Fraunhofer
SCAI

Fraunhofer Institute for Algorithms and Scientific Computing SCAI

Annual Report 2022 | 2023

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Preface

Dear readers,

The world has changed rapidly in recent years. Our society faces tremendous challenges, such as the Corona pandemic, the war in Ukraine, climate change, and the energy crisis. These multi-crises also have a substantial impact on the Fraunhofer-Gesellschaft and Fraunhofer SCAI. Our business environment has been and will be tense. High inflation is placing an additional burden on the economy.

Despite challenging economic circumstances, SCAI has seen prosperous years and an exceptionally successful 2022. In 2021, approximately 52,9 percent of the institute's operating budget came from industrial revenues, mainly arising from software licenses. This result ranked SCAI at the top of the Fraunhofer ICT Group. Last year, the share of industrial revenues reached 60 percent – a record in SCAI's history. This excellent financial performance is due to our employees' high scientific expertise and dedication, most of whom managed the business from their home offices. I would also like to thank our spin-off company, scapos AG, the worldwide distributor of our software solutions.

Although the Corona protection measures have expired, COVID-19 still poses a severe threat to the world. In research, therefore, the struggle against SARS-CoV-2 continues. To address a wide range of pandemic aspects, our *Bioinformatics* department has developed a project portfolio in which the cooperation between Fraunhofer SCAI and the World Health Organization (WHO) deserves special mention. The challenge in this project is to create a 'web of data' using semantic web technologies to better prepare for future pandemics.

Several research projects of Fraunhofer SCAI are addressing the energy transition. For example, SCAI and its partners analyzed the effects of the Russian gas cutoff in 2022 and published the results in July. For the first time, an investigation was available that examined the impact of a supply stop by modeling the actual physical characteristics and properties of the gas network. SCAI's Multiphysical Network Simulator (MYNTS) has been used to simulate the European gas network. In the hydrogen flagship project TransHyDE, funded by the German Federal Ministry of Education and Research, the software is used for modeling a future hydrogen network.

The SONAR project is another vital contribution to the CO_2-neutral transformation of the economy. Together with partners from the European Union and Australia, SCAI is working on novel techniques for redox flow batteries. Flow batteries are particularly suited to store temporary surpluses of electrical energy from renewable sources. The European Commission funds the project.

Finally, we are very grateful to our Advisory Board for providing valuable guidance and to our customers and partners for continued support and fruitful cooperation.

I cordially invite you to read on and learn more about our research.

Prof. Dr. Michael Griebel

Advisory Board meeting in May 2022: Dr. Ulrich Leiner, Dr. Jan Hamaekers, Dr. Richard Trethewey, Dr. Anton Schüller, Dr. Thomas Soddemann, Klaus Wolf, Prof. Dr. Babette Dellen, Victoria Appelbe, Prof. Dr. Martin Hofmann-Apitius, Prof. Dr. Petra Mutzel, Dr. Johannes Landes, Dr. Daniel Oeltz, André Gemünd, Dr. Bram Metsch, Prof. Dr. Hans-Joachim Bungartz, Prof. Dr. Jochen Garcke, Prof. Dr. Michael Griebel, Christiane Stoll, Prof. Dr. Marc Alexander Schweitzer, Prof. Dr. Reinhard Klein (from left)

Profile

Director
Prof. Dr. Michael Griebel
Prof. Dr. Marc Alexander Schweitzer (Deputy)

Business Areas

Bioinformatics	Prof. Dr. Martin Hofmann-Apitius
Optimization	Dr. Ralf Heckmann
Multiphysics	Klaus Wolf
Fast Solvers	Dr. Hans-Joachim Plum
High Performance Computing	Dr. Thomas Soddemann
Network Evaluation Technologies	Dr. Mehrnaz Anvari
Virtual Material Design	Dr. Jan Hamaekers
Numerical Data-Driven Prediction	Prof. Dr. Jochen Garcke
Meshfree Multiscale Methods	Prof. Dr. Marc Alexander Schweitzer
Computational Finance	Dr. Daniel Oeltz

Central Services

Planning and Controlling	Christiane Stoll
Marketing and Communications	Michael Krapp
IT-Services	André Gemünd

Branch Lab Bonn
Dr. Jan Hamaekers

Advisory Board
Dr. Bernhard Thomas, chairman, im.pulse, Köln
Victoria Appelbe, Stadt Bonn
Prof. Dr. Babette Dellen, Hochschule Koblenz, RheinAhrCampus Remagen,
Dr. Bernd Eck, BASF SE, Ludwigshafen am Rhein
Prof. Dr. Reinhard Klein, Universität Bonn
Prof. Dr. Petra Mutzel, Universität Bonn
Prof. Dr. Petra Ritter, Charité – Universitätsmedizin, Berlin

Spin-offs
adiutaByte GmbH, Sankt Augustin
BioSolveIT GmbH, Sankt Augustin
Causality Biomodels Ltd., Kalamassery, Cochin, Indien
scapos AG, Sankt Augustin
SIDACT GmbH, Sankt Augustin

Facts and Figures

Financing and expenditure

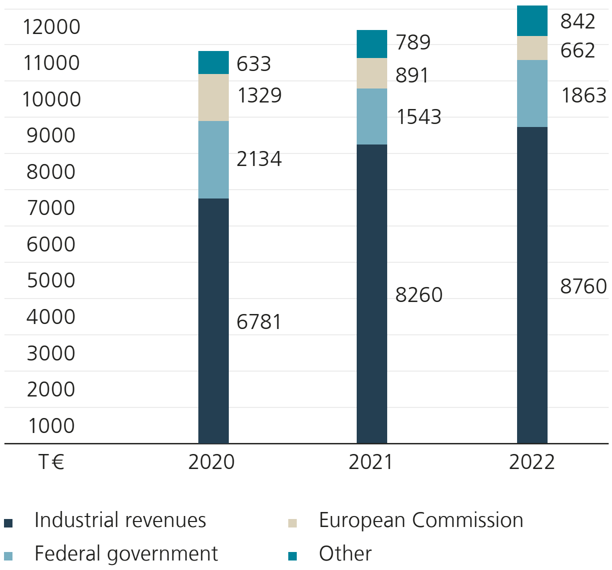
Despite the difficult economic situation in the markets in which Fraunhofer SCAI operates, revenues have increased in recent years. In 2021, the share of industrial revenues in the operating budget had risen from 45.3 to 52.9 percent. Last year, it reached a new record of 60 percent, marking the highest score in SCAI's history. As in previous years, the main reason for the increased industrial revenues totaling 8.8 million euros (2021: 8.3 million euros) is the revenue from licensing the successful software solutions *PackAssistant* (optimized packing of components in transport containers), *AutoNester* (optimized placement of markers on fabric and other material), *MpCCI* (enabling co-simulation with industrial simulation codes) and *SAMG* (library for the highly efficient numerical solution of large sparse systems of equations).

Fraunhofer SCAI's operating budget decreased from 16 to 15 million euros in 2022. Personnel costs declined by about 0.6 million euros, and there were also substantial savings in material costs. During the same period, the institute's overall funding ratio improved by almost ten percent to 83.1 percent (previous year: 73.6 percent).

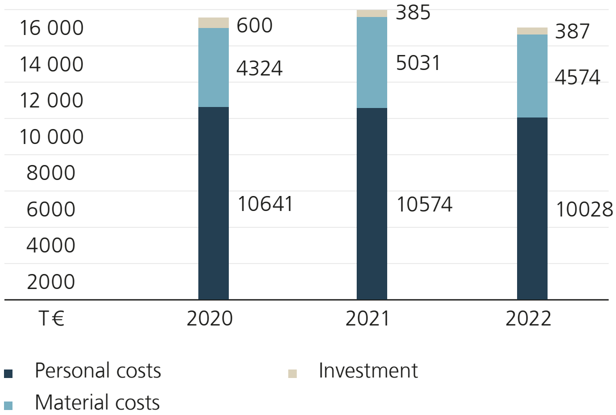
Human resources

At the end of 2022, SCAI's staff dropped by ten employees compared to the previous year. A planned headcount consolidation for 2021 and 2022 followed the significant personnel growth in 2019 and 2020. Meanwhile, the shortage of qualified specialists in the labor market leads to delays and even problems in filling vacant positions.

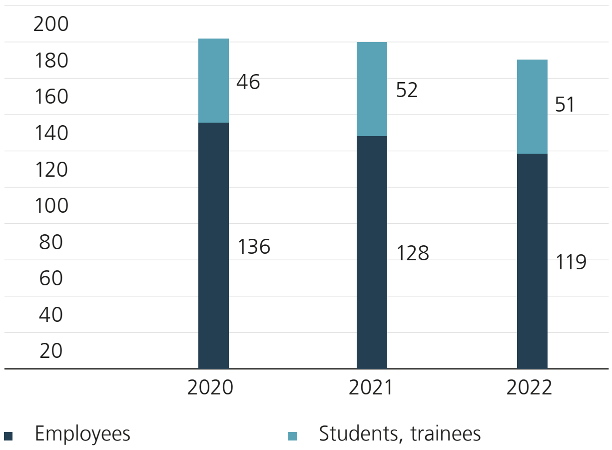
Income



Expenditure



Human resources



Equal Opportunities and Diversity

Diversity is an essential premise for the self-image and prospects of Fraunhofer SCAI

Fraunhofer SCAI highly values diversity in its workforce. Mixed teams are more creative and better at problem-solving. Diversity management aims to create a working environment where all employees can participate equally. Equal opportunities for all employees regardless of ethnic origin, religion, world view, gender, sexual identity, disability, or age is an essential premise for the self-image and prospects of SCAI. The equal rights officer, Dr. Vanessa Lage-Rupprecht, elected by the employees, supports the institute's management in pursuing these goals.

Dr. Vanessa Lage-Rupprecht, Bioinformatics department, is the institute's equal rights officer.

Meeting the demands of childcare and work can be challenging. Fraunhofer SCAI offers assistance for families.

Flexible working hours and comprehensive support services help to balance work and private life

The institute promotes balancing work, family, and private life through flexible working hours. In addition to emergency childcare, homecare/eldercare, and life coaching services provided by pme Familienservice, Fraunhofer offers various information and training courses. Other services at the Fraunhofer Institute Center Schloss Birlinghoven include all-day holiday care during the summer school vacations and play and childcare materials provided for children brought into the office. Workshops and courses on health support and disease prevention complete the offerings.

The TALENTA development program is a career booster for women in science and management

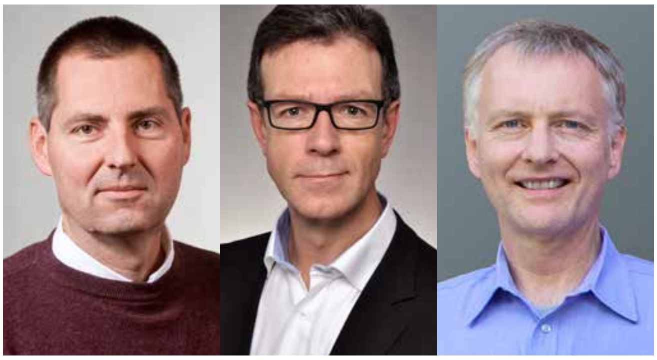
Fraunhofer SCAI supports and takes advantage of the opportunities offered by the Fraunhofer-internal support and development program TALENTA for female scientists. TALENTA focuses on the individual career development of female participants and qualifies them for leadership positions. Dr. Daniela Steffes-lai is promoted in TALENTA speed-up, a program tailored to accelerate the careers of professionally experienced female scientists. Sophia Krix participates in TALENTA start, which offers advice and specific qualification opportunities to women starting their scientific careers.

Dr. Daniela Steffes-lai (l.), Numerical Data-Driven Prediction department, and Sophia Krix, Bioinformatics department

SCAIlights

Fraunhofer appoints a new Advisory Board member and bids farewell to former members

2022/2023 Prof. Dr. Hans-Joachim Bungartz, Technical University of Munich, and Dr. Richard Trethewey, Vice President of Data and Artificial Intelligence Strategy Lead at BASF SE in Ludwigshafen, have left the Advisory Board of Fraunhofer SCAI in 2022. Bungartz has been a board member for ten years and Trethewey for six. Both have shown extraordinary commitment to the institute's progress and have intensively advised the management. Dr. Bernd Eck, Vice President of Scientific Modeling at BASF SE, has been appointed as a new Advisory Board member.



Prof. Dr. Hans-Joachim Bungartz, TU Munich, Dr. Bernd Eck, and Dr. Richard Trethewey, both from BASF SE (from left)

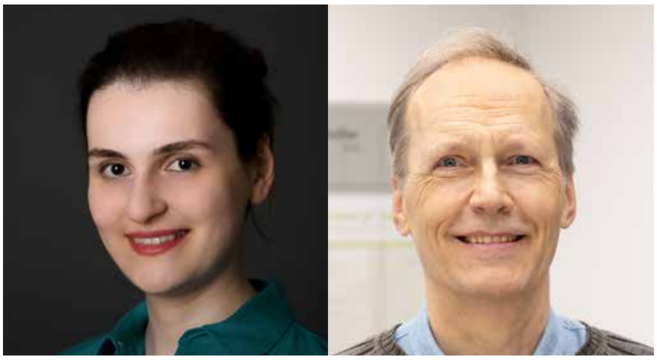
Engaged in research and teaching at b-it: university professors Dr. Martin Hofmann-Apitius (l.) and Dr. Holger Fröhlich

SCAI has been committed to research and teaching at the b-it in Bonn for 20 years

November 2022 The Bonn-Aachen International Center for Information Technology (b-it) in Bonn celebrated its 20th anniversary in November 2022. The b-it is a joint institution of the Rheinische Friedrich-Wilhelms-Universität Bonn, the Rheinisch-Westfälische Technische Hochschule Aachen, the Hochschule Bonn-Rhein Sieg, and Fraunhofer. SCAI's *Bioinformatics* department is involved in the international master's program in Life Science Informatics. The head of the department, Prof. Dr. Martin Hofmann-Apitius, and his deputy, Prof. Dr. Holger Fröhlich, also lead working groups at the b-it.

Anvari succeeds Klaaßen as head of the business area Network Evaluation Technologies

January 2023 Dr. Mehrnaz Anvari is the new head of the business area *Network Evaluation Technologies* of Fraunhofer SCAI. She follows Dr. Bernhard Klaaßen, who now works at the Fraunhofer Research Institution for Energy Infrastructures and Geothermal Systems IEG. Anvari joined SCAI from the Potsdam Institute for Climate Impact Research (PIK). In 2016, the physicist received her Ph.D. from the Carl-von-Ossietzky University Oldenburg. Her research interests include power grids and renewable energy, stochastic thermodynamics, and extreme weather and climate events.

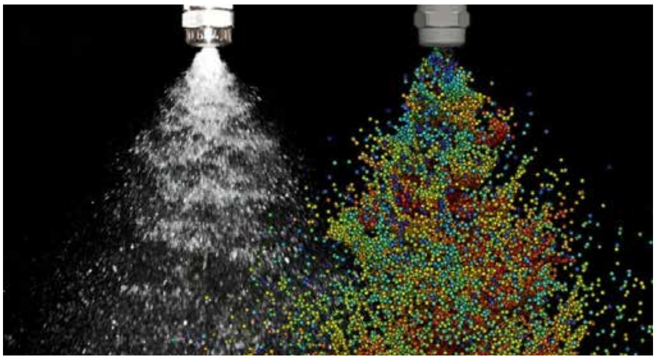


The research topics of Dr. Mehrnaz Anvari and Dr. Bernhard Klaaßen include central aspects of the energy transition.

SCAIlights

Innovative process simulation for the food industry with the software MESHFREE

April 2022 Whether cleaning, stirring, kneading, or injection processes – *MESHFREE* uses a grid-free approach to reliably simulate food technology processes. The Fraunhofer Institutes for Industrial Mathematics ITWM and SCAI have demonstrated the jointly developed software at the *Anuga Food-Tec* trade fair in Cologne from April 26 to 29. In this partnership, the business area *Meshfree Multiscale Methods* of SCAI is responsible for the highly efficient solution of large systems of equations and performance optimization. ITWM develops the underlying numerical methods for the simulation of physical processes.



A spraying full-cone nozzle: left in the experiment, right in the computational simulation

Dr. Thomas Soddemann (SCAI) explains his exhibit to visitors, including Victoria Appelbe, SCAI's Advisory Board member.

Research projects with a focus on sustainability attract visitors to the Bonn Science Night

Mai 2022 "Sustainable research" was the motto of the 13th Bonn Science Night from May 12 to 13. Fraunhofer SCAI presented two exhibits on Bonn's Münsterplatz. The first exhibit explained how better batteries can be developed to store electricity from renewable energy sources. A central research aspect is a computer-aided search for suitable organic electroactive materials for redox flow batteries. The second exhibit used the example of a brewery to demonstrate how costs and energy can be saved through efficient production planning with the help of innovative optimization algorithms.

The MpCCI toolbox supports engineers in creating and assembling customized digital twins

May/June 2022 The Hannover Messe 2022 was a hybrid event from May 30 to June 2. The institute presented its research work on-site in Hannover and at a digital booth. The business area *Multiphysics* of Fraunhofer SCAI showed digital twin solutions for industrial production. The *MpCCI* software toolbox supports engineers in creating and assembling customized digital twins. The goal is better interoperability and smarter engineering workflows. An exhibit from the business area *High-Performance Computing* demonstrated the benefits of material requirements and production planning.

Priyanka Gulati, business area Multiphysics, presents the benefits of interoperability in computer-aided engineering.

SCAIlights

The MYNTS software is used to plan and optimize gas and hydrogen transportation networks.

June 2022 The gas shortage in Germany was one of the main topics at the *E-world energy & water* in Essen from June 21 to 23. SCAI presented MYNTS (Multiphysical Network Simulator), a software that is used by numerous companies. It plans and optimizes networks for gas, electricity, and water. Another exhibit focused on the optimal management and hedging of portfolios of physical assets due to the decentralization of power generation. Dr. Daniel Oeltz, head of the business area *Computational Finance*, advises companies on solving complex optimization problems.

Dr. Bernhard Klaaßen, business area Network Evaluation Technologies , in a discussion at the E-world.

Although students could not attend the summer school on-site at the institute, the course was quickly fully booked.

The SCAI Summer School fascinated students with practical applications of mathematics

July 2022 Due to the Corona pandemic, the 2022 SCAI Summer School was held as an online seminar for the second time since 2021. The math workshop led by Dr. Anton Schüller, *Marketing and Communications group*, quickly filled up. Students in grades 9 to 13 learned modern mathematical methods for solving practical problems in this two-week event. Examples included weather forecasting, traffic simulation, and the mathematical approaches behind the mp3 digital audio coding format. The students also took their first steps with the programming language Python.

A comprehensive program of lectures provided exciting insights into applied research

March 2023 Working at Fraunhofer SCAI offers interesting research topics and numerous career opportunities. This was the experience of forty-two students from the Faculty of Mathematics, Computer Science, and Natural Sciences at the RWTH Aachen University. They visited the institute on March 28 and followed a full program of lectures, including a tour of SCAI's high-performance computing center. For example, Ingo Döpke, a computer scientist in the *Optimization* department, inspired the students with his lecture about developing SCAI's PackAssistant software.

Ingo Döpke, Optimization department, explained how SCAI developed the PackAssistant software.

Selected Software Solutions

PACK Assistant	**Optimized 3D packing design**	*PackAssistant* is a software for optimizing packaging configurations of identical parts in containers. With *PackAssistant*, the exact 3D arrangement of parts with complex shapes can be calculated and displayed already in the design phase. **www.packassistant.com**
AUTO NESTER-T automatic marker making	**Automatic marker creation**	The *AutoNester* software package optimizes the automatic placement of markers on fabrics, sheet metal, wood, and leather hides. By configuring the optimal nesting pattern, the software minimizes the amount of material waste. **www.scai.fraunhofer.de/en/autonester**
AUTO PANEL SIZER	**Reduction of material waste and minimization of manufacturing costs**	*AutoPanelSizer* determines cutting layouts for producing rectangular parts from rectangular stock material and minimizes waste, production times, and manufacturing costs. **www.scai.fraunhofer.de/en/autopanelsizer**
AUTO BAR SIZER	**Optimized cutting plans for the cutting of steel profiles**	*AutoBarSizer* determines optimized plans for cutting steel profiles and other bar materials into shorter parts. The generated solutions are characterized by a high degree of material utilization, and cutting losses are minimized. **www.scai.fraunhofer.de/en/autobarsizer**
CUT PLANNER automatic cut planning	**Automatic cut order planning in textile manufacturing**	*CutPlanner* is a software package used in textile manufacturing for automatically planning cut orders. CutPlanner takes a customer's order for a clothing item and creates a cut plan, including different sizes, fabric types, or colors. **www.scai.fraunhofer.de/en/cutplanner**
CUBO NESTER-C optimal 3D cutting	**Generation of optimized plans for guillotine cuts**	*CuboNester* optimizes the arrangement of cuboid parts in three dimensions. *CuboNester-C* is designed for cutting blocks of material, for example, from metal, marble, graphite, and foam. **www.scai.fraunhofer.de/en/cubonester**
CUBO NESTER-P optimal box packing	**Optimized arrangement of cuboid parts in boxes**	*CuboNester-P* optimizes packing, for example, of disassembled furniture elements into packages. The software is also perfect for online retail that involves ever-varying parts to be shipped. **www.scai.fraunhofer.de/en/cubonester**
SAMG	**Algebraic multigrid methods for systems**	*SAMG* is a software library for the highly efficient solution of large linear systems of equations. Such systems occur, e.g., in fluid and structural mechanics, oil reservoir and groundwater simulation, and process and device simulation. **www.scai.fraunhofer.de/en/samg**
MYNTS	**Simulation and optimization of energy transport networks**	*MYNTS* is a multiphysical network simulator that can be used to analyze and optimize electrical circuits, gas and energy transport, and water distribution. Users can program subnetworks and individual special elements. **www.scai.fraunhofer.de/en/mynts**

MpCCI CouplingEnvironment	**Coupling of simulation programs**	With the *MpCCI Coupling Environment*, it is possible to link simulation programs and thus solve multidisciplinary (multiphysics) problems. Companies use *MpCCI* to optimize the product design. **www.mpcci.de**
MpCCI Mapper	**Handling of data interpolation and conversion between codes**	The *MpCCI Mapper* handles data interpolation and conversion between codes in simulation workflows. In crash simulations, the production process of automotive components is considered, increasing the precision of crash calculations. **www.mpcci.de/mapper**
MpCCI FSIMapper	**Data interpolation between CFD- and FEM-meshes**	The *MpCCI FSIMapper* interpolates the data between different simulation meshes used for computational fluid dynamics (CFD) or finite element method (FEM) simulations, considering different mesh densities or orders. **www.mpcci.de/fsimapper**
PROMINER	**Identification of gene and protein names**	The software tool *ProMiner* identifies and normalizes the names of genes and proteins in scientific literature. This identification is based on automatically generated dictionaries. **www.scai.fraunhofer.de/en/prominer**
SCAIVIEW	**Knowledge discovery in life sciences**	*SCAIView* facilitates the rapid identification of aggregated information from large text sources. To this end, it integrates the results of ProMiner with the associated text and allows for semantic search. **www.scai.fraunhofer.de/en/scaiview**
Model Compare	**Comparison of similarly discretized finite element models**	*ModelCompare* is a plug-in for finite element (FE) pre- and postprocessing tools. It compares two similarly discretized FE models and identifies their differences in geometry (mesh), material, and thickness. **www.scai.fraunhofer.de/en/modelcompare**
SimCompare	**Towards automatic event detection for crash simulations**	*SimCompare* is a tool for detecting events – in this context, deviations, such as anomalies or strange variations in deformations – arising from similar simulation runs for crashworthiness analysis using FE models. **www.scai.fraunhofer.de/en/simcompare**
SimExplore	**Tool to support analysis of FEM or CFD simulations**	*SimExplore* is a software tool for explorative analysis and visualization of engineering data from FEM or CFD simulations. By applying non-linear dimension reduction, intrinsic patterns and similarities in the data can be identified. **www.scai.fraunhofer.de/en/simexplore**
TREMOLO X	**Numerical simulation in molecular dynamics**	*Tremolo-X* is a massively parallel software package for numerical simulation in molecular dynamics. It has been successfully used in various application fields, such as nanotechnology, materials science, biochemistry, and biophysics. **www.tremolo-x.com**
MESHFREE	**Powerful simulation tool for complex geometries and physics**	In simulation workflows, grid generation can be a time-consuming and, therefore, costly process. *MESHFREE*, follows a point cloud approach that allows engineers to analyze their product design without the deficiencies of meshes. **www.meshfree.eu**

scapos

Fraunhofer SCAI's software packages are distributed by scapos AG: **www.scapos.com**

Bioinformatics

The fight against SARS-CoV-2 has significantly impacted research since the spring of 2020, and it continued when the pandemic was over. 2022 has seen an impressive transfer of technology and problem-solving approaches developed initially for translational computational biomedicine in the neurodegeneration and neuropsychiatry context to the COVID-19 topic.

Research in the business area *Bioinformatics* of Fraunhofer SCAI represents the entire data-based value chain of translational biomedical research in academia and industry – from unstructured information mining to knowledge graph technologies and models that combine data and knowledge to actionable insights and decision support.

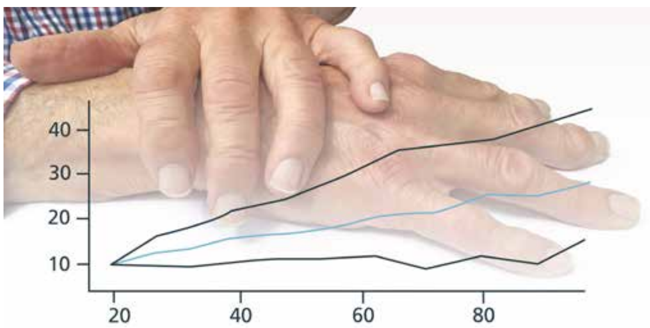
Automated processes extract biomedical knowledge from the specialist literature and make it available in a searchable, structured form. Semantic technologies help to represent complex biological and medical knowledge in rich, disease-specific knowledge graphs. Widely recognized are the knowledge assemblies representing the complex biology of neurodegenerative diseases such as Alzheimer's or Parkinson's in computable cause-and-effect models. These knowledge-based models are then used to interpret and model patient-related data and to make individualized predictions. This means an essential step towards precision medicine.

Tightly linked to this approach are data-driven models in drug development. Cause-and-effect models integrate knowledge about drug-target relationships in a disease-specific fashion. Big data architectures, modern machine learning methods, and artificial intelligence (AI) are used here.

When combining data and knowledge-driven approaches, things get particularly exciting in science and industrial applications. This work is attracting significant interest from pharmaceutical and biotechnology companies. The health research industry (biotech to pharma to eHealth) is investing massively in "AI in biomedicine." SCAI works closely with industrial partners, including small and medium-sized enterprises, to improve competitiveness by transferring knowledge and technology from academic research to industrial application. The collaborative research and development projects provide solutions for the pharmaceutical, biotech, and life sciences software industries.

COVID infections cause detectable changes in the human brain

SCAI has a clear profile in computational biomedicine in neurodegenerative diseases and neuropsychiatry. At first sight, research on COVID-19 does not fit in with this. But COVID-19 is still a major threat to the world. Though the pandemic is over, alarming signs and symptoms can be observed following SARS-CoV-2 infections, which may link the virus to the original research topic of the business area *Bioinformatics*: neurology. Recent studies suggest that COVID-19 infections cause detectable changes in the human brain and induce neuroinflammatory processes. Based on the internal Fraunhofer project COPERIMOplus, SCAI has developed an entire project portfolio that addresses various aspects of the pandemic. Among them is the German-French project



Neurodegenerative diseases affect million patients in Western societies – with an upward trend.

How can pandemics be detected earlier and people be warned of the dangers? Collaborating with the WHO, SCAI uses semantic web technologies to improve global pandemic preparedness.

AIOLOS. The research focuses on harnessing AI for pandemic preparedness and critical aspects of alerting and monitoring outbreaks. AIOLOS focuses on all types of communicable respiratory diseases. It is also a reference project for the *Health Emergency Preparedness and Response* initiative of the European Commission.

COPERIMOplus was also paving the way towards collaborating with the World Health Organization (WHO), particularly its *Pandemic Intelligence Hub* in Berlin. WHO started this Hub due to the COVID pandemic, aiming to increase pandemic preparedness globally. In a joint project, WHO and SCAI try to establish a "web of data" using semantic web technologies. The challenge is integrating information about geographic localization with information about virus genomes, mobility patterns, and food markets – the Rockefeller Foundation, New York, is funding the project.

While SCAI continues to contribute to COVID-19 and pandemic intelligence, it has strengthened its project portfolio in the core areas of neurodegeneration and neuropsychiatry. Examples include:

- ADIS: This project focuses on identifying biomarkers for earlier diagnosis of Alzheimer's disease. In particular, patients' blood and sleep patterns are being studied for this purpose. The results are analyzed using AI methods. The German Federal Ministry of Education and Research funds the project as part of the European Commission's Joint Programming Initiative (Neurodegenerative Disease Research). ADIS will run from July 2022 to June 2025.
- PSYCH-STRATA: One-third of patients with mental disorders develop resistance against drug therapy. The project will investigate the biological mechanisms underlying resistance. SCAI is developing AI/ML algorithms to predict the emergence of the mechanisms and feed them into a recommendation system for physicians. PSYCH-STRATA started in October 2022. The European Commission provides funding for five years.
- ParKInsonPredict: The joint research project of the Technische Universität Dresden and Fraunhofer SCAI aims to predict disease progression in Parkinson's disease. SCAI is contributing in-house developed AI algorithms to the project. The German Federal Ministry of Education and Research funds the project from September 2022 to February 2024.
- eBrain-Health: The project will integrate data at multiple levels into the ultimate simulation engine for the human brain, The Virtual Brain. SCAI brings to the project, coordinated by Charité in Berlin, its work in integrative data semantics, knowledge graphs, and AI methods for predicting drug effects. eBRAIN-Health started in July 2022 and will be funded by the European Commission for four years.

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(Deputy, Head of Group Software and Scientific Computing)
scai.fraunhofer.de/en/bio

Optimization

The efficient utilization of resources and associated cost savings are of fundamental importance in industry. When optimizing transport and storage capacities, material usage, or operating production facilities, complex optimization tasks have to be solved. Algorithms can bring about notable improvements by solving application problems and help to reduce costs, save energy, and reduce material consumption and environmental impact.

The business area *Optimization* of Fraunhofer SCAI has developed several sophisticated software solutions for optimization problems arising in many branches of industry, commerce, or transport. Typical areas of application are:

- **Production:** cutting and packing, machine scheduling, work schedules, material consumption
- **Logistics:** transport optimization, route planning, choice of location
- **Material flow:** utilization of transportation means, machines, and workers, cycle times of workpieces, inventory of buffers and intermediate storages, dimensions of resources
- **Planning:** optimal utilization of area and space

The CuboNester software can optimally arrange disassembled parts of furniture in outer packaging.

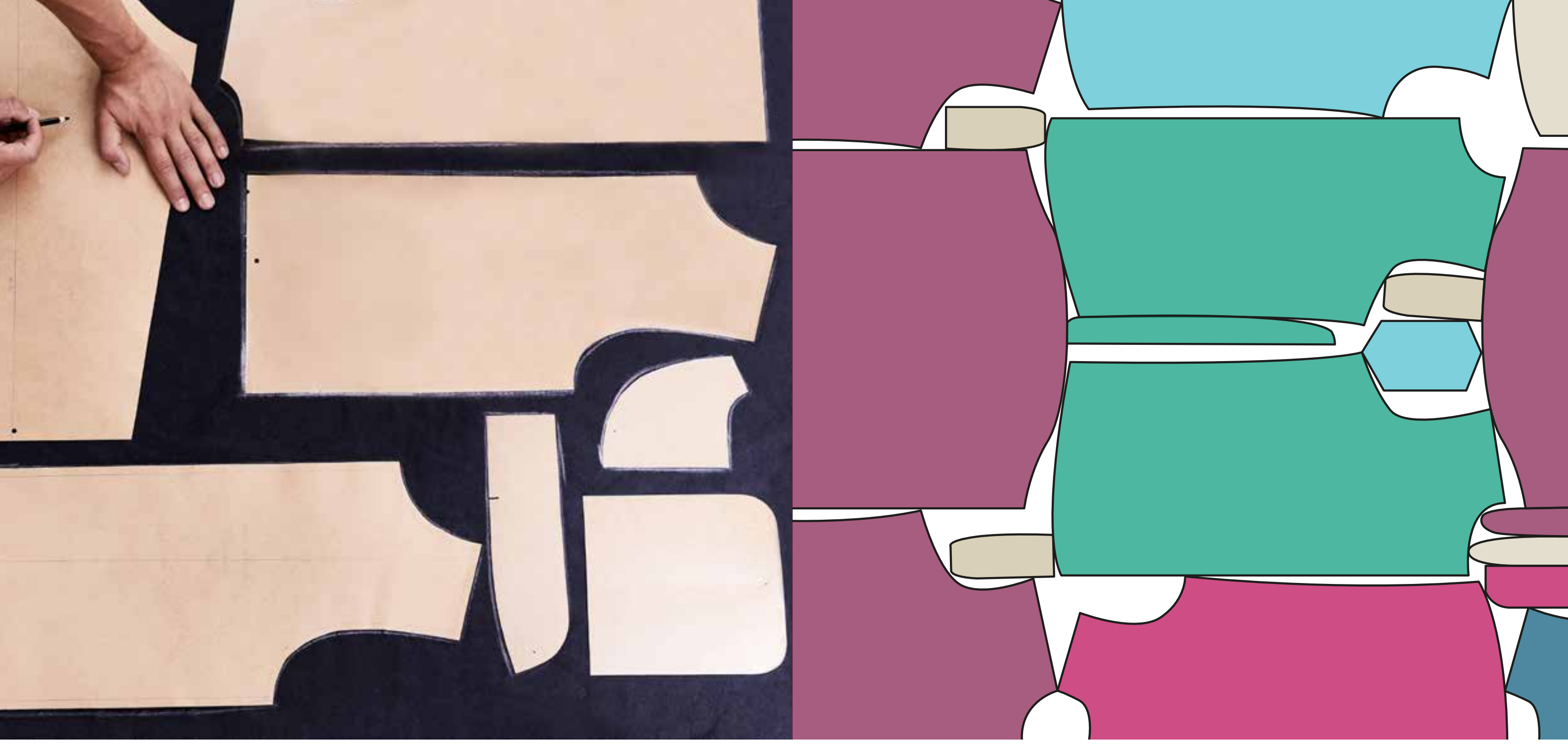
Optimized 3D packaging planning for increased transportation and storage capacity

Optimal container filling saves time and money regarding transportation and storage capacity. That's why experienced packaging planners sometimes fiddle around for a long time when packing parts with complex geometries. The world's leading software *PackAssistant* helps packaging planners find the ideal way to fill containers with identical parts in just a few minutes. *PackAssistant* facilitates packaging with rigid or flexible interlayers, with compartments or in stacks, as well as the simulation of bulk goods. The latest development is an automation module that allows data to be transferred to *PackAssistant* without user interaction. Companies can use it to automatically calculate a large number of containers and parts and determine critical key figures for their logistics.

Software solutions for optimized cutting patterns in 1D and 2D

AutoNester is a world-leading software package for the automatic creation of markers on fabrics, leather, sheet metal, wood, or other materials. *AutoNester* is capable of optimally nesting any quantity of parts in a very short time, minimizing material waste and respecting various constraints. The efficiency of the markers achieved by *AutoNester-T* is competitive to experienced human nesters.

Software companies can seamlessly integrate the *AutoNester* optimization kernel into their software (such as CAD systems). Recently, SCAI achieved significant speed increases and improved material utilization, as well as developing special algorithms for incremental nesting and regular cutting patterns.



Hand-nesting patterns to avoid offcuts can be a tedious puzzle. SCAI's AutoNester software does the job in a matter of seconds.

AutoPanelSizer determines optimized cutting plans for producing rectangular parts from rectangular stock, thus minimizing waste, manufacturing time, and manufacturing costs. The resulting plans can be produced with straight end-to-end cuts. This meets the constraints of common standard saw technologies, especially in the wood industry, but also in the glass, metal, and plastics industries. Fraunhofer SCAI continuously improves and enhances the software, most recently by adding support for tension-free cuts and robotic de-stacking.

AutoBarSizer generates optimized layouts for cutting steel profiles (for example, metal beams) and other bar materials into shorter pieces. The calculated solutions minimize cutting loss. Various parameters allow the planner to find a balance between material utilization and the additional organizational effort caused by the generation of reusable remnants. *AutoBarSizer* includes unique algorithms for minimizing cutting loss between miter parts. *AutoBarSizer* can be used for planning in rolling mills, by steel manufacturers, in the woodworking industry, and by manufacturers and processors of all types of bars.

Production planning in the textile industry saves material and reduces manufacturing costs

CutPlanner is a software package for automatic cut order planning in the textile manufacturing industry. Starting from a customer order for a garment in different sizes and fabrics, the tool creates a "Cut Plan," a compilation of sizes on cutting patterns. The number of layers necessary to fulfill the required order quantity is calculated for each of these cutting patterns. *CutPlanner* aims to save material and reduce manufacturing costs.

Perfect packings for online retail that involves ever varying parts to be shipped

CuboNester went live with a pilot customer in 2022 and early 2023. Like *PackAssistant*, *CuboNester* optimizes packings of parts in 3D but specializes in the case of cuboid or nearly cuboid parts. It can combine a large number of different parts in one arrangement. *CuboNester* thus optimally arranges boxes in one or more larger boxes. *CuboNester* is available in the variants *CuboNester-P* for packing and *CuboNester-C* for cutting.

CuboNester-P can be used, for example, to pack disassembled furniture or to pack heterogeneously filled shipping cartons in online retail. The calculation is based on configurable rules describing the allowed packages.

CuboNester-C addresses the cutting of metal blocks, e.g., metal, foam, or graphite. Only cutting plans that can be produced with straight, end-to-end (guillotine) cuts are generated. Among other constraints, *CuboNester-C* can consider reusable remnants, known defects in the material, preferred orientation of the material, and size limitations of the saw.

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Multiphysics

Designing sustainable products virtually and developing material-saving production procedures are key goals of the industry. For this purpose, simulation models from different engineering disciplines and tools from several software providers are combined in virtual engineering workflows. Multi-physical simulations consider the influence of manufacturing history on product properties and the interdependencies of physical effects.

One of the main focuses of the business area *Multiphysics* of Fraunhofer SCAI is the development of methods and software solutions for tasks in which engineers have to evaluate the effects of several physical disciplines. In the center of these developments stand the software packages *MpCCI CouplingEnvironment* and *MpCCI Mapper*. These tools provide a vendor-independent solution for simulation coupling and file-based data transfer and support commercial as well as research codes from numerous application disciplines. *MpCCI* provides an open application program interface (API) for connecting to internal or new commercial software codes.

SCAI collaborates with the leading vendors of commercial simulation programs as well as developers of university research codes. In further developing *MpCCI*, the institute cooperates with the world's leading software providers. The aim is to continuously improve the *MpCCI* interface and to develop coupling solutions for new application fields in multiphysics.

These applications include creating and using high-performance ceramics in gas turbines that can withstand significantly higher temperatures (joint project BonoKeram, funded by the German Federal Ministry of Economic Affairs and Climate Action) or developing a highly efficient electric motor for compressors in hydrogen fuel cells (Fraunhofer-internal project HABICHT).

Work with a methodological-algorithmic focus addresses the development of adaptive and self-learning coupling methods for fluid-structure interactions and the continuous development of robust methods for model correlation and data transfer in integrated process chains.

Broad range for multiphysics simulations in the industry

Multiphysics problems arise in numerous industrial applications:

- Aeroelasticity and mechanical engineering (aerodynamics in racing cars, aeroelastic effects in aeronautics, deformation of turbine blades)
- Vehicle and machine dynamics (extreme loads on particular components, dynamic behavior of elastic components under flow loading, for example, in valve flaps or hoses)
- Thermal stress analysis in vehicles, engines, or turbines (influence of hot flows on components)
- Thermal management in automotive engineering (combination of computational fluid dynamics with efficient radiation models, whole vehicle models)
- Electrical systems (dynamic loads and vibrations in electric motors, thermal stresses in electronic devices)
- Integrated process chains (complex and multi-step manufacturing processes)

Digital twins rely on interoperable data to unleash their full potential

Multiphysics phenomena are paramount to many industrial applications and production lines. They are directly related to efficient and safe production processes or the integrity of produced parts. As multiphysics simulations are embedded in process chains and design tasks, they are successively undergoing enormous automation and optimization. In this way, they are part of Digital Twins, i.e., virtual versions of real systems. The Digital Twins contain the properties of a given

Standardization of data interfaces in computer-aided engineering is essential for all industries where simulation processes are central to product and process design.

system and map the life cycle of a product or process in the form of data and metadata.

Artificial intelligence (AI) and machine learning (ML) methods are used for this data to be combined and used appropriately. With ML, it is possible, for example, to create fast-running data-based surrogate models, compare data from real measurements with the results of numerical calculations, and to intelligently evaluate uncertain simulation variables. This is crucial to merging and reusing data from heterogeneous sources and engineering disciplines. The digital twins can, therefore, only be created based on a robust and interoperable data backbone. This backbone includes the machine-interpretable semantic definition of the data, metadata, interfaces, and formats and describes them in machine-readable ontology models. Concrete implementations of such digital twins occur in the Fraunhofer internal project DigitalTPC, funded from 2019 to 2022, and PIONEER, funded by the European Commission from January 2023 to December 2025.

Unidirectional continuous fiber reinforced thermoplastic tape

VMAP standard improves data interoperability in virtual engineering workflows

The vendor-neutral standard for storing data in computer-aided engineering – VMAP – improves the interoperability of software packages in virtual engineering workflows. Various industry partners have already adopted their CAE workflows to the VMAP standard and could benefit significantly from saving time and implementation efforts. VMAP is the result of collaborative research within the European ITEA VMAP project. The project, coordinated by Fraunhofer SCAI, ran from August 2017 to October 2020 and was funded by the German Federal Ministry of Education and Research through the ITEA 3 cluster of the European research initiative EUREKA.

Applications stem from multi-stage manufacturing processes for components made of hybrid materials, injection molding of plastics, composite materials for lightweight vehicles, or integrative simulation and optimization workflows for blow-molded plastic parts. Due to the positive reception, 16 partners from industry, software development, and research founded the association *VMAP Standards Community e.V.* (www.vmap.eu.com) in December 2022 to disseminate the VMAP standard and to continue to develop it as required.

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Fast Solvers

Emerging hardware resources allow for more complex computer simulations in different industrial design processes. This further raises the quality of innovative products, reduces the need for experiments and prototypes, and improves product and process design cost-efficiency. The pre-requisites for such advanced simulations are efficient and robust linear solvers.

Linear solvers are the kernel of numerical simulations in various industrial applications. Such simulations transfer a physical model into a linear problem with a finite number of unknowns to approximate a solution that is not analytically known. These linear systems need to be solved frequently in a simulation: for each time step and, possibly, linearization step. Therefore, the linear solution is the most time-consuming part and requires fast and robust solver methods. This is especially true as emerging hardware developments allow for more complex physics at higher model resolutions. The linear systems feature millions and even billions of unknowns and structures that often enough prevent the robust application of textbook algorithms.

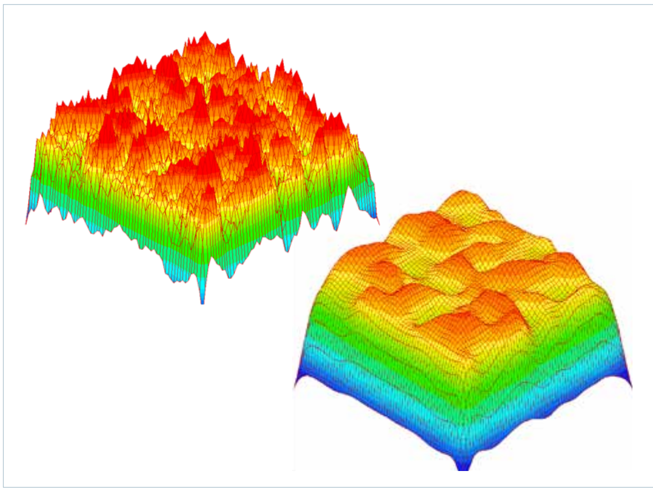
The business area *Fast Solvers* of Fraunhofer SCAI develops the library SAMG (Algebraic Multigrid for Systems). The software contains a vast variety of linear solver algorithms for the efficient and robust solution of linear systems. Hierarchical multigrid methods are used as the core strategy, offering numerical scalability: Solution efforts for doubling the number of unknowns only roughly double. This is unique to hierarchical methods and makes them superior to classical solver methods, particularly for large problem sizes.

SAMG is a toolbox for application-tailored solver solutions

SAMG provides not only a fixed solution algorithm but a versatile toolbox of solver ingredients that users can combine to create a solver strategy tailored to a specific kind of simulation. These components are implemented in a highly tuned manner and feature parallelization options that provide computational scalability.

SAMG is a licensable software solution applied in industrial and scientific practice to reduce computational time for increasingly complex simulations drastically. In several applications, it is the key to allowing for a certain level of complexity.

The fields of application of *SAMG* comprise flow processes such as fluid dynamics in the automotive and machinery industry, optimization processes in material design, geological simulations of oil reservoirs and groundwater processes in the energy and construction sector as well as the simulation of casting, plating, and molding processes. Moreover, *SAMG* is applied in circuit and battery aging simulations and various applications from structural mechanics in numerous applications from electronics to construction engineering to the automotive and machinery industry.



Visualization of the error smoothing procedure in AMG, which is fundamental for the overall hierarchical solution procedure.

Parallel scalability is a mandatory feature for large-scale workloads in computer-aided engineering, particularly for the linear solver, which is the inner core of simulations based on finite differences, finite elements, finite volumes, and meshfree approaches.

SAMG is developed further in close cooperation with the industrial praxis

Industrial and academic users and partners apply *SAMG* in all these fields. They all have various requirements for the software. Along with the different underlying physics, the structures of the linear systems may differ to some extent. Therefore, *SAMG* is further developed in close cooperation with its user base and project partners. World-leading experts support the development of both linear solvers and the underlying physics.

SCAI is offering more than just granting licenses for *SAMG*. In cooperation and evaluation projects, the *SAMG* team provides consultancy for the best, custom-tailored way of applying *SAMG*. These highly interdisciplinary projects consider a simulator's underlying physics and requirements and then assemble those parts of the solver toolbox within *SAMG* that best fit a certain kind of simulation. Once this initial layout is settled, it can be used in industrial practice without further intervention.

SAMG provides access to efficient solver algorithms without requiring expert knowledge of solvers

This consultancy provides the *SAMG* user easy access to highly efficient solver schemes. Moreover, it allows coping with more involved physics by exploiting algorithmic solutions beyond the textbook standard. No expert level is required for the simulation developer here. Still the entire linear solution process is encapsulated within the *SAMG* library. This easy access to various highly efficient solver options to form a best-fit solver strategy is unique to *SAMG*.

SAMG provides different software modules, bespoke for different kinds of simulations

This user-relation approach is also featured in the design of the *SAMG* library with different interoperable software modules. Among these, some are mainly developed for a specific field of application. Knowledge about the underlying physics allows for tailored, pre-defined solver strategies that are directly accessible:

- Reservoir simulations and geomechanics (*SAMG-Oil*)
- Groundwater processes (*SAMG-Modflow*)
- Elasticity problems from structural mechanics (*SAMG-Elasticity*)
- Constraint problems, e.g., from contact formulations (*SAMG-Constraints*)
- Meshfree simulations (*MESHFREE*)
- Highly parallel fluid dynamics simulations (*SAMG-MPP*)

These application-specific extensions are accompanied by modules that enhance the usability of *SAMG*:

- Particularly addressing the different physics in a coupled system model (*SAMG-Coupled*)
- Apply machine learning tools to optimize *SAMG* parameters (*SAMG-ASC*) on-the-fly

These modules are grouped around the core *SAMG* library that implements the various linear solver algorithms, all with different options for more complicated cases.

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High Performance Computing

Optimization problems arise in many fields of industry. For example, material requirements and production planning are essential for the efficient operation of manufacturing facilities. Modern mathematical methods allow tailor-made solutions to be engineered for specific customer problems. Quantum computing has the potential to solve particular optimization problems in seconds instead of days or years.

The research work in the business area *High-Performance Computing* of Fraunhofer SCAI concentrates especially on two domains:

- optimization in the mathematical sense with a focus on combinatorial optimization and heuristic solvers
- optimization of code performance on various hardware systems

The goal is to develop tailored solutions to the optimization problems of various industries. SCAI has supported customers in several projects in solving their specific optimization problems. This includes optimization problems for finding the optimal position of articles on the shelves of a warehouse, e.g., by minimizing distances traveled by the workers during the picking process. Another task was to assist dispatchers when stocking shelves or assigning loading bays to loading actions.

Over the last two years, SCAI has created an algorithm suite that tackles the problem of solving the so-called *Job Shop Scheduling Problem* when liquids are processed. This suite can be successfully applied to food manufacturers (e.g., breweries) or in processing chemicals, such as paint manufacturing. SCAI demonstrated the optimization solutions at the Hannover Fair 2022, which sparked considerable interest from potential customers.

For the retailer *Galeria Karstadt Kaufhof* in Essen, SCAI created a solution for the optimal distribution of returned articles to online shops and department stores. This project is ongoing, and SCAI is working closely with its partner Fraunhofer IAIS and the customer's logistics provider. The combinatoric problem, in this case, is a combination or variant of a multi-knapsack and a bin packing problem.

Quantum computers could solve optimization problems faster and more precisely in the future

Many scientists believe that quantum computing will eventually enable us to solve the above optimization problems more precisely and in less time. In the project QuantumQAP, SCAI is porting its patented solver for the so-called *Quadratic Assignment Problem* (QAP) to include quantum computers in finding the optimal solution. The German Federal Ministry of Education and Research funds the three-year research project, which began in January 2022.

QuantumQAP aims to apply post-quantum cryptography algorithms to protect the encryption against being broken by Shore's Algorithm with the help of quantum computers. In this project, not the algorithms are developed, but their implementation is optimized.

Post-quantum cryptography algorithms can protect encryption from being broken by quantum computers.

Determining the optimal location of articles on a warehouse shelf, for example, to minimize the distance workers walk during the picking process, can be a complex optimization problem.

Since those algorithms demand a lot of computing power on digital hardware compared to current cryptography algorithms such as Rivest–Shamir–Adleman (RSA), the aim is to execute them on dedicated hardware, such as Field Programmable Gate Arrays (FPGAs) and possibly Application-Specific Integrated Circuits (ASICs).

In the design phase, the synthesization, where the program implementing the algorithm is converted into the binary description and then uploaded to the FPGA or the assembly plan for a given ASIC platform built, a QAP optimization problem has to be solved. In this way, fast and reliable execution of the code is ensured.

In particular, the project aims to solve the so-called place-and-route problem, which targets the uses of compute blocks by exploiting neighborhoods and minimizing the maximum length of a signal traveling through the hardware quasi simultaneously. The number of hops or stops is proportional to the clock ticks it takes to execute the implemented algorithm on the hardware and, hence, determines the performance.

Optimized processing of sensor data helps improve scanning systems at security checkpoints

With its partners, *Thales* in Paris and *Quantum Brilliance* in Stuttgart, Fraunhofer SCAI is trying to take the next step and use quantum computers. With the help of the two companies, it should be possible to shorten the turnaround time in developing an implementation and quickly arrive at a better solution. For this to work, the algorithm has to be divided into small pieces to be partly executed on quantum hardware. This approach is also called hybrid quantum computing. Essentially, this kind of parallelization should also work on purely digital computers. At the end of the project, a study will compare the results for quantum computers with purely digital execution available at that time with both old and new algorithm versions. The knowledge gained should make it possible to project the results onto future quantum hardware.

In other projects, SCAI optimizes the processing of data emitted from a multitude of radar sensors. The aim here is to create an image of the scene which can, e.g., identify broken or defective items on a conveyor belt or persons carrying weapons at a security checkpoint. In 2022, SCAI and its partners Fraunhofer FHR and ONERA (Frankreich) successfully tested the system in a subway station of Rome's metro. Here, the team has demonstrated that the technology can reliably detect weapons on people moving in front of a radar sensor array.

The essential advantage of such a system is that people do not have to stop moving to be scanned for illegal items. They simply pass through a gated area equipped with the new sensor array, and the system detects objects while people move. That significantly reduces the time for inspection. Also, it is now possible to introduce security measures in subways or at large events, for example. Scanners currently used to check people at airports or in sensitive buildings are not suitable for such purposes.

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Network Evaluation Technologies

Efficient and high-performance transport networks for gas, electricity, heat, and water are crucial for transforming European energy use toward climate neutrality. Smart grids are becoming increasingly important, as are future hydrogen transport networks. The intelligent networking and control of power generators, storage facilities, consumers, and network resources are major economic and ecological challenges.

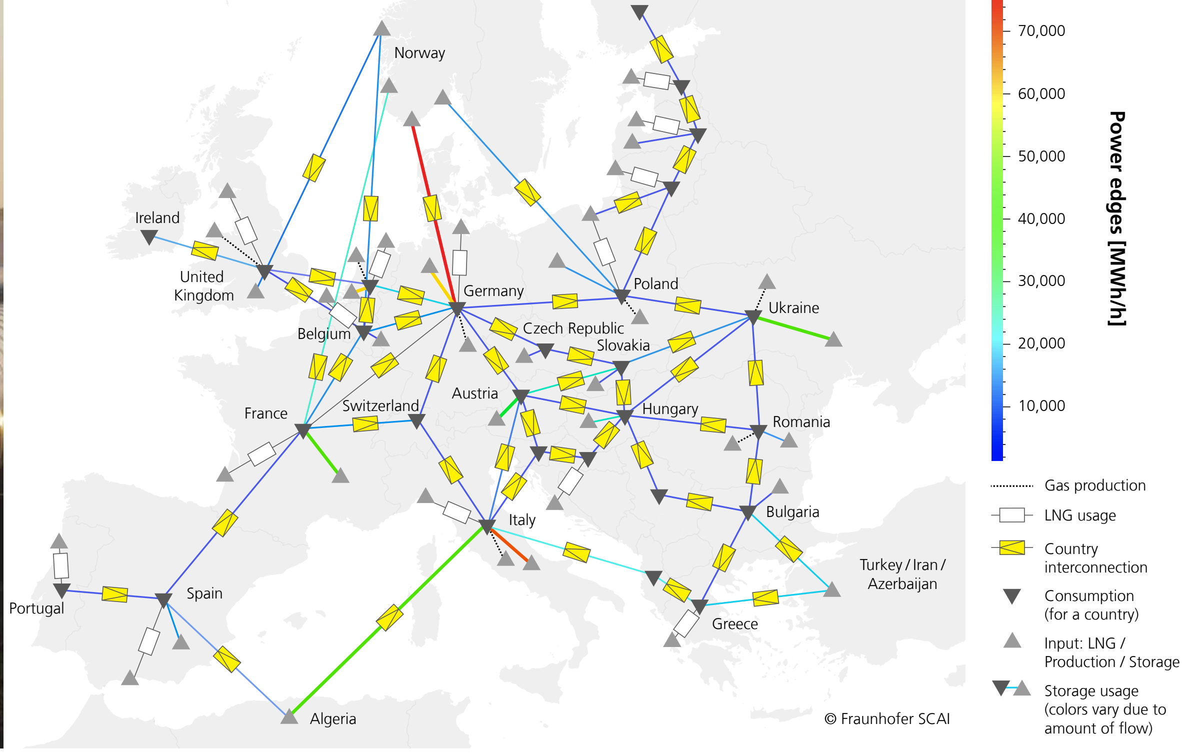
The methods and software packages developed in the business area *Network Evaluation Technologies* of Fraunhofer SCAI are suitable for modeling, simulating, analyzing, and optimizing networks. These are energy networks for transporting gas (including hydrogen), water, electricity, district heating, and oil. The tools from SCAI are also suitable for modeling CO_2 in its liquid state. For this purpose, SCAI develops and implements methods from physical modeling, numerical mathematics, data mining, and machine learning.

MYNTS software also models transport networks for hydrogen and liquefied carbon dioxide

Analyzing and optimizing their networks is an essential competitive factor for energy suppliers and large consumers. For this purpose, SCAI has developed the *MYNTS* (MultiphYsical NeTwork Simulator) software package. *MYNTS* can be used to plan complex networks and predict, analyze, and optimize their behavior during operation. The software models transport networks for energy or water. The simulation shows how changes in certain factors affect the network. *MYNTS* can be used, for example, to calculate how temperature fluctuations change flow rates and how the failure of subnetworks affects the other network components. For network operators, this makes energy conversion and grid expansion more flexible. They save energy and money and also increase the security of their infrastructure.

MYNTS is also suitable for networks transporting hydrogen or liquefied carbon dioxide. For this reason, the software is a sought-after tool for modeling the transition to hydrogen infrastructure in research projects or industrial planning. The future infrastructure of energy transport networks is also the subject of the joint project TransHyDE-Sys, funded by the German Federal Ministry of Education and Research. *MYNTS* plays a central role in the toolchain, and several other institutes in the project use the software from SCAI.

SCAI's portfolio also comprises the simulation and analysis of electrical power networks, such as power flow analysis.



Europe in Winter 2025: The simplified topology model represents the natural gas flows between regions. The network infrastructure reconstruction measures and savings are already taken into account in the picture.

Gas pipeline companies, including Germany's largest gas transmission company, Open Grid Europe (Essen), and the Federal Network Agency in Bonn, use the software for network development and planning tasks.

Investigating the security of the European gas supply until 2025

In the spring of 2022, the urgent question arose if Europe could make up the energy shortfall in case of a complete stop of Russian gas supplies. To give answers, ESYS – a joint initiative of the science academies acatech, Leopoldina, and Academy Union – asked Fraunhofer IEG, Fraunhofer SCAI, and TU Berlin to investigate the situation. The result: By 2025, the expected supply gap could be closed through an infrastructure expansion, an expected decline in gas demand, and savings.

The researchers examined the effects of a supply stop by accurately modeling the actual physical characteristics and properties of the gas network. Other studies only work with highly simplified "balance sheet" models. The new approach allows recommendations to be made regarding concrete measures to optimize the infrastructure. The focus is on which technical changes to the gas network are necessary to supply all countries in the European Union and the Ukraine with gas.

The study inquires when gas no longer flows from Northeastern Europe to Western and Southern Europe but in the opposite direction from Western and Southern Europe (where most LNG terminals are located) to Eastern Europe. Even with this flow direction reversal, supplying all countries with similar volumes would be impossible. From the large density of high-volume pipelines in Eastern Europe, the network branches out like the circulatory system in the human body. Flow reversal in such a network is a complex problem because there are only a limited number of entry points with technically limited capacity. The new German LNG terminals, where liquefied natural gas delivered by ship flows into the pipeline system, can mitigate but not solve the problem. Norway, Algeria, and Turkey can only increase their gas supplies by a few percentage points – indispensable but not suited to be game changers. Thus, the report concludes that short-term efforts to reduce natural gas demand are essential.

MYNTS has been successfully used for several such studies, serving the industry, research, and advisory policy support.

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Virtual Material Design

New materials with tailored properties are becoming increasingly important in many industrial application areas. Developing them quickly and efficiently is achieved by applying mathematical methods and combining scientific and engineering knowledge with modern data-driven approaches. In this process, machine learning techniques play an essential role.

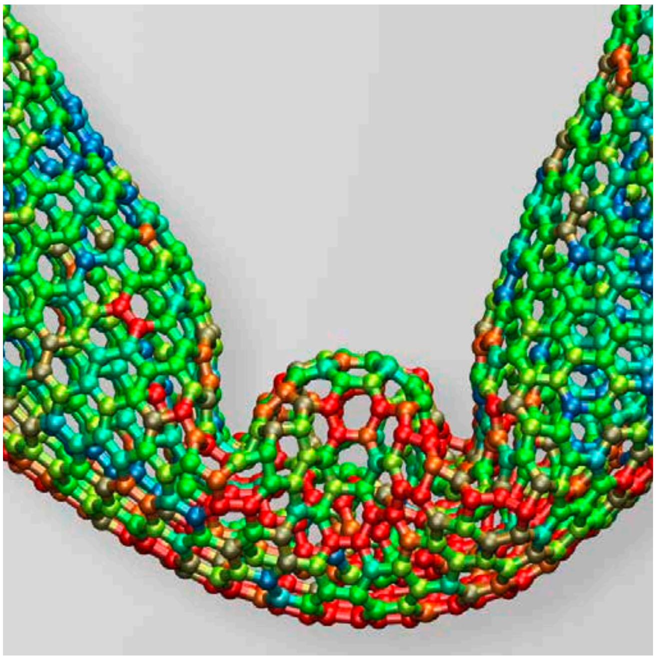
The work in the business area *Virtual Material Design* of Fraunhofer SCAI aims to use the computer as a virtual laboratory within a data-driven design approach to develop and investigate new materials and molecules. This strategy can significantly reduce development costs for new materials and optimize manufacturing processes.

For most materials design problems, the design space size increases exponentially with the number of parameters. Hence, a conventional trial-and-error approach is not applicable. To this end, SCAI follows a so-called data-driven design technique to efficiently explore the design space, including an iterative feedback loop to elaborate the optimum systematically. However, some potentially required material properties are not directly available by straightforward, efficient physical model numerical simulation.

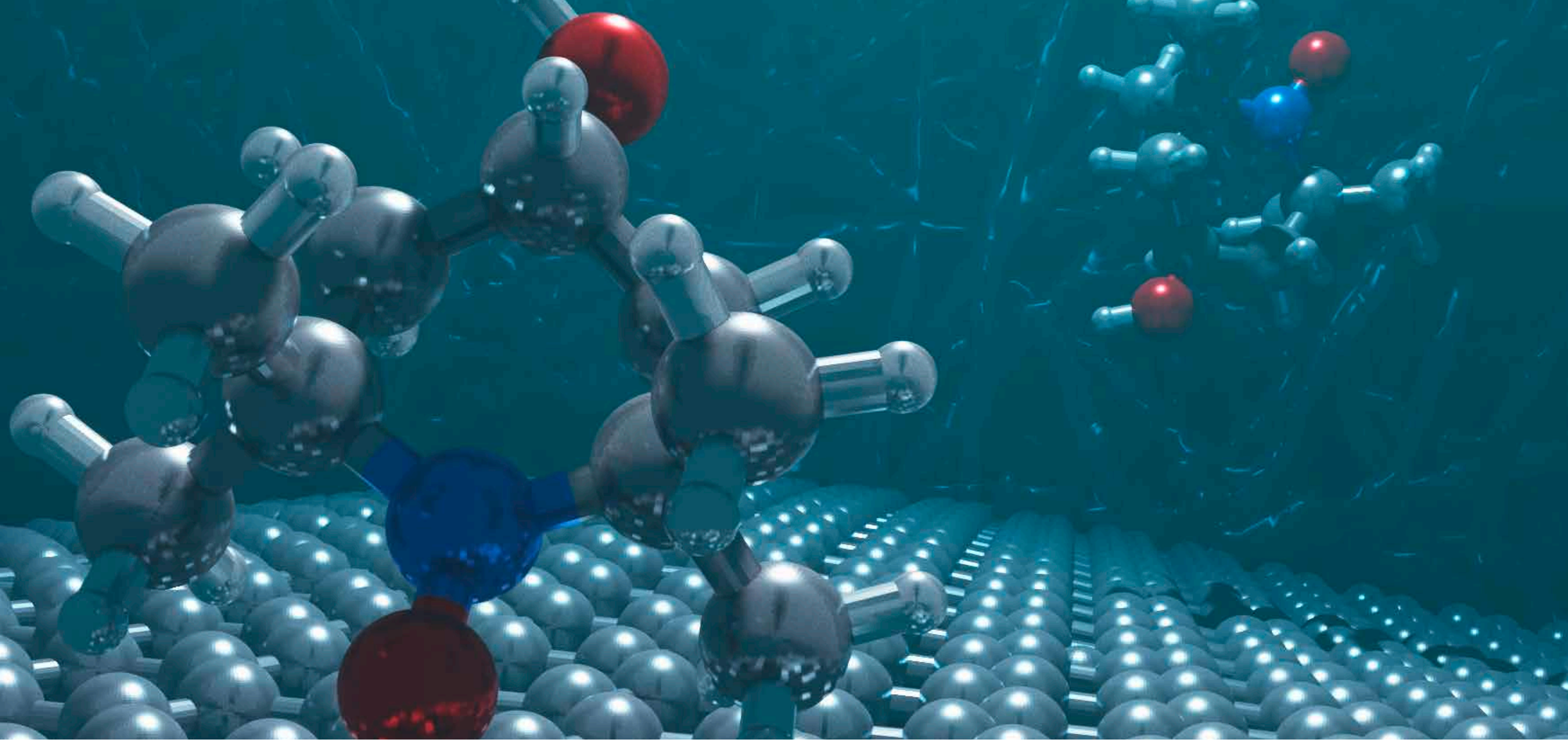
Therefore, the workflow involves an informed machine learning approach based on a smart mixture of black-box and white-box models, i.e., so-called grey-box models. Note here that the aim of white-box models is an accurate physical description of the modeled system. In contrast, a black-box model's purpose is to reproduce just the input-output behavior of a system. However, in many cases, establishing white-box models is too complex. The amount and quality of data available to create black-box models is often insufficient, but their mixture can potentially be applied.

For the outer optimization loop, optimization methods such as Bayesian optimization, are employed to balance the exploration and exploitation of the design space. In each iteration, based on the current surrogate models, new potential candidates for the most practical experiments will be suggested by the inverse design step.

Then, the newly generated experimental data are utilized to improve the involved predictive surrogate models leading to new suggestions of promising candidates for experiments in the next iteration. This way, the data-driven workflow will exploit existing data and lead to the application of further investigations within the materials development and design process. Note here, in particular, that learn-on-the-fly machine learning methods are applied such that the involved predictive models will be automatically improved using the workflow. This substantially reduces the number of necessary tests and simulations.



Tremolo-X includes computations in nanotechnology: Simulation of the bending of a double-walled carbon nanotube.



In redox flow batteries, electron exchange occurs in an electrochemical cell (stack). Within the cell, graphite felt is used to increase the surface of the electrodes. The picture shows a redox pair on the surface of a felt fiber.

Tremolo-X supports nearly all conventional interaction potentials for modeling materials

Tremolo-X is a massively parallel software package for efficient molecular dynamics simulations. The software, developed by SCAI, is also the numerical backend of the *QuantumATK* simulation toolkit marketed by the company *Synopsys*. Tremolo-X supports nearly all conventional interaction potentials for modeling materials and core-shell and reactive potential models. The applicability of molecular dynamics methods to a problem usually depends on the existence of a suitable interaction potential. Therefore, the software also includes interaction potentials based on machine learning (ML) methods and tools to efficiently train both these and conventional potentials. In this way, suitable interaction potentials for a given problem can be generated almost automatically.

Better batteries for storing temporary surpluses of renewable energy

Organic redox flow batteries (RFBs) are a promising approach for storing temporary surpluses of renewable energy generation. The SONAR project aims to capture the entire RFB development process digitally, to accelerate screening to identify suitable materials, and to adapt the design of a battery system to specific conditions. To this end, the partners are developing tools and workflows for investigating electroactive materials and combining simulation methods on multiple physical scales. Factors such as cost, lifetime, and performance are included to compare competing energy storage technologies comprehensively. The European Commission funds SONAR from January 2020 to December 2023.

ML methods improve polyurethane and glass composition design

The joint project MaGriDo aims to develop ML methods that require fewer data or can make predictions consistent with existing knowledge. To this end, the project partners create deep neural networks for industrial applications so that existing domain knowledge is incorporated into the architecture of the networks.

Application examples include polymers and glasses. For instance, it is possible to adjust the properties of polyurethane coatings (hardness, scratch resistance or gloss) by varying the base materials used in their production. However, elaborate experiments are necessary to develop a new coating with specific properties. MaGriDo is intended to make these investigations largely superfluous and thus to accelerate the development process. In the project, SCAI is responsible for the software-technical aspects, the engineering connection, and the subsequent exploitation of the project results. The German Federal Ministry of Education and Research funded MaGriDo as part of the *Mathematics for Innovation* program from April 2020 to March 2023.

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Numerical Data-Driven Prediction

Data-driven approaches are becoming increasingly important in Industry 4.0. The interplay of efficient data analysis algorithms, large amounts of sensor data, or numerical simulations to incorporate domain knowledge is promising. Machine learning methods provide targeted insights from data that support decision-making or the automation of process control.

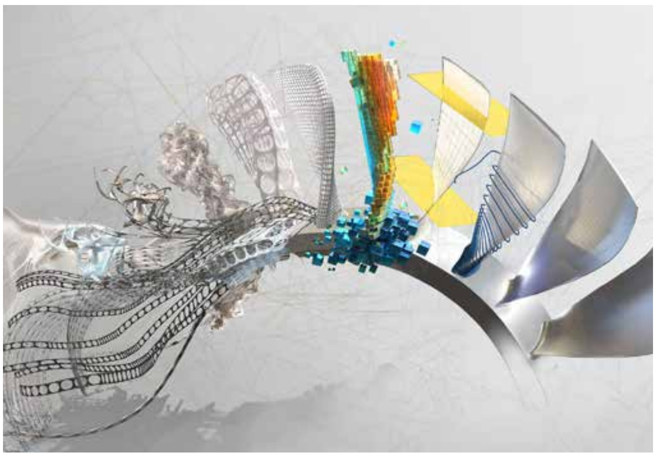
The work in the business area *Numerical Data-Driven Prediction* of Fraunhofer SCAI focuses on dealing with complex data from physical-technical applications, especially to meet the challenges of Industry 4.0. SCAI combines mathematics, machine learning, and engineering knowledge to develop robust, scalable, and domain-adapted data analysis concepts and methods. Applications can be found, for example, in virtual product development using computer-aided engineering, in condition monitoring, including predictive maintenance of wind turbines, or in the realization of digital twins.

One research and development focus is the integration and use of engineering knowledge in machine learning (ML). Other topics are the efficient processing and analysis of large complex data sets, time series or numerical simulation results, the quantification of uncertainties, contributions to transfer learning, and approaches for robust design.

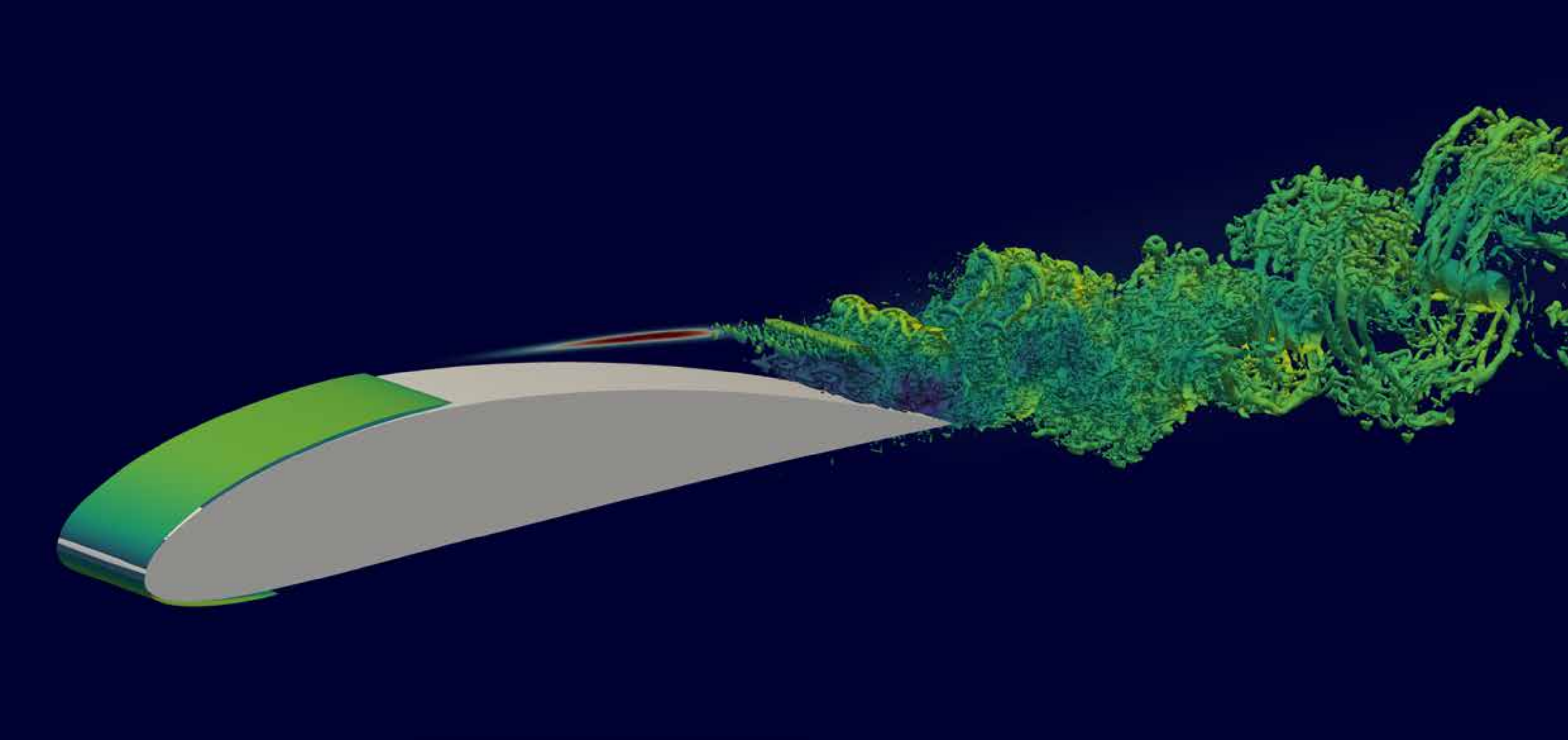
SimExplore supports engineers by providing a browsable overview of crash simulation results

Computer-aided engineering (CAE), based on reliable numerical simulations, is a core pillar in many engineering domains. Particularly in the CAE-based crashworthiness analysis process, the large number of design possibilities combined with increasing requirements and regulations for crash safety lead to large so-called development trees. A key challenge is to learn useful designs from a set of model changes and corresponding simulation results, for example, to mitigate undesired deformations. In addition to the software tools *ModelCompare* and *SimCompare*, already on the market for comparing two design variations and their impact, SCAI has extended its framework for automatic data analysis and event detection to the interactive exploration of many simulation results with the newly developed software SimExplore. It supports CAE engineers in their simulation data analysis workflow by providing a browsable overview of many crash simulation results, e.g., in terms of clusters and outliers based on deformations and mesh functions.

SCAI uses its specifically developed, patented dimensionality reduction technique to compute geometry-driven features representing the displacements or mesh functions from the selected parts. Moreover, *SimExplore* provides a web-based application for interactive visualization. *SimExplore* thus represents a breakthrough towards automatic event detection for car crash simulations within the overall crashworthiness data analysis process.



The vision of the EVOLOPRO project is the automatic adaptation of production processes to rapidly changing requirements.



Large Eddy Simulation of the turbulent flow around a wing section, including the quantification of the uncertainty in the mean velocity field computed during runtime (‚in-situ').

EVOLOPRO: Transfer-learning speeds up the optimization of CAM process parameters

The big vision of Industry 4.0 is the automatic adaptation of production processes to rapidly changing requirements. In the last four years, the Fraunhofer Leitprojekt EVOLOPRO has pushed developments to come a step closer to this vision. Seven institutes have jointly investigated how design features of natural organisms that promote flexibility and robustness can be transferred to production processes. The aim is to increase flexibility and robustness in production concerning changing conditions such as new product requirements.

An essential contribution by SCAI is the development of a general framework for system flexibility optimization that allows to systematically study the integration and flexibility contribution of design features. Based on this framework, SCAI has investigated how transfer and multi-task learning can help to optimize processes and to train deep-learning-based surrogate models more efficiently. A key result is a transfer-learning-based algorithm that speeds up the optimization of computer-aided manufacturing (CAM) process parameters for milling by a factor of up to 14. The algorithmic developments of SCAI contribute to leveraging the potential of digital twins for powerful and efficient design and parameter space explorations.

EXCELLERAT: Simulation results can be processed in more detail with 'in-situ' data analysis

Computational fluid dynamics (CFD) simulations usually have many degrees of freedom that lead to high computational costs and large amounts of data to be stored. SCAI took a novel approach in the EXCELLERAT project to overcome these challenges. Data is analyzed during the runtime of the simulation while it is still in memory, also known as 'in-situ analysis.' In this context, SCAI developed data analytics algorithms that can be applied in a streaming fashion. Besides a significant reduction of data in- and output, the advantages of an in-situ approach lie in the much higher resolution of the input data and earlier availability of results. Compared to standard offline post-processing, this allowed us to extract more knowledge from each simulation, for example, in the form of surrogate models that can be applied for multiple purposes such as design optimization, uncertainty quantification, or system identification.

Another focus in EXCELLERAT was the development and application of methods for the identification of trends and similarities in simulations. In this way, it is possible to monitor simulations and to define stop criteria if unwanted behavior occurs, thus saving time and computing resources. On a technical level, SCAI relied on standard in-situ interfaces to facilitate a simple integration of our analysis tools with multiple flow solvers and engineering application fields. The project EXCELLERAT continues with a second funding phase from 2023 on.

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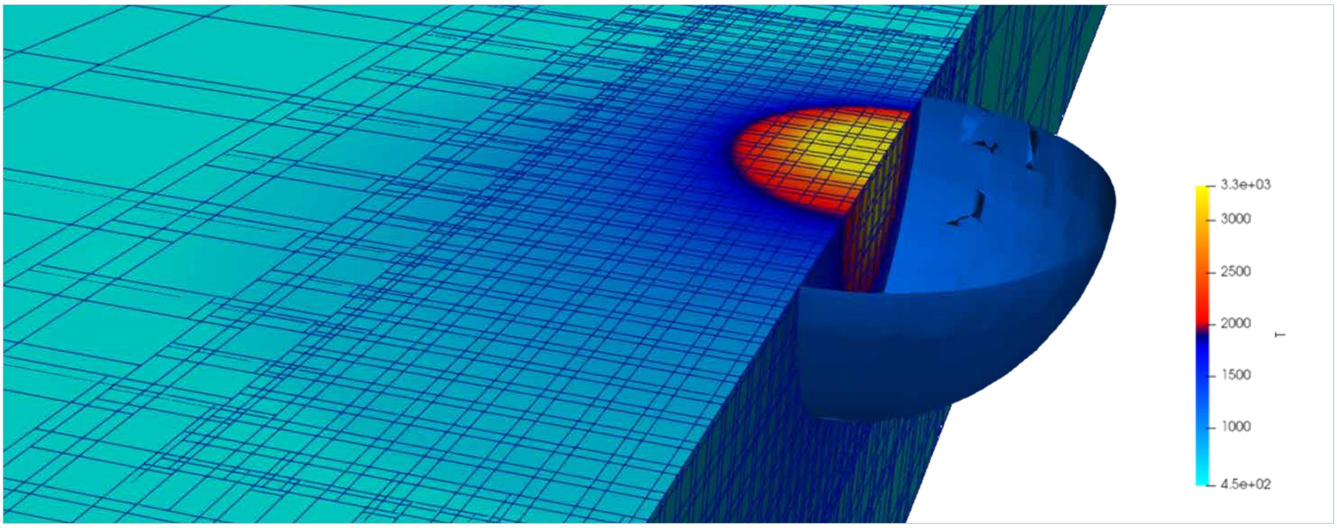
Meshfree Multiscale Methods

The pre-processing step of computational mesh generation and adaptation in established simulation workflows is time-consuming and costly. Meshfree simulation methods overcome these problems and allow engineers to design products significantly faster. They are highly attractive for complex industrial use cases, for example, in the automotive, chemical, and hydropower industries.

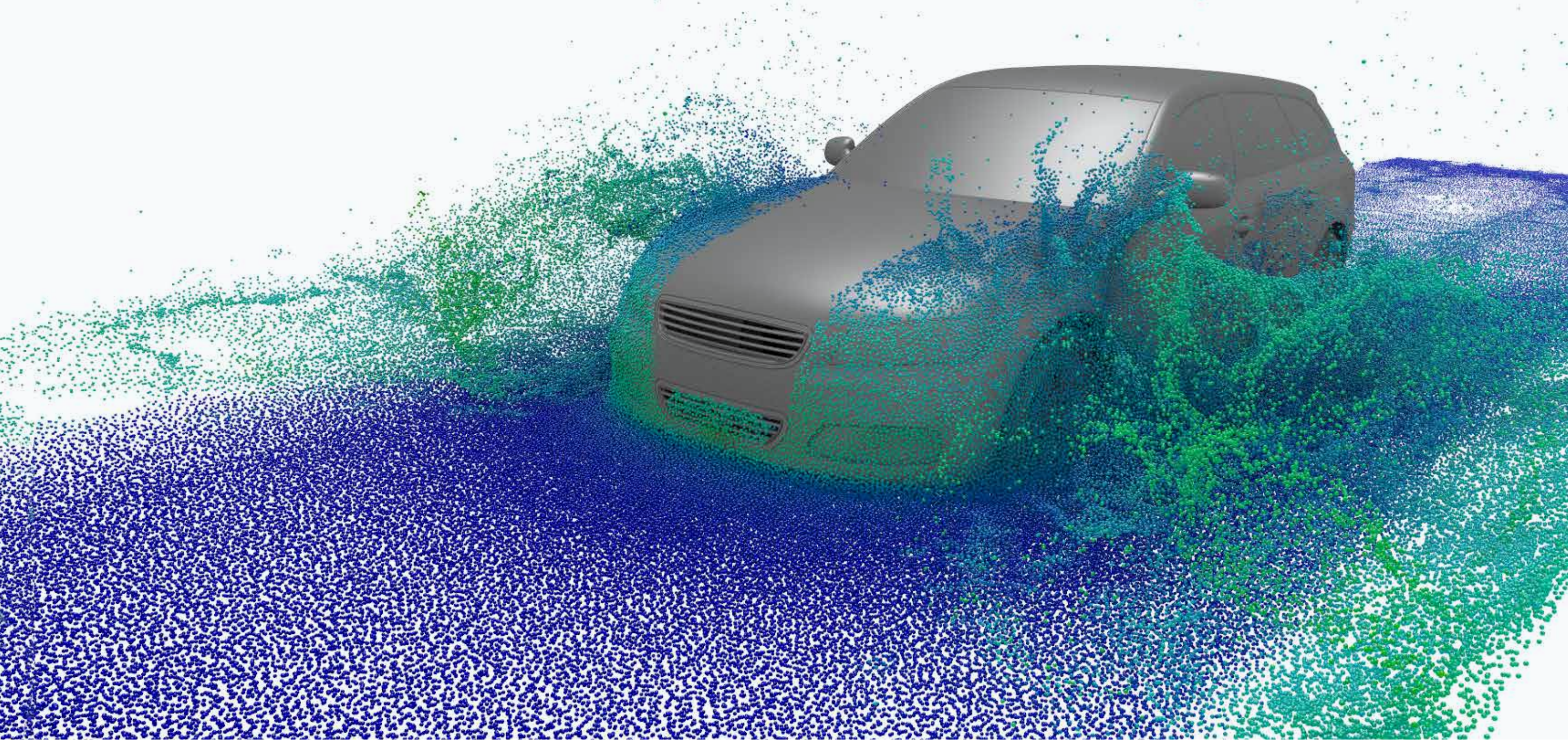
Today's product design processes typically involve highly complex geometries and fine details. The required resolution of these geometric details – which may deform and change over time – leads to the use of very fine meshes which need to be generated appropriately, i.e., adaptively refined and coarsened locally, in classical numerical simulation tools. The computational costs associated with mesh generation and local mesh adaptation pose a severe bottleneck so that simulation methods that do not require the availability of a computational mesh become highly attractive for such complex use cases. Thus, the work in the business area *Meshfree Multiscale Methods* of Fraunhofer SCAI focuses on developing efficient multiscale algorithms, e.g., the generalization of the finite element (FE) method or particle-based multiscale methods.

MESHFREE provides customers with essential features to reduce cost

Together with Fraunhofer ITWM in Kaiserslautern, SCAI develops the simulator *MESHFREE* which is built on a generalized finite difference approach and only involves a point or particle cloud instead of a classical mesh – which is far simpler to create and refine. *MESHFREE* is used by customers and project partners, e.g., in the automotive sector, chemical engineering, and hydropower industry, in many application areas typically involving fluid flow. The implicit *MESHFREE* solver employs SCAI's *SAMG* fast linear solvers to attain robustness and efficiency independent of geometric details and material properties.



During a laser powder bed fusion process in additive manufacturing, the metal vaporizes, forming a liquefied pool of molten metal. The PUMA software toolkit can be used to simulate this process.



Where is the risk for rainwater intrusion in a car body? Using MESHFREE, engineers can track the paths of water.

Most industrial applications today involve the interaction of solids and liquids, which needs to be captured during the simulation to attain the required accuracy. To this end, *MESHFREE* is extended with the help of SCAI's Open Co-Simulation tool (OCoS), designed to couple particle-based and mesh-based methods in a robust and scalable way. Customers can thus take full advantage of *MESHFREE* in conjunction with all classical simulation tools employed in their existing workflows. OCoS is used, for instance, in the power management sector to provide three-code coupling for joint modeling of electromagnetic effects, fluid flow, and elastic behavior.

Moreover, SCAI is also improving the usability of *MESHFREE* and customers' user experience via the Computational Model Builder (CMB) and Simulation Modeling Toolkit (SMTK) frameworks. With the help of these industry standards, even non-experts can operate the simple-to-use graphical user interface (GUI) for all stages of a simulation workflow. The extendability of these frameworks makes it easy to provide application- and customer-adapted GUIs. These features are essential for customers from small and medium-sized enterprises to reduce the total investment cost when adopting a novel software tool and integrating it into their workflows.

PUMA allows for rapid prototyping via a simple Python user interface

Another meshfree simulation product in development is *PUMA*. The software toolkit is based on the partition of unity method (PUM) – a meshfree generalization of the FE method. PUMA enables engineers to rapidly implement simulation applications using generalized FE techniques based on the PUM. Compared to classical FE methods, the PUM allows immediate use of the user's special knowledge of the problem to be solved, of domain-specific information, and of physics-based basis functions to improve the approximation properties of the model and to reduce the computational effort.

A key advantage of PUMA is its rapid prototyping capabilities via a simple Python user interface. It allows for the easy input of complex computational models, i.e., coupled systems of partial differential equations, and the utilization of built-in or user-specified enrichment functions, which provide superior approximation properties compared with classical polynomial-based FE approaches. For instance, PUMA provides built-in enrichment functions for fracture mechanics problems, composite materials, and quantum mechanics. Currently, a specialized version of PUMA is in the pipeline, targeting the advanced modeling of additive manufacturing, particularly the laser powder bed fusion process. Furthermore, SCAI works in the joint project PADME-AM on novel mathematical models that can represent advanced laser profiles, multiple laser sources, high-resolution enrichment functions, and geometric design capabilities in PUMA. SCAI's partners are the Deutsches Zentrum für Luft- und Raumfahrt (DLR), Access e.V., and the Rheinische Friedrich-Wilhelms-Universität Bonn. The German Federal Ministry of Education and Research is funding PADME-AM from November 2022 to October 2025.

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Computational Finance

Computational Finance is an interdisciplinary area of scientific computing. The main goal is to develop efficient and robust algorithms for financial mathematics. Machine learning methods, which form the basis of many applications in artificial intelligence (AI), play an essential role here. SCAI contributes to making AI models understandable, to quantifying uncertainties of the financial market, and to analyzing blockchains.

The focus in the business area *Computational Finance* of Fraunhofer SCAI is to develop efficient and robust algorithms for financial mathematics. The scopes of application include

- the valuation of financial and physical assets,
- the calculation of sensitivities and hedging strategies (risk management strategies used by short- to medium-term oriented traders and investors to hedge against unfavorable market developments),
- risk measurement and risk management, and
- big data analysis for market or blockchain data.

For these applications, numerical methods such as (quasi-) Monte Carlo methods, techniques for the discretization and solution of partial differential equations, graph algorithms, and machine learning models are used and further developed.

In its research and project work, SCAI focuses on the following main areas of activity.

Energy asset optimization and valuation of green power purchase agreements

The optimal control and hedging of portfolios of physical assets are gaining importance due to the advancing decentralization of power generation. Suppose one wants to take future price uncertainties into account during optimization. In that case, the solution to the problem often becomes computationally intensive. Additionally, it requires experienced developers who can make necessary adjustments to the parameterization of the algorithm when the portfolio composition changes. SCAI applies reinforcement learning techniques to develop a generic framework for describing and

The challenge for energy suppliers today is to create and manage a cost-optimal portfolio of renewables, flexible resources, and storage that guarantees customers a certain amount of green power.

Cryptocurrencies are also popular with criminals because of their anonymity. Analytical methods can be used to detect money laundering or theft.

solving tasks. With its help, companies can optimally manage their portfolios and thus save costs and effort.

In addition, SCAI enhances methods for hedging physical energy asset portfolios and for valuing green power purchase agreements. During the last year, SCAI completed a project for the optimal control of a gas power station using reinforcement learning algorithms and a project that used neural networks to optimize gas storage management.

Explainable artificial intelligence for quantitative financial applications

Artificial intelligence models, especially in deep learning, are often "black boxes" for users. It is hardly understandable how these models come to important decisions. In explainable artificial intelligence (XAI), SCAI is working on techniques to help explain decisions made by AI models. For that, domain-specific characteristics, like data sets that include categorical data, need to be considered.

One example is determining the influence of individual input data on the result at a selected data point. Another approach is to describe complicated models with simpler ones, making it easier to understand decisions. If, for example, an algorithm must decide whether a loan is granted, such a procedure can clarify which factors are relevant to the decision in individual cases. This is essential for a justification to customers and superiors and regarding applicable regulations.

Furthermore, such approaches help improve AI models and detect data bias.

Blockchain analysis for cryptocurrencies and smart contracts

Cryptocurrencies and smart contracts have become more and more relevant in the finance domain during the past several years. Technically, smart contracts are programs stored in a blockchain that map the logic of contractual arrangements. They are executed when certain conditions are met. SCAI introduces procedures for analyzing blockchain data and is working on a project to visualize transaction graphs. These procedures rely on graph algorithms and use machine learning methods. One challenge lies in the tremendous amount of time-dependent data.

The methods can be applied for various purposes, for example, analyzing the trading behavior of market participants. Since cryptocurrencies such as Bitcoin or Ether offer a space for criminal activities due to anonymity, an important aspect is detecting and examining activities such as money laundering or coin theft.

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Founded in 1949, the Fraunhofer-Gesellschaft currently operates 76 institutes and research units throughout Germany. Over 30,000 employees, predominantly scientists and engineers, work with an annual research budget of €2.9 billion. Fraunhofer generates €2.5 billion of this from contract research. Industry contracts and publicly funded research projects account for around two thirds of that. The federal and state governments contribute around another third as base funding, enabling institutes to develop solutions now to problems that will become crucial to industry and society in the near future.

The impact of applied research goes far beyond its direct benefits to clients: Fraunhofer institutes enhance businesses' performance, improve social acceptance of advanced technology and educate and train the urgently needed next generation of research scientists and engineers.

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The prestigious nonprofit Fraunhofer-Gesellschaft's namesake is Munich scholar Joseph von Fraunhofer (1787–1826). He enjoyed equal success as a researcher, inventor and entrepreneur.

Academic Partnerships

Institute for Numerical Simulation (INS), University of Bonn

The INS is a mathematical research institute at the University of Bonn focusing on scientific computing, numerical analysis, and numerical simulation. In its research work, the institute develops tools for numerical simulation in natural sciences and engineering, geosciences, medicine, life sciences, business, and finance.

A part of the *Virtual Material Design* department of Fraunhofer SCAI is located at the INS and is headed by Dr. Jan Hamaekers.

Prof. Dr. Michael Griebel, Institute Director of Fraunhofer SCAI, Prof. Dr. Jochen Garcke, head of the *Numerical Data-Driven Prediction* department of SCAI, and Prof. Dr. Marc Alexander Schweitzer, head of the *Numerical Software* department of SCAI, also lead working groups at the INS.

Bonn-Aachen International Center for Information Technology (b-it)

The b-it is a joint institution of the University of Bonn, the RWTH Aachen University, the University of Applied Sciences Bonn-Rhein Sieg, and the Fraunhofer-Gesellschaft. The *Bioinformatics* department of Fraunhofer SCAI, headed by Prof. Dr. Martin Hofmann-Apitius, participates in the international Master Program in *Life Science Informatics*. Hofmann-Apitius and Prof. Dr. Holger Fröhlich, group leader *AI and Data Science*, each lead working groups at the b-it.

Hochschule Bonn-Rhein-Sieg, University of Applied Sciences, Sankt Augustin

The cooperation with the Bonn-Rhein-Sieg University of Applied Sciences is comprehensive and multifaceted, covers several topics, and involves students in SCAI's project work.

Hochschule Koblenz, University of Applied Sciences, RheinAhrCampus, Remagen

The cooperation with the RheinAhrCampus of the Koblenz University of Applied Sciences focuses on new machine learning methods and applications.

SCAI is active in several Fraunhofer alliances and networks:

- Fraunhofer Information and Communication Technology Group
- Fraunhofer Big Data and Artificial Intelligence Alliance
- Research Center Machine Learning within the Fraunhofer Cluster of Excellence *Cognitive Internet Technologies*
- Fraunhofer Network Simulation
- Fraunhofer Competence Network Quantum Computing

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