competence in Financial Mathematics, Stochastics and Data Science

The “Financial Mathematics” department focuses on the business areas “Life Insurance”, “Settlement Audit” and “Flexible Loads in the Energy Industry”.

Its applications range from the classification of pension products and the support of digital business processes to risk controlling in the energy sector. The business areas are strengthened by a flexible modular system of research focuses.

Currently, this includes the modules of financial and actuarial mathematics, statistics, Machine Learning (ML), data science, stochastic simulation, time series analysis and quantum computing. In addition to long-standing research focuses, a strong network of national and international partners and collaborations has been established, particularly in the still young research area of quantum computing.

The department also includes the junior research group “Decision support for business processes using new AI methods”.

**www.itwm.fraunhofer.de/en/fm**

# Division “High Performance Computing”

### Innovation, Disruption and Holistic Thinking in the World of Distributed Computing

Simulations and calculations are the basis for many industrial and scientific applications. Increasingly stringent requirements mean that the complexity of hardware and software is constantly growing. This development requires new methods and solutions for high-performance computing and forms the scientific basis of the department.

The distribution of data and the communication of computing units play an important role in the efficient and high-performance execution of highly parallel calculations. Efficiency also plays a central role in the development of new processor and system architectures, in the development of tools and applications for quantum and neuromorphic computing, in finding optimized models for artificial intelligence and in the control of energy flows in the field of renewable energies.

The department is also the central point of contact for the optimization of algorithms in various domains and in particular in the field of seismic data processing.

**www.itwm.fraunhofer.de/en/hpc**

# Department "Materialcharacterization and Testing"

### Seeing through With Millimeter, Terahertz and Optical Waves

The "Materialcharacterization and Testing" (MC) department develops and builds industrial-grade systems for non-destructive testing using electromagnetic waves in the spectral range from visible light to radar frequencies. The necessary laser sources, electronic circuits, emitters and detectors, particularly in the terahertz and radar range, are partly developed and improved in-house. The necessary scientific foundations include lithographic know-how (2D and 3D structuring), in-depth knowledge of linear and non-linear optics, laser physics and quantum optics.

The department is an international leader in the development of model-based evaluation algorithms for layer thickness measurement and tomography with a priori information, which allow the reliable detection of defects in the volume. With the realization of the principle of measurement with undetected photons in the terahertz range, the department has broken new scientific ground, which in the long term will make it possible to dispense with the detection of terahertz waves in general. With the development of the first laser-based optical FMCW radar, the thickness measurement of cathode and anode layers in battery production has also been achieved for the first time.

**www.itwm.fraunhofer.de/en/mc**

# Division "Mathematics for Vehicle Engineering"

### Simulation-Supported Development and Production Optimization

The "Mathematics for Vehicle Engineering" (MF) division is divided into two departments, "Dynamics, Loads and Environmental Data" (DLU) and "Mathematics for the Digital Factory" (MDF), as well as the Tire Simulation project group and the MF Technical Center cross-sectional unit, which is responsible for testing and measurement technology.

The "DLU" department develops methods and tools for system simulation, taking into account environmental data and usage variability. In particular, the vehicle development attributes of operational stability, reliability, energy efficiency and ADAS/AD as well as the development of sustainable mobility solutions are addressed. In line with this, there is research and development in the area of vehicle-environment-human interaction and tire modeling and simulation. The "MDF" department bundles the activities for the development of software tools for virtual product development and creation.

**www.itwm.fraunhofer.de/en/mf**

# Division “Optimization”

### Interactive Decision Support Based on Models and Data

The “Optimization” (OPT) division comprises the three departments “Optimization in the Life Sciences” (OPT-LS), “Optimization – Operations Research” (OPT-OR) and “Optimization – Technical Processes” (OPT-TP). “OPT-LS” develops and provides innovative and customized mathematical-methodological approaches as well as software solutions and services for various fields of application in medicine, healthcare and social services, medical and bioprocess engineering.

“OPT-OR” develops individual (software) solutions for strategic, tactical and organizational issues in production and process planning with the declared aim of providing decision-makers from industry and society with tools for weighing up conflicting planning objectives.

“OPT-TP” deals with multi-criteria decision support based on modeling, simulation and optimization of technical processes in various manufacturing industries.

**www.itwm.fraunhofer.de/en/opt**

# Department “Flow and Material Simulation”

### Industrially Applicable Multi-Scale Simulation and Customized Software Solutions

The “Flow and Material Simulation” (SMS) department develops models, efficient solution methods and software for industrial problems of fluid and solid mechanics, heat conduction and electrochemistry, including fluid-structure interaction, reaction-convection-diffusion and multiphysics tasks, in heterogeneous media.

The “SMS” department thus offers expert research and development support in modelling, simulating and optimizing the production, function and application behaviour of porous and composite materials. It creates simulation-based digital twins down to the material level in order to sustainably improve your production processes (infiltration, foaming, pressing, etc.) and your product development (e.g. filters, batteries, textiles, lightweight components) as well as to quantitatively evaluate raw material and energy balances.

**www.itwm.fraunhofer.de/en/sms**

# Department "System Analysis, Prognosis and Control"

### Analysis and Prediction of Complex System and Process Behavior

The "SYS" department develops mathematical methods for the resource-optimized real-time operation of components, drives and systems. Areas of application include the energy sector and industrial production facilities in plant and mechanical engineering. The scientific issues include the development of real-time, multivariate signal analysis methods and ML algorithms, in particular deep neural networks, as well as their hardware connection and integration for condition monitoring and predictive maintenance.

In addition, "SYS" develops model- and data-based methods for the predictive control of drives and production systems with the target variables of quality, quantity and use of resources. The scientific challenges here lie in low data availability, data and information gaps and complex process diversity.

**www.itwm.fraunhofer.de/en/sys**

# Department "Transport Processes"

### Mathematical Modelling, Simulation and Optimization of Transport Processes

The core competence of the "Transport Processes" department is the mathematical modeling of complex industrial problems and the development of efficient algorithms for their numerical solution. The problems are located in a technical and scientific context (fluid dynamics, heat and radiation transport, structural mechanics, etc.) and, from a mathematical point of view, lead to differential equations, which in many cases can be characterized as transport equations. For years, the department has continuously pursued two scientific focal points with strong unique selling points: the mathematical modelling, simulation and optimization of the dynamics of threads, fibres and filaments and the development of the grid-free continuum mechanical simulator MESHFREE. In addition, new research topics are constantly being taken up with university partners.

One example is the transient simulation, optimization and control of energy and supply networks. Fluid dynamic shape optimization is an important topic for the future and one in which we have already built up considerable expertise.

**www.itwm.fraunhofer.de/en/tv**

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