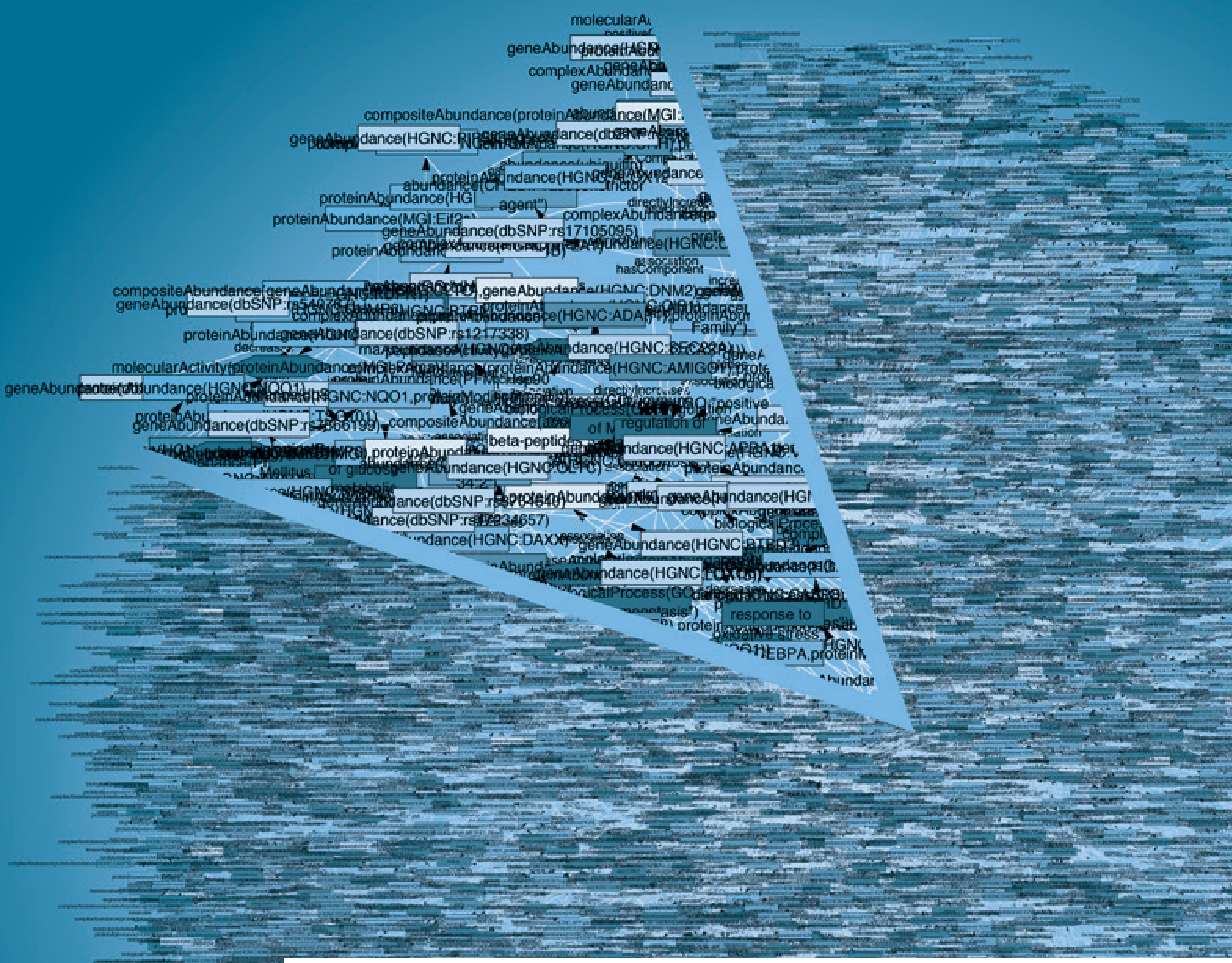
Fraunhofer SCAI

FRAUNHOFER INSTITUTE FOR ALGORITHMS AND SCIENTIFIC COMPUTING SCAI



ANNUAL REPORT 2018|2019

COVER
Semi-automatically generated multiscale biomedical cause-and-effect networks help to gain insights into disease mechanisms.

ANNUAL REPORT 2018|2019

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PREFACE

Dear reader,

The German economy has been in a steady upswing for many years. New technologies and innovations are fundamental to this success, to which the Fraunhofer-Gesellschaft makes a significant contribution. Fraunhofer SCAI also continues to grow. We were again able to increase our earnings last year. Revenues from software licenses rose to a record level of 5.1 million euros in 2018. For many years, the share of our income from industry in operating expenses has been over 50 percent. In 2018, we achieved 54.4 percent.

Our economic success goes hand in hand with success in research. The high scientific quality of the institute's research work is, for example, reflected in the careers of two female scientists: Dr. Tanja Clees, the former head of the institute's Department of High Performance Analytics, now teaches as a professor at the *Bonn-Rhein-Sieg University of Applied Sciences*. Dr. Juliane Fluck, the former deputy head of the Department of Bioinformatics, has been appointed professor of "Intelligent Information Retrieval and Pattern Recognition" at the *University of Bonn*.

Another scientific success in 2018 was the renowned "Hugo-Geiger-Prize" for Dr. Alpha Tom Kodamullil. She developed innovative methods to systematically explore new correlations in medical data sets on neurodegenerative diseases. The newly discovered mechanisms contribute to the development of new diagnostic procedures and active pharmaceutical ingredients.

A cross-sectional topic for the institute is machine learning. SCAI is part of the *Research Center for Machine Learning*, which is one of three centers in the Fraunhofer Cluster of Excellence *Cognitive Internet Technologies.* Here, SCAI is working with other Fraunhofer institutes on innovative algorithms and methods that combine data-driven learning with automated modeling and domain- and application-specific expert knowledge.

SCAI is also involved in the Fraunhofer flagship project EVOLOPRO. The aim is to give industrial production systems the ability to autonomously adapt to new requirements and environmental conditions. Fraunhofer SCAI coordinates algorithm development in EVOLOPRO at the interface of transfer and multitask learning, evolutionary exploration strategies, and multi-fidelity modeling.

Of course, the work described in this report would not have been possible without the dedication and the extraordinary commitment of our employees. For this reason, I want to thank them for their strong commitment and their first-class performance.

I would also like to thank our customers and partners for their valuable cooperation and the Members of our Advisory Board for their beneficial support.

I cordially invite you to have a look on some highlights of our work on the following pages!

Prof. Dr. Michael Griebel

Advisory board meeting in May 2018 at Schloss Birlinghoven: Stephan Springstubbe, Prof. Dr. Martin Hofmann-Apitius, Klaus Wolf, Dr. Ulrich Leiner, Victoria Appelbe, Prof. Dr. Petra Ritter, Prof. Dr. Michael Schäfer, Dr. Jan Hamaekers, Prof. Dr. Michael Griebel, Dr. Bernhard Thomas, Carl Vogt, Prof. Dr. Hans-Joachim Bungartz, Prof. Dr. Reinhard Klein, Kuno Blank, Dr. Richard Trethewey, Dr. Thomas Soddemann, Christiane Stoll (from left).

PROFILE

Director

Prof. Dr. Michael Griebel
Carl Vogt (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. Bernhard Klaassen
Virtual Material Design	Dr. Jan Hamaekers
Numerical Data-Driven Prediction	Prof. Dr. Jochen Garcke
Meshfree Multiscale Methods	Prof. Dr. Marc Alexander Schweitzer
Computational Finance	Prof. Dr. Michael Griebel (acting)

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. Hans-Joachim Bungartz, *TU München*
Prof. Dr. Babette Dellen, *RheinAhrCampus Remagen, Hochschule Koblenz*
Prof. Dr. Reinhard Klein, *Universität Bonn*
Dr. Claus Axel Müller, *Gauss Centre for Supercomputing, Bonn*
Prof. Dr. Petra Ritter, *Charité – Universitätsmedizin, Berlin*
Prof. Dr. Michael Schäfer, *TU Darmstadt*
Ulrich Schüller, *Bundesministerium für Bildung und Forschung, Bonn*
Dr. Richard Trethewey, *BASF SE, Ludwigshafen am Rhein*

Spin-offs

BioSolveIT GmbH, Sankt Augustin
scapos AG, Sankt Augustin
SIDACT GmbH, Sankt Augustin
adiutaByte (presently launched), Sankt Augustin

FACTS AND FIGURES

Financing and expenditure

In 2018, approximately 54.4 percent (about 5.9 million euros) of the operating budget of the Fraunhofer Institute SCAI came from revenues from industry – mostly arising from software licenses. For 2019, the aim is to exceed the value of six million euros turnover from industry for the first time.

In 2018, the operating budget (personnel expenses and operating expenses) was 10.9 million euros, the overall budget (operating budget plus investments) was 12.4 million euros.

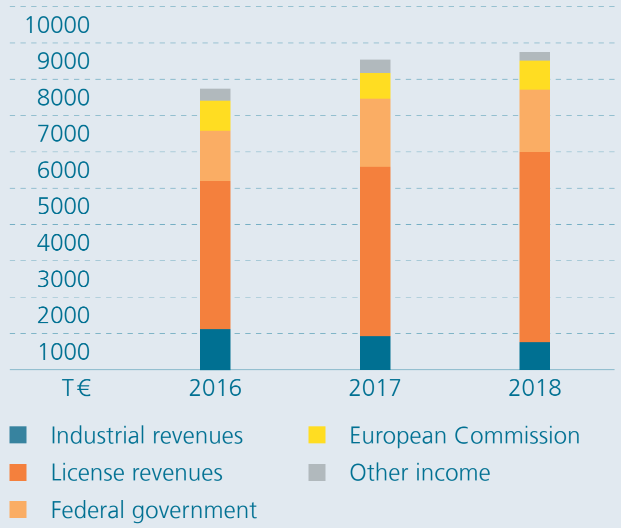
Overall expenses have remained relatively constant over the last few years. Personnel expenses are the main cost factor and account for nearly 75 percent of the operating budget.

The top-selling software packages of the institute are the AutoNester group of products (automatic placement of markers on fabric and other materials), PackAssistant (optimized packaging of components in transport containers), SAMG (library for the highly efficient numerical solution of large sparse systems of equations), and MpCCI (enabling co-simulation with industrial simulation codes).

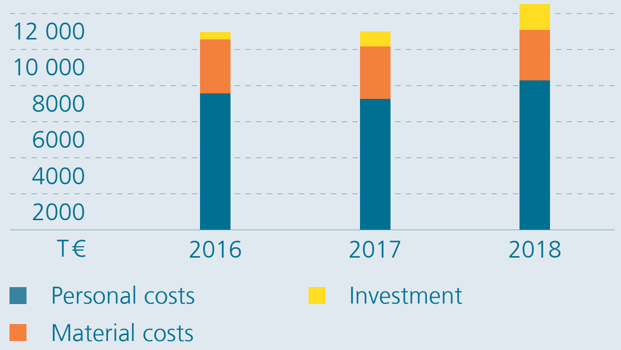
Human resources

At the end of 2018, the institute's staff consisted of 161 employees, including 21 Ph.D. students as well as 45 graduate students and student assistants, mainly from the *University of Bonn* and the *Bonn-Rhein-Sieg University of Applied Sciences*. In the future, we expect a further growth of the institute, in particular due to a strengthening of the links to the *University of Bonn*.

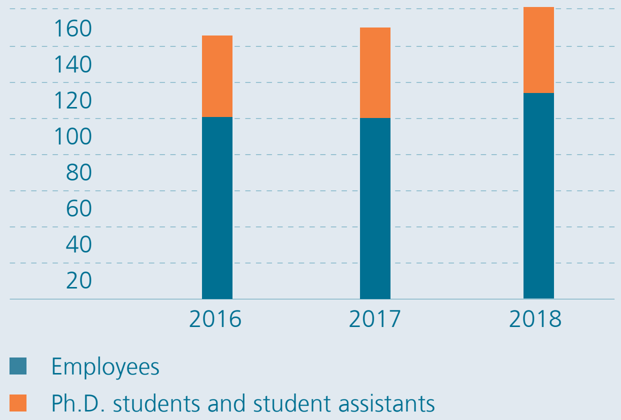
Income



Expenditure



Human resources



SCAI LIGHTS

The optimization of energy networks is Clees' topic in research and teaching

February 2018 Dr. Tanja Clees, former head of the institute's Department of *High Performance Analytics*, has started teaching as a professor at the *Bonn-Rhein-Sieg University of Applied Sciences*. As head of the High Performance Analytics department at SCAI, Clees worked on energy management. An important result of the work of Clees and her team has been the development of the Multiphysical Network Simulator MYNTS. At the university, Clees continues her research on optimization of energy networks, digitization and sector coupling.

Professorship for intelligent information retrieval at the University of Bonn

October 2018 Dr. Juliane Fluck, the former deputy head of the Department of *Bioinformatics*, has been appointed professor of "Intelligent Information Retrieval and Pattern Recognition" at the *University of Bonn*. In addition, she leads the program area Applied Research at the *German National Library of Medicine (ZB MED) – Information Centre for Life Sciences*, also based in Bonn. A cooperation between Fraunhofer SCAI and ZB MED is in preparation. At SCAI, Fluck developed the ProMiner software, which identifies gene and protein names in scientific texts.

Petra Ritter was welcomed as a new member of the institutes' Advisory Board

May 2018 Prof. Dr. Michael Griebel welcomed Prof. Dr. Petra Ritter, Head of the Section Brain Simulation at the *Charité Department of Neurology with Experimental Neurology* in Berlin, as a new member of the Advisory Board. Ritter is also coordinating the European research project VirtualBrainCloud in which Charité, SCAI, and 15 other institutions intend to set up a cloud-based neuroinformatics platform to simulate the brains of individual patients. This is important because the progression of neurodegenerative diseases such as Alzheimer´s varies greatly.

SCAI researcher Alpha Tom Kodamullil wins renowned Hugo Geiger Prize

February 2019 Dr. Alpha Tom Kodamullil was awarded the renowned Hugo Geiger Prize of the *Bavarian Ministry of Economic Affairs, Regional Development and Energy*. Her innovative approach to the analysis of the causes of Alzheimer's disease contributes to the development of new diagnostic methods and drugs. In her doctoral thesis, Kodamullil systematically combined relevant information on neurodegenerative diseases in so-called knowledge graphs. This work provides new insights into the relationships between different processes in the human body.

SCAI LIGHTS

Two of SCAI´s student assistants awarded with Ada-Lovelace-Prize for their theses

December 2017/18 Clelia Albrecht (right photo), student assistant at SCAI, has been awarded the Ada-Lovelace Prize for her master thesis. The mathematics graduate worked on the parallelization of adaptive gradient augmented level set methods. Albrechts colleague Andrea Cremer received the Ada-Lovelace-Prize for her bachelor thesis. She investigated how different methods of machine learning can be used to solve differential equations numerically. Both prizes are awarded by the Institute for Numerical Simulation at the *University of Bonn* and honor female mathematicians.

Bachelor thesis on deep learning strategies in Alzheimer´s diagnostics receives prize

September 2018 Helena Balabin, student assistant at Fraunhofer SCAI, was honored for her bachelor thesis. The University Society of the *University of Applied Sciences Bonn-Rhein-Sieg* awarded the work of the student in computer science with a prize money of 1000 euro. In her thesis, Balabin investigated the generalizability of deep learning strategies in Alzheimer's diagnostics. One of the advisors of Balabin's bachelor thesis was Prof. Dr. Martin Hofmann-Aptitius, head of SCAI's Department of Bioinformatics.

Prize honors excellent training of apprentices at the institute

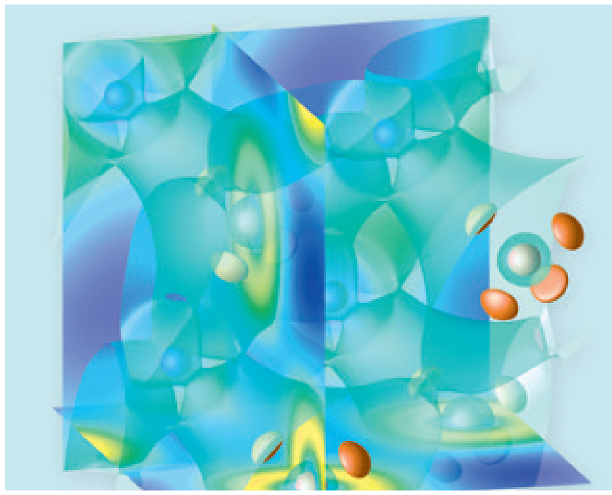
October 2018 Elisa Kagelmaker was awarded a certificate for her excellent final examination by the Chamber of Industry and Commerce (IHK) Bonn/Rhein-Sieg. At Fraunhofer SCAI, Kagelmaker completed her training as a mathematical-technical software developer (MATSE). The institute was also honored for its achievements in the training of apprentices. The institute offers the MATSE training as part of the "Scientific Programming" dual study program at the *FH Aachen University of Applied Sciences*, Cologne branch.

Spin-off project adiutaByte: Optimized route planning saves time for patient care

June 2018 SCAI presented the spin-off project adiutaByte at the CeBIT in Hannover. adiutaByte develops algorithms that optimize route planning enabling outpatient care services staff to spend less time on the road and more time with patients. Unexpected staff shortages or traffic jams are taken into account automatically and in real time. The algorithms can also be used in other business areas, for example, for optimal spatial planning in hospitals, optimized loading of container ships, and planning tasks in mail order.

Science Year 2018: optimum cutting of steel profiles as a child´s play

August 2018 SCAI participated in the Science Year 2018 with an interactive exhibit on the topic "Working Environments of the Future". The Science Years are an initiative of the *German Federal Ministry of Education and Research*. SCAI presented its software AutoBarSizer for optimized cutting of steel profiles on the science ship "MS Wissenschaft". Visitors were invited to try out whether their manual optimization corresponds to the solution provided by the software. AutoBarSizer helps planners in industry to avoid waste and to reduce production costs.



Fraunhofer SCAI contributes to the Cluster of Excellence at the University of Bonn

September 2018 SCAI is a partner in the *Hausdorff Center for Mathematics – Mathematics: Fundamentals, Models, Applications*, one of six clusters of excellence at the *University of Bonn*. SCAI contributes to the Interdisciplinary Research Unit (IRU) "Data driven material science". One aim is to advance the data-driven approach of material science from a mathematical perspective. Both empirical and simulated data are combined with data analysis methods, machine learning, high dimensional optimization and multiscale techniques.

Prof. Dr. Jochen Garcke

INTERVIEW: NEW METHODS FOR MACHINE LEARNING

Machine learning (ML) is a key technology for cognitive systems, intelligent products and digital assistants and plays a crucial role in the digital transformation of our economy and society. It is also changing computational science and engineering in fundamental ways. For realistically-sized problems, ML and its applications require a systematic use of HPC technologies. There is need to analyze, design, develop, and deploy ML methods as well as to develop scalable implementations for HPC and embedded systems.

What is machine learning?

Jochen Garcke: In its core, machine learning involves algorithms that automatically find patterns, signals, or structures within massive data sets. The exact nature of these patterns and structures is unknown and may be hidden. Therefore, it is not possible to program an algorithm exploiting them explicitly before a thorough analysis of the data. Instead, machine learning methods are employed for their semi-automatic detection. SCAI develops new intelligent and scalable methods for machine learning and adapts data analysis methods to concrete applications. We also investigate the mathematical basis of machine learning methods.

Are there efforts in the Fraunhofer Gesellschaft to meet the challenges of transferring ML into industrial practice?

In 2018, the Center for Machine Learning was launched as one of three centers in the Fraunhofer Cluster of Excellence *Cognitive Internet Technologies*. Here, SCAI and three other Fraunhofer institutes work on new algorithms and methods that combine data-driven learning with automated modeling as well as domain- and application-specific expert knowledge.

At SCAI, ML is a cross-sectional topic. Moreover, SCAI is involved in the Fraunhofer flagship project EVOLOPRO. The aim of this project is to give industrial production systems the ability to autonomously adapt to new requirements and environmental conditions. Fraunhofer SCAI leads the algorithm development in EVOLOPRO at the interface of transfer and multitask learning, evolutionary exploration strategies, and multi-fidelity modeling.

CONTACT

Prof. Dr. Jochen Garcke
Phone +49 2241 14-2286
jochen.garcke@scai.fraunhofer.de

www.scai.fraunhofer.de/en/ml

What are the key research areas of SCAI in ML?

It is well known that high-dimensional data – and this is usually the case with ML applications – typically form low-dimensional structures. Discovering and reconstructing these structures is important. Once they are known, it is possible to achieve a better understanding of the relationships in the data or to significantly reduce the computing times required for training an ML model. Our methods can discover and calculate such low-dimensional representations of the data, e.g., to represent data from simulations in a geometry-aware basis. Another focus of our work is informed machine learning.

What is informed machine learning?

In many real life machine learning applications, there are situations where data-driven approaches find their limits, in particular in engineering. Often, there is not enough labeled data to train good ML models. Or a data-driven model is not physically consistent or does not follow constraints stemming from regulatory or security guidelines. Here, informed machine learning comes into play as a form of hybrid learning, where domain knowledge is directly integrated into the ML process. This also helps to make ML models more transparent, interpretable, and explainable. A specialty of SCAI is ML for physical-technical applications, where, for example, domain knowledge is exploited in the form of numerical simulations. This is also called simulation-based ML.

Which applications benefit from informed ML?

Particularly in the natural and engineering sciences, an informed ML approach offers much more reliability for predictive analysis. We develop mathematical concepts that integrate physical properties and behaviors into ML methods. They simplify work processes and allow engineers to focus on the important aspects of their work.

Can you give an overview of the explored applications?

Examples for applications of ML at SCAI are manifold:

- In the predictive maintenance of technical systems using sensor data, ML methods form the algorithmic core. For example, we have investigated wind turbines. ML methods are able to detect anomalies in the data of vibration sensors, which were originally measured to detect the formation of an ice layer. But these measurements of the vibration of the rotor blades provide more information and – using ML – possible future damages become apparent.
- In biomedicine we use ML in particular to recognize patterns and correlations in the data. Here, it becomes increasingly important to compare the personalized data directly with the current knowledge, which is present in the current medical literature. The use of text mining methods helps to extract relevant data and connections. For example, an information extraction workflow from SCAI can be used for knowledge representation and assembling causal biological network models.
- In virtual product development, ML methods simplify and accelerate the research and development process, for example in the automotive industry.
- Further application areas are data-driven energy management, virtual material design, finance, and smart robot systems that can cooperate safely with humans.

How will ML influence the future work of engineers?

The design process of machines and plants is changing, e.g. through "digital twins" – a representation of the machine as a data set. Simulations of an overall system like, e.g., an aircraft, will become the rule for many other applications. ML makes it possible to combine and analyze the data from real operations together with the development and simulation data. In this way, the entire process can be understood much more precisely, better products can be developed, and the operation of plants can be optimized.

Prof. Dr. Martin Hofmann-Apitius

INTERVIEW: COMPUTER SCIENCE FIGHTS ALZHEIMER'S

More than 46 million people worldwide suffer from Alzheimer's disease (AD) – with an upward tendency. And there are still no drugs that can cure AD. The causes of AD have hardly been researched although they are crucial in the search for agents. The AETIONOMY project, funded by the European Innovative Medicine Initiative (IMI), has identified more than 120 disease mechanisms. Until the end of 2018, Fraunhofer SCAI, together with its European partners, investigated the molecular causes of AD and Parkinson's disease. In the last few months, three follow-up projects were launched. Prof. Dr. Martin Hofmann-Apitius, Head of the Department of Bioinformatics, explains what has been achieved so far and what is planned for the future.

What were the key challenges in AETIONOMY?

Martin Hofmann-Apitius: The processes that lead to Alzheimer's are believed to start 20 to 30 years before the diagnosis. The challenge we faced was to understand the activators of the disease without being able to examine the affected brain at that time. Therefore, we first used the knowledge discovery software SCAIView, an advanced literature mining tool, to extract relevant knowledge from existing publications and to link the extracted information in "cause-and-effect" networks. The resulting knowledge graphs show connections between molecular and physiological processes in the human body. By applying this method at a large scale, we systematically compared the knowledge graphs of healthy and diseased brains. This is how we were able to identify more than 120 disease mechanisms.

AETIONOMY provided even more insights. You have developed a new system for classifying Alzheimer subtypes.

Exactly. Based on these mechanisms, we have developed a new system for the classification of Alzheimer's subtypes and we have tested it with independent data. In order to validate our first version of a mechanism-based taxonomy, we even did our own clinical study on Parkinson's patients in AETIONOMY. For the validation of our Alzheimer mechanism-based taxonomy, we await eagerly the first data from the IMI project EPAD, which has recruited thousands of AD patients for a prevention trial platform. Testing our taxonomy on the EPAD cohort will allow us to check even pre-symptomatic patients, i.e., we test our taxonomy on subjects that do not yet show any clinical symptoms. If the taxonomy works in the EPAD cohort, this would mean a breakthrough.

CONTACT

Prof. Dr. Martin Hofmann-Apitius
Phone +49 2241 14-2802
martin.hofmann-apitius@scai.fraunhofer.de

www.scai.fraunhofer.de/en/bio

What are the advantages of this classification system?

Until now, diseases have been classified on the basis of clinical symptoms. The roots for our current disease classification system go back to the work of William Farr in 1855. This was a long time before we even had the slightest idea about what "genes" and what "proteins" are. Accordingly, drug discovery research has been dominated by a focus on disease symptoms. New findings – for example from molecular biology – have not been taken into account for some time, but of course, the pharmaceutical industry is adapting fast now. Research on molecular causes significantly increases the chances of finding a drug that prevents dementia. Understanding mechanisms is therefore a pre-requisite of what we call "precision medicine". And of course: Different causes of disease require different agents that interfere with different pathophysiology mechanisms. The mechanism-based taxonomy we have developed considers the different molecular causes of neurodegenerative diseases and thus will hopefully make it possible to find the right drug for the patient in question.

Recently, three more projects have been launched. What are the goals of these projects?

With the »VirtualBrainCloud« project, we want to lay the foundations for personalized simulation of neurodegenerative processes. In this project, we bring the outcome of AETIONOMY to the most powerful brain simulation environment worldwide: The Virtual Brain (TVB). So far, TVB could not make use of already existing knowledge as a "prior" for its simulation. However, knowledge graphs, as we have generated them in the course of AETIONOMY, can be used to constraint simulations. If we know what mechanisms actually influence essential pathophysiology processes in the brain, we can use this "a priori" knowledge to constrain the quantitative simulation of these pathophysiology mechanisms in TVB.

The aim of the IMI project RADAR-AD is to develop digital signatures that are objective measures for cognitive impairment or cognitive decline of AD patients. The concept is to make use of sensors and digital devices (e.g. smartphones) and to create a wealth of digital signatures that can be correlated with cognitive decline and onset of dementia in follow-up studies. SCAI's contribution concerns the correlation between digital signatures and the progression of disease as modeled in the course of EPAD.

The ROHAN project, which is part of the medical informatics platform of the Human Brain Project, aims at generating ontologies for brain diseases and at preparing them in such a way that they can be used for literature mining and metadata annotation. Ontologies and terminologies are essential building blocks for explicit and shared semantics in any project and whenever we want to enable other researchers to find and access our data, whenever we make our data interoperable and re-useable, we need this sort of "shared semantics". This is why we contribute not only ontologies and terminologies, but also the software services that allow to use them.

How would you summarize the role of the department?

Understanding correlations, simulating brain communication pathways, and identifying causes of diseases – these are important topics in our AD research. We always understood our role as builders of bridges – bridges between different funding programs and communities. Our portfolio of projects in AD shows how important this bridge-building can be.

SELECTED SOFTWARE SOLUTIONS

PACK Assistant	Optimized 3D packing design	*PackAssistant* is the leading 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 the production of rectangular parts from rectangular stock material and minimizes waste, production times and manufacturing costs. It generates layouts that can be produced with straight, continuous (guillotine) cuts. **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 material (long material) into shorter parts (fixed dimensions). The generated solutions are characterized by a high degree of material utilization, cutting losses are minimized. **www.scai.fraunhofer.de/en/autobarsizer**
CUT PLANNER automatic cut planning	Automatic cut order planning	*CutPlanner* is a software package for use in the textile manufacturing industry for the automatic planning of cut orders. *CutPlanner* takes a customer's order for a clothing item and creates a cut plan for that item, including different sizes, fabric types, or colors. **www.scai.fraunhofer.de/en/cutplanner**
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* in order to optimize the product design. **www.mpcci.de**
MpCCI Mapper	Considering the manufacturing of automotive components in crash simulations	The *MpCCI Mapper* handles data interpolation and data conversion between codes in complex simulation workflows. In crash simulations, the manufacturing process of automotive components is taken into account, which increases 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 CFD or FEM simulations, taking care of different mesh densities or orders. **www.mpcci.de/fsimapper**

SAMG Algebraic Multigrid Methods for Systems	Algebraic multigrid methods for systems	*SAMG* is a software package for the highly efficient numerical solution of large systems of equations. Such systems occur, for example, in fluid and structural mechanics, oil reservoir and ground water simulation, process and device simulation, and circuit simulation. **www.scai.fraunhofer.de/en/samg**
MYNTS	Simulation and optimization of energy transport networks	*MYNTS* is a multiphysical network simulator which can be used for the analysis and optimization of electrical circuits, gas and energy transport, and water distribution. Users can program subnetworks and individual special elements. **www.scai.fraunhofer.de/en/mynts**
PRO MINER	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. *ProMiner* can handle voluminous lexica, complex thesauri and large expert-controlled vocabularies. **www.scai.fraunhofer.de/en/prominer**
SCAI VIEW	Knowledge discovery in life sciences	*SCAIView* is a knowledge discovery software used in the life sciences. It 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. *ModelCompare* compares two similarly discretized FE models and identifies their differences in geometry (mesh), material and thickness. **www.scai.fraunhofer.de/en/modelcompare**
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 projects addressing a wide range of application fields, such as nanotechnology, materials science, biochemistry and biophysics. **www.tremolo-x.com**
MESHFREE	Powerful simulation tool for complex geometries and physics	MESHFREE is a software tool for flow and continuum mechanics. It is developed in cooperation with Fraunhofer ITWM. MESHFREE is particularly suited for transient flows with moving geometry parts, free surfaces, phase boundaries, and large deformations. **www.meshfree.eu**
scapos	Fraunhofer SCAI's software packages are distributed by scapos AG: www.scapos.com	

DIGITAL TWINS

As part of the digital transformation, more and more industries realize the potential of digital twins for system optimization and behavior prediction. Research and development at Fraunhofer SCAI address several aspects of this promising but highly complex topic.

A digital twin is a detailed digital representation of a physical system that describes the current and potentially past states of the system. Early versions of this concept from around the year 2000 implied a comprehensive database of digital information spanning the entire life cycle of the system. Today, it is clear that the full potential of the concept can only be exploited if a digital twin entails integrated multi-physics-multi-scale simulations that are matched against sensor data and provide high-quality, real-time predictions of system behavior.

Apart from few quite specific applications, high-fidelity digital twins are currently more vision than reality. The National Aeronautics and Space Administration and the Air Force in the United States, which define the digital twin as a key technology in their technical roadmaps, estimate a 25 year development frame to realize full-fledged digital twins. The general challenges are heterogeneity of data, complexity in the interaction of models, and flexibility in the event of unforeseen changes in requirements. However, with digital sensor technology and computational resources constantly improving, the concept is becoming more and more interesting for various branches of industry. Fraunhofer SCAI – with its strong background in machine learning, optimization, and numerical simulation – contributes in many ways to progress in the development of digital twins. Application areas at SCAI include new materials, manufacturing, and life sciences, while digital twins for energy networks are starting to emerge as a component for the energy transition.

Simulation, coupling, and standardized interfaces

A new ingredient for the realization of digital twins are numerical simulations. Here, SCAI has developed numerous software packages for the simulation and optimization of industrial applications. Recent developments are the flexible simulation environments PUMA and MESHFREE, which are particularly suited for large changes in geometry and topology.

With the MpCCI CouplingEnvironment, SCAI offers a vendor-neutral solution for the coupling of simulation programs for different physical disciplines. MpCCI thus allows a more comprehensive digital simulation than conventional mono-disciplinary codes and has established itself as the de facto standard for multiphysics simulations.

Complex engineering workflows represent a further step in the direction of digital twins. The lack of software standards in virtual engineering workflows and incompatible interfaces for the transfer of virtual material information not only causes additional costs and complex manual adjustments, but also leads to inflexible IT solutions, loss of information, and considerable delays in the entire design process. The standardization of material interfaces in computer-aided engineering (CAE) is therefore of decisive importance whenever material behavior is at the center of product and process design. The European VMAP project, coordinated by Fraunhofer SCAI, aims at a common understanding and interoperable definitions for virtual material modeling in CAE.

Model generation and validation

High-fidelity simulations continue to be too expensive for many applications such that meta modeling remains a highly relevant topic. In the context of digital twins, model validation based on local quantities of interest reaches its limits. It requires more complex similarity and quality measures that take complete geometries into account, e.g., to gain a deeper understanding of car crashs. In several projects, compact data-driven representations for large simulation bundles have been developed. The SCAI software DesParO, a toolbox for the intuitive exploration, automatic analysis, and optimization of parameterized problems in production processes, supports the generation of multi-level meta models. The new Fraunhofer flagship project EVOLOPRO investigates methods of multitask and transfer learning to enable more efficient surrogate modeling across multiple stages in process chains. In the MADESI project, SCAI investigates how the interaction of sensor data and numerical simulation can be used to increase the capabilities of machine learning methods for the predictive maintenance of wind turbines.

Digital twins down to the material level

Experiments and simulations are used on many scales to better understand processes and improve their usage. In addition to macroscopic simulations as mentioned above, SCAI is addressing high-resolution sensor data in the millimeter range in the Fraunhofer DigitalTPC project. This requires the acquisition and processing of high-resolution sensor data. This information is used to detect defects in the fiber structures of thermoplastic composite tapes at an early stage and to optimize subsequent work steps (e.g. laying processes) accordingly. The heterogeneous microstructure of the composite material and its influence on the manufacturing process poses a challenge for process control and quality assurance and requires continuous digitization of the production process. In this context, SCAI is involved in numerical simulations for the development of new materials with improved properties, in particular with the software Tremolo-X for material models on the atomistic scale.

Virtual patients in dementia research

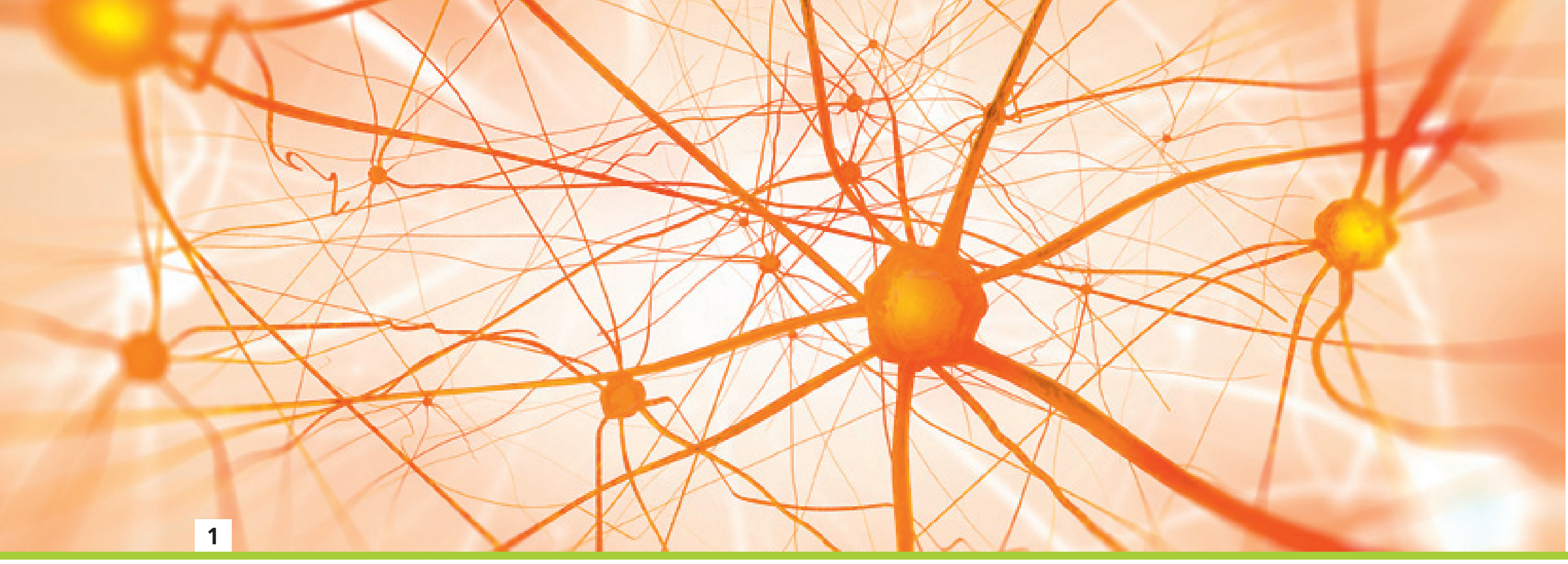
The concept of a digital twin has recently also been adopted by the Innovative Medicine Initiative (IMI) project AETIONOMY in the form of a virtual dementia cohort (VDC). A complete VDC is a derivative of a real-world clinical study; it represents all relevant variables and the dependencies between these variables that have been measured in the clinical study. Such VDCs allow to simulate huge numbers of virtual patients that do not differ from real-world patients. VDCs open completely new perspectives for Alzheimer research – ranging from sharing of patient-level data without compromising patient-data privacy to clinical trial simulation.

CONTACT

Prof. Dr. Jochen Garcke
Phone +49 2241 14-2286
jochen.garcke@scai.fraunhofer.de

www.scai.fraunhofer.de/en/dt

Digital twins help to optimize the operation of wind turbines.



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BIOINFORMATICS

Worldwide, there is no shortage of ideas on how neurodegenerative diseases such as Alzheimer's can develop. However, there is a definite lack of a comprehensive model of such a disease with which new targets can be identified. The work in the business area *Bioinformatics* contributes to the development of knowledge-based models for neurodegenerative diseases.

Bioinformatics covers a broad spectrum of technologies and competencies, ranging from data, information and knowledge management in the life sciences to technologies for information extraction and retrieval. The department cooperates closely with partners from industry – including small and medium-sized enterprises – to improve their competitiveness through the transfer of knowledge and technology from academic research to industrial application. The collaborative research and development projects of the business area provide solutions for the pharmaceutical industry, the biotech industry and the life science software industry.

Positioned at the interface between commercial and academic research, the department maintains strong links to both communities and actively participates in various national and European research initiatives. Furthermore, the department is involved in the education of students of the Life Science Informatics curriculum of the *Bonn-Aachen International Centre for Information Technology* (B-IT).

The activities of the department cover four research fields: modeling of neurodegenerative diseases, information and knowledge extraction in the life sciences, applied chemistry informatics, and scaling life science software services.

Modeling of neurodegenerative diseases

The modeling of neurodegenerative diseases addresses an emergent research area in the field of dementia diseases. The competencies in this field include

- the generation of knowledge maps for psychiatric indications such as the post-traumatic stress syndrome,
- the generation of entire semantic frameworks that include disease-specific ontologies (e.g. Alzheimer´s Disease Ontology, Parkinson´s Disease Ontology or Epilepsy Ontology) as well as specific terminologies,
- the modeling of neurodegenerative diseases such as Alzheimer's or Parkinson's,
- the development of predictive longitudinal models based on data from clinical studies,
- the further development of algorithms for the analysis of knowledge-based models, which establish causal and correlative relationships between genes and clinical parameters (patient-level data).

CONTACT

HEAD OF BUSINESS AREA
Prof. Dr. Martin Hofmann-Apitius
Phone +49 2241 14-2802
martin.hofmann-apitius@scai.fraunhofer.de

www.scai.fraunhofer.de/en/bio

Information and knowledge extraction in the life sciences

Biomedical knowledge is for the most part not available in databases, but only in unstructured text (publications in journals and on websites). Due to around 3500 new biomedical publications per working day, up-to-date information can only be extracted with the help of computers. Our modular information extraction services can be flexibly combined and thus quickly adapted to different requirements.

Applied chemistry informatics

Chemistry informatics is a key application of computer science in the pharmaceutical industry. It mainly deals with methods for the description, modeling, simulation and prediction of low molecular weight substances and high molecular weight biopolymers including their interactions. In this field of research SCAI is developing a novel knowledge resource, the "Human Brain Pharmacome" (HBP). The HBP is a so-called drug-target network, which comprises the majority of active substances active in the human brain and their target proteins. In addition to this model-like representation of knowledge, HBP also allows for the prediction of new potential active substances and supports the simulation of drug-target interactions.

Scaling life science software services

Here SCAI develops a new scientific benchmark, the mapping of the entire PubMed literature database as a gigantic knowledge graph. This knowledge graph will be linked to the human genome as far as it contains specific human objects such as genes and proteins, miRNAs and gene polymorphisms. This approach results in a graph density distribution and a graph topology of knowledge *about the genome* that can be used to predict *unknown knowledge*. The genome has its own topology, which can be visualized by specialized 3D genome browsers. The next big challenge is to improve the genome topology with its implicit functional relationships to the topology of the knowledge graph.

Project AETIONOMY

Until recently, research on the modeling of neurodegenerative diseases was not computer-driven; the AETIONOMY project, however, has impressively shown that current hypotheses on the development of Alzheimer's can be represented in computeable models. The candidate mechanisms predicted in the computer can distinguish patient subgroups in clinical data and thus prove that a mechanism-based taxonomy can be generated even in the context of idiopathic diseases. However, the more empirical disease hypotheses of clinical partners showed no real potential for mechanism-based stratification of patients. AETIONOMY has thus demonstrated the potential of computer science methods in dementia research.

1 Neurons in the human brain.
2 Knowledge graphs illustrate the information extracted from medical literature on a brain affected by Alzheimer's (left) and a healthy brain.
3 Information extraction from medical texts using the SCAI software ProMiner.

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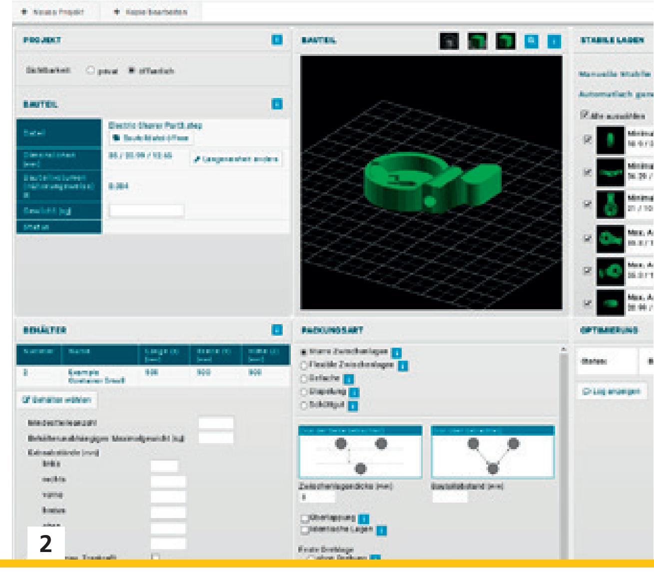

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OPTIMIZATION

The efficient utilization of resources and associated cost savings are of fundamental importance in industrial practice. Whenever transport and storage capacities or existing material are to be exploited optimally or when production facilities are to be operated efficiently, complex optimization tasks have to be solved. In such cases, algorithms can provide amazing improvements in production, trade, and transportation of goods by solving the corresponding application problems.

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

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

Depending on the structure of the problems to be solved and according to the underlying problem specific constraints, the software packages employ the most appropriate state-of-the-art optimization techniques, enriched with the special knowledge and improvements of SCAI. Typical optimization techniques for such optimization problems are branch and bound, simulated annealing, great deluge, record-to-record travel, genetic or evolutionary algorithms, simulated trading, greedy algorithms, tabu search, linear and integer programming, multi-objective optimization, or ant colony optimization.

AutoNester

AutoNester is a software package for the automatic marker making on fabrics, sheet metal, wood or other materials. It is widely used in the garment and upholstery manufacturing industry. AutoNester is able to nest any set of pieces within a very short time in an optimal way, minimizing wasted material while taking various types of constraints into account. The efficiency of the markers achieved by AutoNester is competitive with experienced human nesters. The AutoNester software is organized as a Dynamic Link Library (DLL) that can be used as a developer tool kit. Developers of CAD systems can integrate AutoNester-T into their software.

The business area also offers the creation of custom-made stand-alone applications for the end user which can be used to create markers from special data formats. A special version for automatic marker making on leather hides is available, too.

CutPlanner

CutPlanner is a software package for use in the textile manufacturing industry for automatic cut order planning. A cut plan is an assignment of sizes and fabric types to markers. For each of these markers, the required number of plies is computed to fulfill the requirements of the order. The objective of CutPlanner is to minimize overall production costs.

PackAssistant

PackAssistant calculates the ideal filling of (storage or transport) containers with identical parts in just a few minutes. The software is used worldwide by numerous manufacturers and suppliers, especially in the automotive industry. PackAssistant enables the user to handle different types of packaging. These include packing with solid or flexible intermediate layers, with compartments or in stacks, and the simulation of bulk goods.

AutoPanelSizer

AutoPanelSizer determines optimized cutting layouts for the production of rectangular parts from rectangular stock material and minimizes waste, production times and manufacturing costs. All layouts generated by AutoPanelSizer refer to straight, continuous (guillotine) cuts. For interlinked plants, the number of existing cutting stages is also taken into account. Thereby, the software models a common cutting technology, applied in the machining of wood and also in the glass, metal, and plastics manufacturing industries.

AutoBarSizer

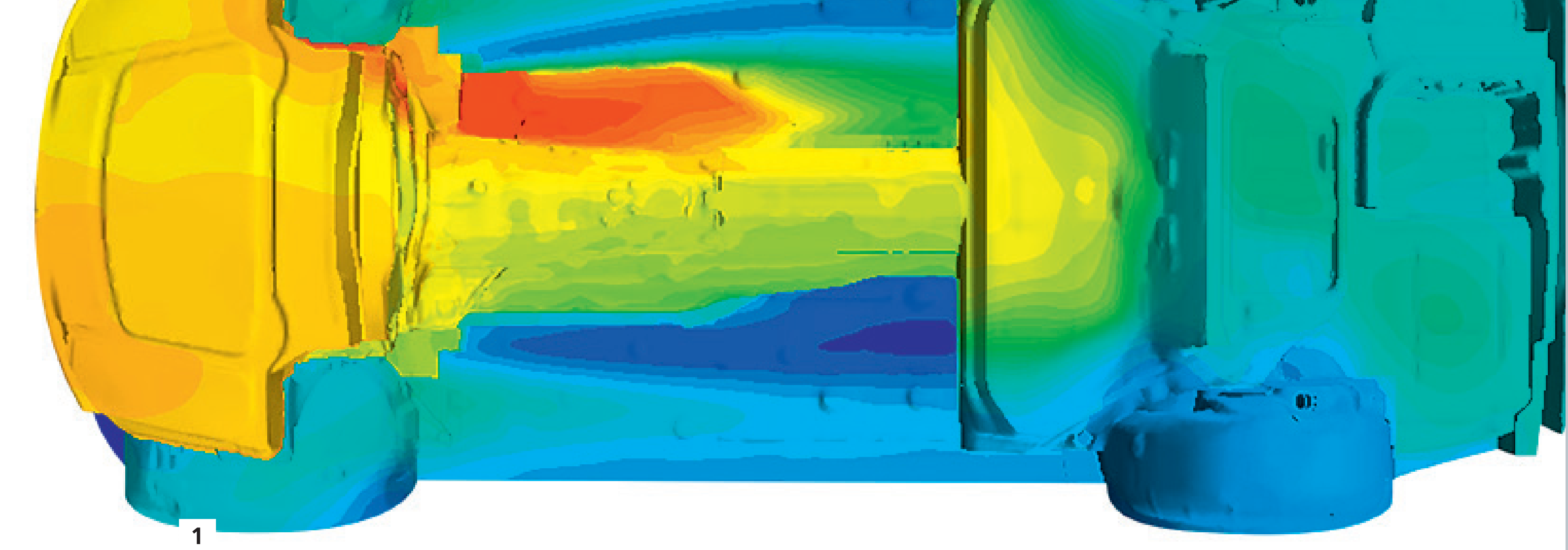
AutoBarSizer generates optimized layouts for the cutting of stock items, namely steel profiles (metal beams) and other bars and rods, into shorter pieces. The generated layouts achieve an extremely high degree of material utilization (yield), i.e. the cutting waste is minimized. The planner can also use various parameters to balance yield and additional organizational effort caused by the reusable remainders produced. When creating layouts with miter cuts, AutoBarSizer also optimizes the interleaving (nesting) of parts. The software solves planning issues not only for rolling mills and steel traders, but also for the woodworking industry and manufacturers of »material strips« of all kinds.

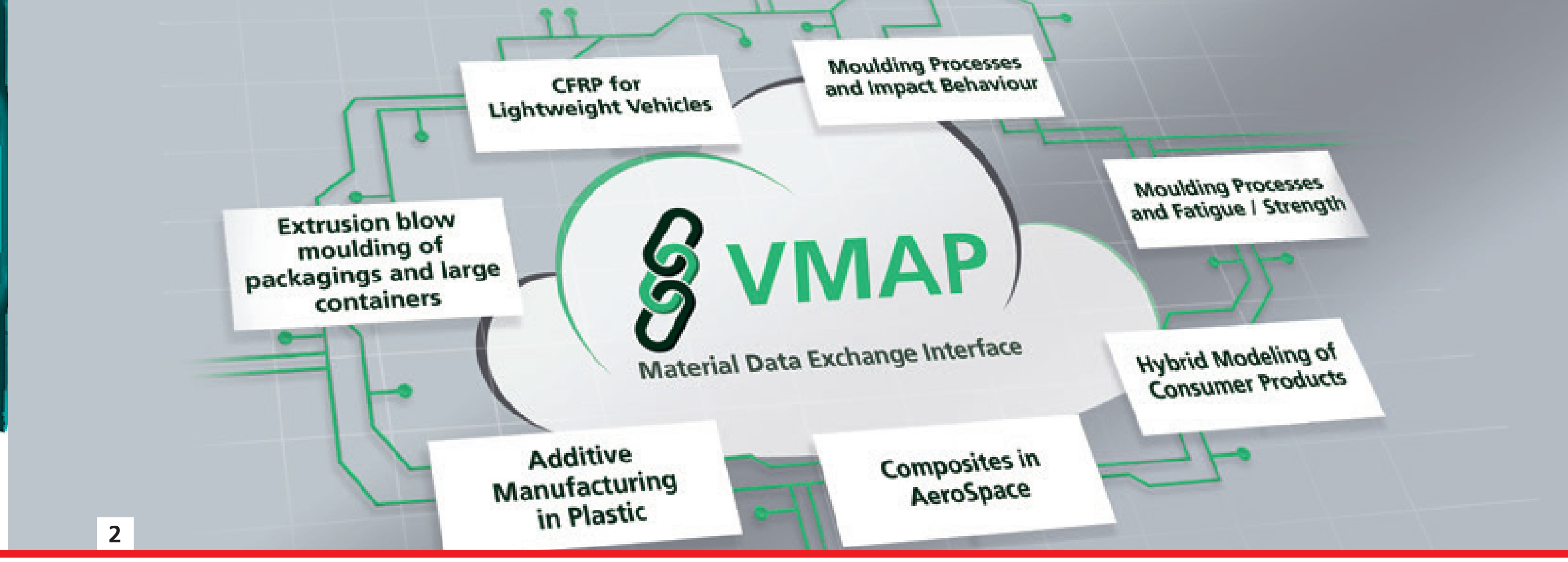
CONTACT

HEAD OF BUSINESS AREA
Dr. Ralf Heckmann
Phone +49 2241 14-2810
ralf.heckmann@scai.fraunhofer.de

www.scai.fraunhofer.de/en/opt

1 Cutting layouts generated by AutoPanelSizer.
2 The newly designed PackAssistant 4 user interface enhances navigation and leads to a more intuitive operation.
3 AutoNester-T minimizes wasted material. The picture shows an optimized nesting layout for skirts.





MULTIPHYSICS

Aeroelasticity in aircraft design, deformations and thermal loads in turbomachinery, car-ground interaction, automotive thermal management, electric arcs in switching devices, in-vitro toxicology, aortic stent design, and complex manufacturing workflows – all these applications have one thing in common: They make use of multiphysics simulations.

The term multiphysics denotes simulation applications that combine different physical disciplines, e.g., fluid-structure interaction. Depending on the application, the interaction of the individual simulation disciplines can be realized by bidirectional simulation couplings or by a file-based result exchange.

Key topics in the *Multiphysics* business area are the development of methods and software solutions for tasks in which effects from several physical disciplines have to be taken into account. The core of these developments is the *MpCCI Coupling Environment*. This software provides a vendor-independent solution for simulation coupling and file-based data transfer and supports a large number of commercial and research codes from different application disciplines. *MpCCI CouplingEnvironment* has an open interface to application programs (API) which can be used to connect internal or new commercial codes.

The business unit *Multiphysics* conducts research, software development and application modeling on several levels:

- Expansion and improvement of MpCCI interface software and internal algorithms
- Development of application solutions
- Engineering services and participation in research and development projects on new topics in the field of multiphysics

The department cooperates with many providers of commercial simulation programs and developers of university research codes. In the ongoing development of MpCCI, the business area works closely with the world's leading software vendors, including

- ANSYS Inc.
- CD adapco Group
- Cedrat SA
- Ceetron
- CEI
- JSOL
- Mentor Graphics
- MSC
- NUMECA Intl.
- SIMPACK AG
- Simulia 3DS
- ThermoAnalytics Inc.

CONTACT

HEAD OF BUSINESS AREA
Dipl.-Inform. Klaus Wolf
Phone +49 2241 14-2557
klaus.wolf@scai.fraunhofer.de

www.scai.fraunhofer.de/en/mp

Applications

Multidisciplinary problems arise in many fields of application. Some application areas in which MpCCI has recently been used are:

- Aeroelasticity and mechanical engineering (aerodynamics in racing vehicles, aeroelastic effects in aviation)
- Turbomachinery applications (influence of turbine blade deformation on flow)
- Vehicle and machine dynamics (extreme loads on individual components, influence of external flows on vehicle dynamics)
- Thermal management in automotive engineering (combination of numerical fluid mechanics with efficient radiation models, complete vehicle models)
- Electrical installations (electric arc in switches, dynamic loads and vibrations in electric motors)
- Process chains for passive safety (crash behavior and lifetime prediction through integrated process chains in computer-aided engineering, comparison of simulation and experiment)
- Numerical simulation in the life sciences (development of a system for aerosol measurement, microfluidics)

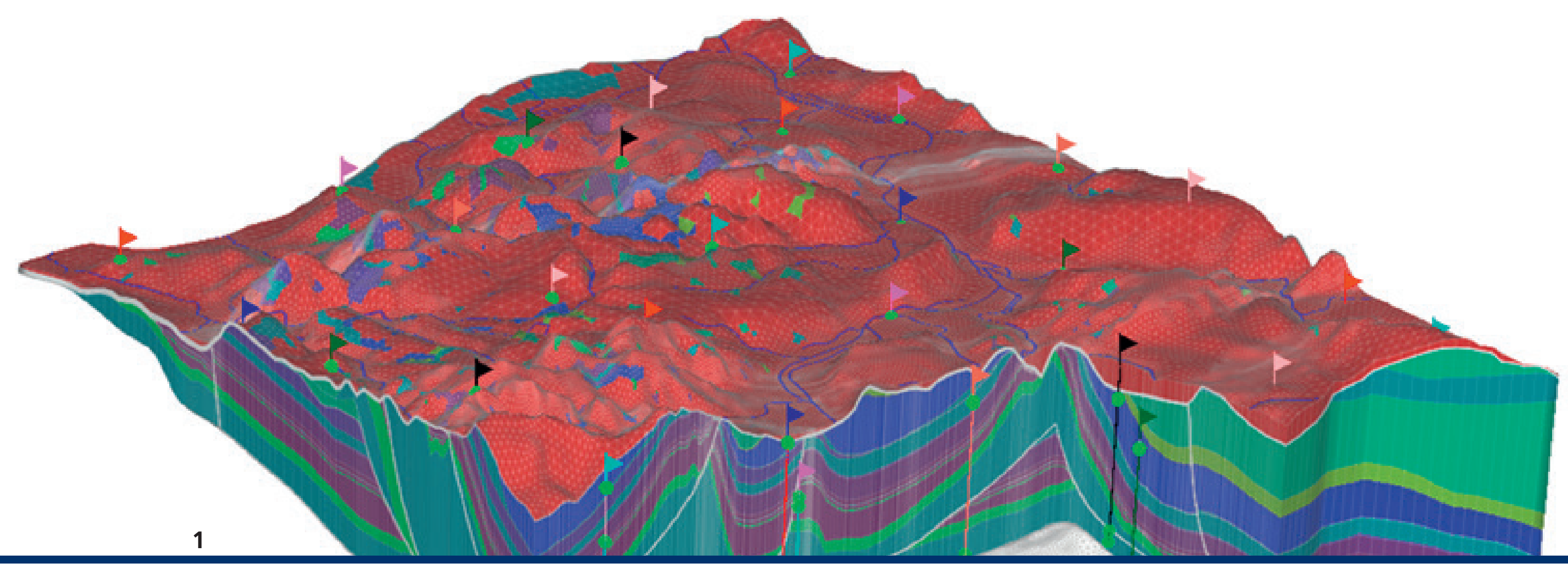
Further examples of multiphysics applications are thermal stress analysis in vehicles, engines or turbines (influence of hot flows on structural components), the dynamic behavior of flexible components under flow loading (valve flaps, aircraft wings, hoses) or process chain integration (complex manufacturing processes) for vehicle body components.

Project VMAP – virtual material modeling in manufacturing

The lack of software standards in virtual engineering workflows causes enormous additional costs for manufacturing companies. Incompatible interfaces for the transfer of virtual material information require complex manual adaptation work, lead to inflexible technical solutions, cause loss of information, and finally lead to long delays in the overall design process.

The VMAP project will create new concepts for a universal material exchange interface for virtual engineering workflows. These concepts will be concretized in an open software standard. They will be implemented in a number of software tools and the benefits of integrated material handling will be demonstrated with six industrial use cases from different manufacturing areas and industry segments. VMAP is funded by the *German Federal Ministry of Education and Research* via the ITEA3 cluster of the European EUREKA initiative. The project started in September 2017 and will be finished by the end of August 2020.

1 Thermal management for automotive underhood.
2 Industrial use cases in the project VMAP.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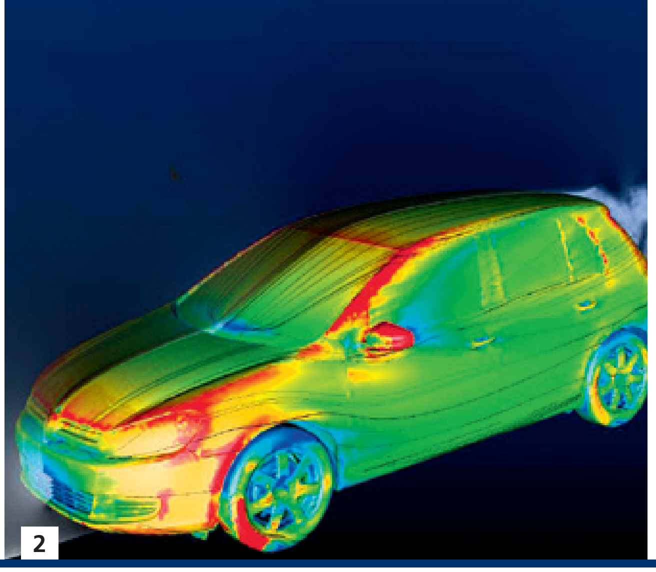
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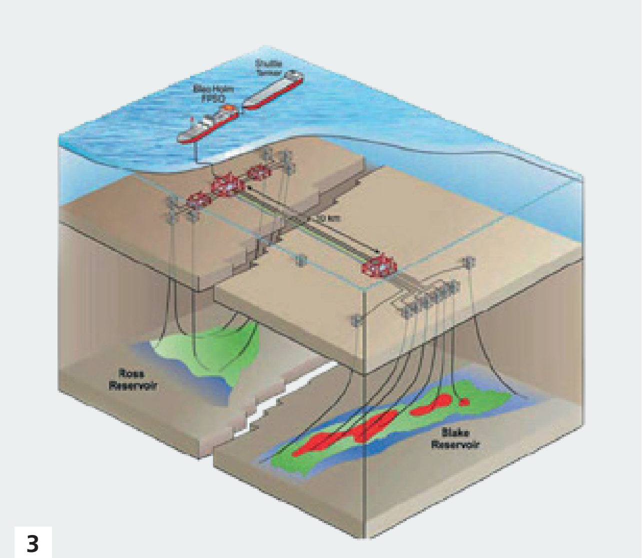

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FAST SOLVERS

With increasing modeling complexity and problem size, the computing times of almost all simulation codes become a bottleneck. Large simulations often enough take far too long to be used efficiently in industrial practice. Typically, the solution of huge linear equation systems with millions of unknowns is by far the most time-consuming part of many numerical simulations. Thus, it becomes increasingly important to reduce the computing times for the solution of large systems of equations in simulation software.

Computer simulations are used in many branches of industry to reduce development times, to replace complex experiments, to design prototypes more cost-effectively, or to optimize production processes. In many cases, large systems of linear equations with sparse matrices have to be solved. This task usually requires a large, often even the largest part of the computing time for the overall simulation. The SCAI library SAMG (Algebraic Multigrid Methods for Systems) contains algorithms for the highly efficient solution of such systems of equations. It is offered to customers from industry and science as a licensed product. Efficient parallel versions are available, too.

Compared to classical methods (e.g., preconditioned conjugated gradients), SAMG uses hierarchical multigrid techniques, which have the unique feature of numerical scalability. This means that the larger the systems of equations are, the greater the acceleration that can be achieved with SAMG compared to classical solution methods. This scalability of SAMG leads to significantly shorter computation times in industrial practice and makes highly complex simulations possible.

SAMG is constantly being enhanced according to customer requirements. The properties of new classes of systems of equations to be solved with SAMG, regardless of their sheer size, also become mathematically more and more complicated. The purely numerical research for the extension of SAMG is therefore an ongoing process.

SAMG is used commercially in many areas, such as oil reservoir simulation, fluid mechanics, structural mechanics, foundry technology, groundwater simulation (for which the special version SAMG-MODFLOW was developed), hydrothermal simulation, process simulation in semiconductor physics and circuit simulation.

CONTACT

HEAD OF BUSINESS AREA
Dr. Hans-Joachim Plum
Phone +49 2241 14-2350
hans-joachim.plum@scai.fraunhofer.de

www.scai.fraunhofer.de/en/samg

SAMG is available in several versions:

- SAMG, OpenMP parallel (for users who need pure multicore / multithreading parallelism)
- SAMGp, MPI / OpenMP hybrid parallel (for computing clusters with distributed parallelism, combinable with multithreading)
- XSAMG (uses the parallelism of a computing cluster by automatically distributing the data to several nodes; the higher-level simulation program itself does not need to be designed for a parallel cluster infrastructure)

SAMG offers certain add-on features and interfaces for some specific application areas:

- Oil reservoir simulation and geomechanics
- Groundwater modeling
- Elasticity
- Meshless simulations
- Problems with constraints

Approaches and working methods of the team

The SAMG team not only supports and advises customers from industry and science, but also works on the further development of the software and on projects – publicly or bilaterally with current and potential customers. The consulting services are customer- and application-specific. The team supports customers in the optimal integration of SAMG into their applications and in the choice of optimal parameter settings for SAMG, tailored to their respective applications. SAMG includes the most relevant multigrid approaches in optimized form. The department cooperates with global leading experts (Marian Brezina, John Ruge, Klaus Stüben).

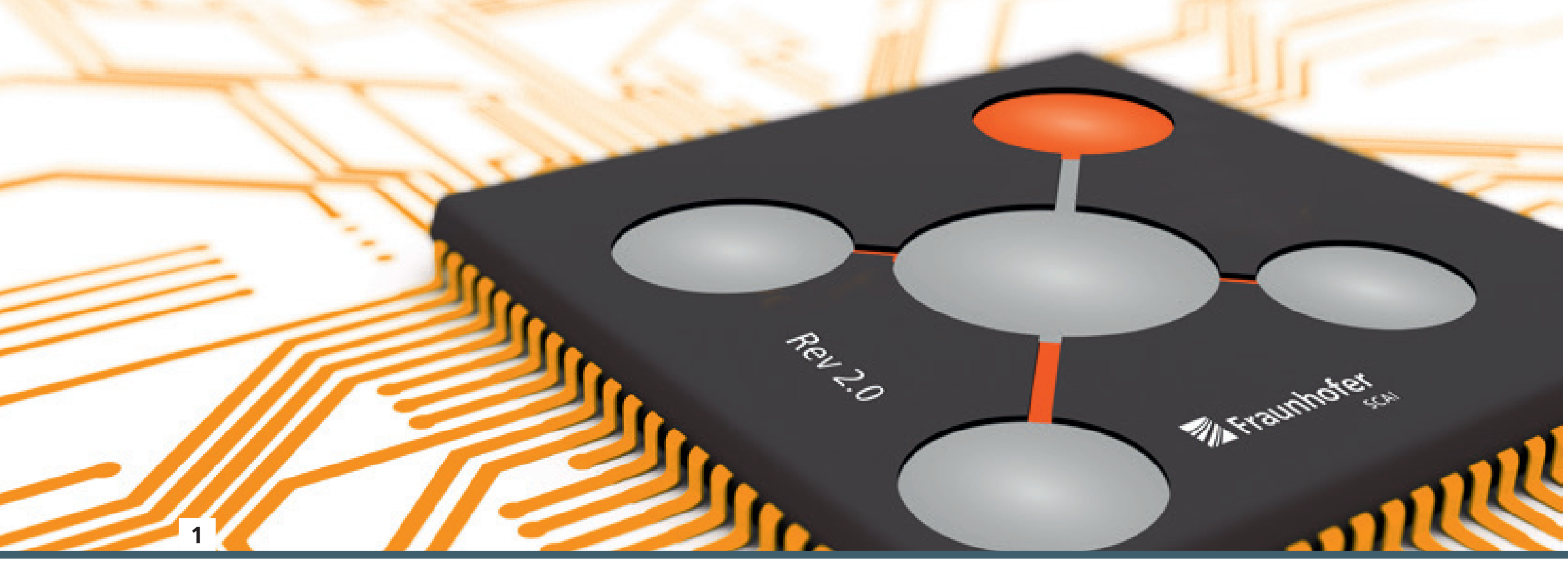
Selected applications

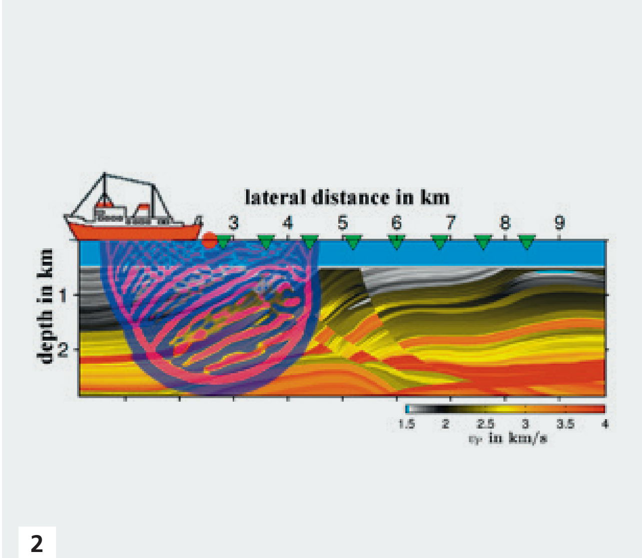
Oil reservoir simulations are essentially based on structures which are predestined for the application of algebraic multigrid methods. However, the high physical complexity prevents these structures from being directly usable. Rather, a preparatory step and a targeted adaptation of the AMG strategy are required in order to be able to successfully use algebraic multigrid methods. The new interface SAMG-OIL performs the adaptations in a graybox manner by taking basic physical information into account.

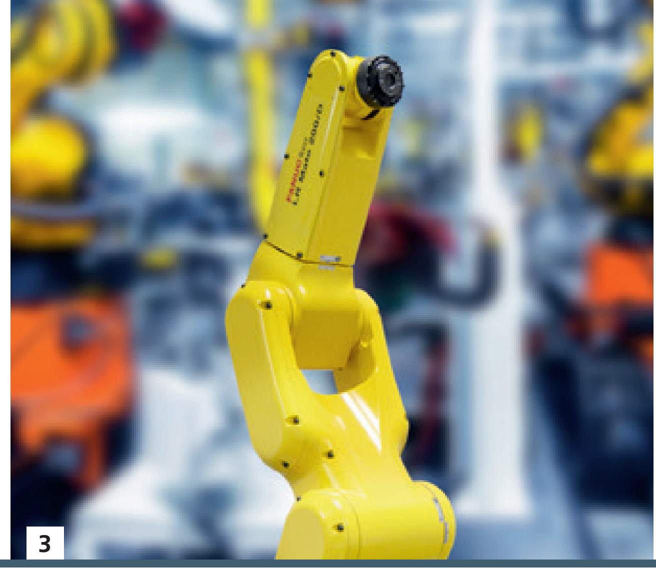
A version of the OpenFOAM computational fluid dynamics software package in which SAMG has been integrated is of particular interest to the automotive industry. An important aspect here is the parallel scalability of SAMG: Customers are now routinely computing on configurations of up to 2000 to 4000 processes.

Another interesting SAMG application for the automotive industry is the calculation of heat generation in the interior of cars under solar radiation.

1 Nuclear waste repository simulation in a complex geologic formation.
2 Numerical flow simulation around a complete vehicle.
3 Exemplary illustration of different wells and surface facilities of an off-shore field.







HIGH PERFORMANCE COMPUTING

High Performance Computing (HPC) is an enabler of the recent developments and tremendous success in the field of machine learning and big data. It connects research from mathematics, computer science (including hardware and software), and application fields such as engineering, natural sciences, economics, and many more.

In the business area *High Performance Computing*, Fraunhofer SCAI develops solutions to make computationally expensive algorithms quickly and efficiently executable on different hardware. The spectrum of target architectures ranges from embedded systems to multicore PCs, high-performance workstations with hardware accelerators and graphics processors to traditional upscaling supercomputers and – in the medium term – also to quantum computers.

There are two conflicting aspects in HPC: the optimal utilization of the features of different computer architectures and the minimization of the amount of code that has to be adapted to the hardware properties. SCAI´s approach is to separate the technical aspects of the implementation from the tuning of relevant parts for a specific hardware architecture. For this reason, the SCAI researchers use their own domain language approaches and compiler frameworks.

This approach is suitable for applications in many areas, such as intelligent machine control, satellite data analysis or a complex simulation program. The department supports partners and customers in optimizing applications from various areas for current hardware architectures.

At the same time, the department ensures that all software developments are prepared for a seamless transition to future hardware architectures. This not only keeps maintenance costs low. Above all, it allows developers to keep an eye on their algorithms.

Fraunhofer SCAI provides a powerful computer infrastructure to execute order computations. The offer also includes HPC test systems that customers can use for development purposes.

LAMA – a versatile framework for performance and maintainability of compute-intensive code segments

The high-performance software framework LAMA is a valuable tool for cross-hardware code optimization. With the help of LAMA, it is possible for developers

- to create fast and scalable software that runs efficiently on almost any computer architecture in a simple and hardware-independent way,
- to significantly reduce the time required to develop new software,
- to automate the transition to new hardware developments as far as possible and
- to facilitate the maintenance of existing software considerably.

The solution of equation systems, as they occur, for example, in flow and structural mechanic simulations, is a typical field of application of LAMA. The strength of LAMA lies in the approach to support distributed and hierarchical storage models seamlessly and with high performance. The fields of application for LAMA are manifold. Especially software developers who implement complex algorithms from numerical mathematics, optimization and machine learning benefit from the software library.

WAVE – simulation and inversion of wave fields

The aim of the WAVE project (duration 02/2016 – 07/2019) funded by the *German Federal Ministry of Education and Research* is the development and implementation of a portable HPC toolbox for the simulation and inversion of wave fields (reverse time integration). This toolbox supports

- generic numerical data structures and algorithms and
- load balancing.

In addition, it contains 3D finite difference wave field simulators for acoustic, elastic and electromagnetic waves on spatially variable grids. The toolbox takes into account the characteristics of current and future HPC architectures, especially regarding their size, heterogeneity and hierarchical structure.

RoKoRa – safe human-robot collaboration

The project RoKoRa (duration 07/2017 – 06/2020) is about protecting humans from injuries by robots. Compact radar systems are used for this purpose. They offer many advantages: Radars operate independently of any lighting and are largely insensitive to environmental conditions. In addition, radar sensors can measure not only the distance to the sensor, but also the motion vector of the targets detected. The sensor system significantly improves the safety of personnel in human-robot collaboration. In RoKoRa, SCAI develops the "brain" of the robot using methods of machine learning. It is responsible for environmental perception, decision-making, and robot control.

adiutaBYTE – optimized processes and scheduling

Planners, schedulers, dispatchers and many other professional groups face complex optimization problems on a daily basis, which are difficult to solve for humans. It is still state of the art that plans are created manually in the morning and adapted with great effort throughout the day. This can be the daily roster in a hospital or for outpatient care, fleet planning in a parcel service or shelf planning in a department store. Creating such a plan in itself is already highly complex and many factors have to be considered. In practice, unpredictable events occur and require additional tasks. These have to be taken into account in the plan since they have a direct influence on the given situation and the options for action.

SCAI currently prepares the launch of the spin-off adiutaByte. This company will provide an efficient software support for such problems.

CONTACT

HEAD OF BUSINESS AREA
Dr. Thomas Soddemann
Phone +49 2241 14-3414
thomas.soddemann@scai.fraunhofer.de

www.scai.fraunhofer.de/en/hpc

1 Software developers benefit from LAMA when implementing complex algorithms.
2 WAVE is used to simulate wave fields.
3 Safe cooperation between humans and robots.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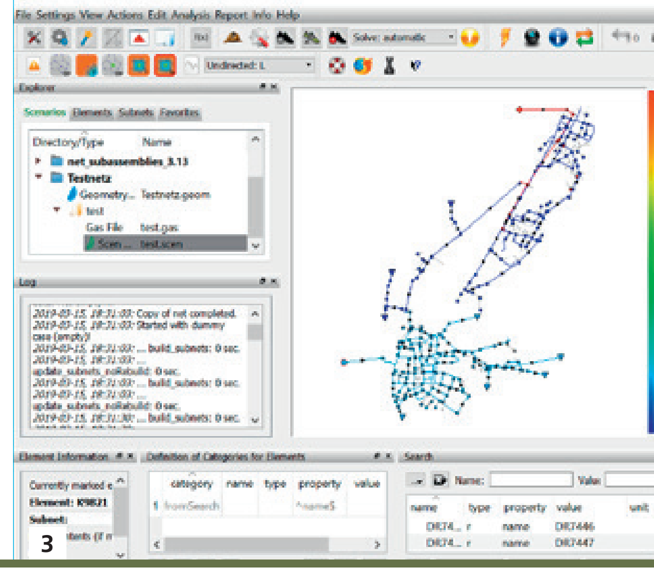
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NETWORK EVALUATION TECHNOLOGIES

Efficient transport networks for gas, electricity and water are of paramount importance in industrialized countries. To enable and expand the use of renewable energies, the German government is supporting the modernization and construction of thousands of kilometers of new power networks. Smart grids are becoming increasingly important. The intelligent networking and control of power generators, storage facilities, consumers and network resources is one of the great economic and environmental challenges.

The research and development within the business area *Network Evaluation Technologies* (NET) focuses on the analysis, simulation and optimization of networks for the transport of water, electricity, and energy carriers. The developed applications are particularly important in several areas:

- Networks: modeling, simulation, analysis/optimization in the fields of gas, water, electricity, district heating, oil, cooling circuits in data centers and office buildings
- Analysis of measurement data for monitoring and control of energy networks

NET employs methods from numerical mathematics, data mining and machine learning. For example, solvers for differential algebraic equation systems, methods for creating interpolation or approximation models (response surfaces) and statistical methods are developed and implemented. The department also uses proprietary patented methods for statistical analysis and robust optimization of parameter-dependent chains of (simulation) processes.

Software MYNTS

The analysis and optimization of their networks is an essential competitive factor for energy suppliers and large energy consumers. For this purpose, NET has developed the software package MYNTS (Multiphysical Network Simulator). With MYNTS, complex networks can be planned and their behavior in operation can be predicted, analyzed and optimized. MYNTS models transport networks for gas, electricity, district heating or water. The simulation immediately shows how changes in certain factors affect the network. For example, MYNTS can be used to calculate how temperature fluctuations change the flow rates and how the failure of sub-networks affects the other network components. This makes energy conversion and network expansion more flexible for network operators, saves energy and money, and also increases security.

The software is also interesting with regard to smart grids. To face the challenges of a power supply which largely depends on natural resources, local solutions can also make important contributions. Improved time management and savings, especially for energy-intensive companies, could cut consumption peaks and bring electricity and gas consumption into line with supply. However, this increases complexity, costs and susceptibility.

MYNTS is currently used for network development and planning tasks in industrial companies, among them the largest German gas transport company *Open Grid Europe* (located in Essen, Germany) and in several research projects as described below.

CONTACT

HEAD OF BUSINESS AREA
Dr. Bernhard Klaaßen
Phone +49 2241 14-2851
bernhard.klaassen@
scai.fraunhofer.de

www.scai.fraunhofer.de/en/net

Project MathEnergy

In the context of the energy turnaround, many new challenges are emerging. The project MathEnergy addresses these challenges through the development of new mathematical approaches. In order to adapt the workload and the expansion of the energy networks, offers and demands have to be adjusted and flexibilities among the energy sources have to be utilized. For this purpose, network-transcending models and model-based monitoring, controlling and evaluation concepts are developed.

The goal of the project MathEnergy is to create a software package for hierarchical complex network models. The solution shall support stochastically varying input data and workflows for the integrated simulation and analysis of network-transcendent scenarios of the energy supply with power and gas. In the future, this software will be used to significantly improve the control of the entire energy network in Germany.

MathEnergy is funded by the *German Federal Ministry for Economic Affairs and Energy* (BMWi). The project was launched in October 2016 and will be finished by the end of September 2019.

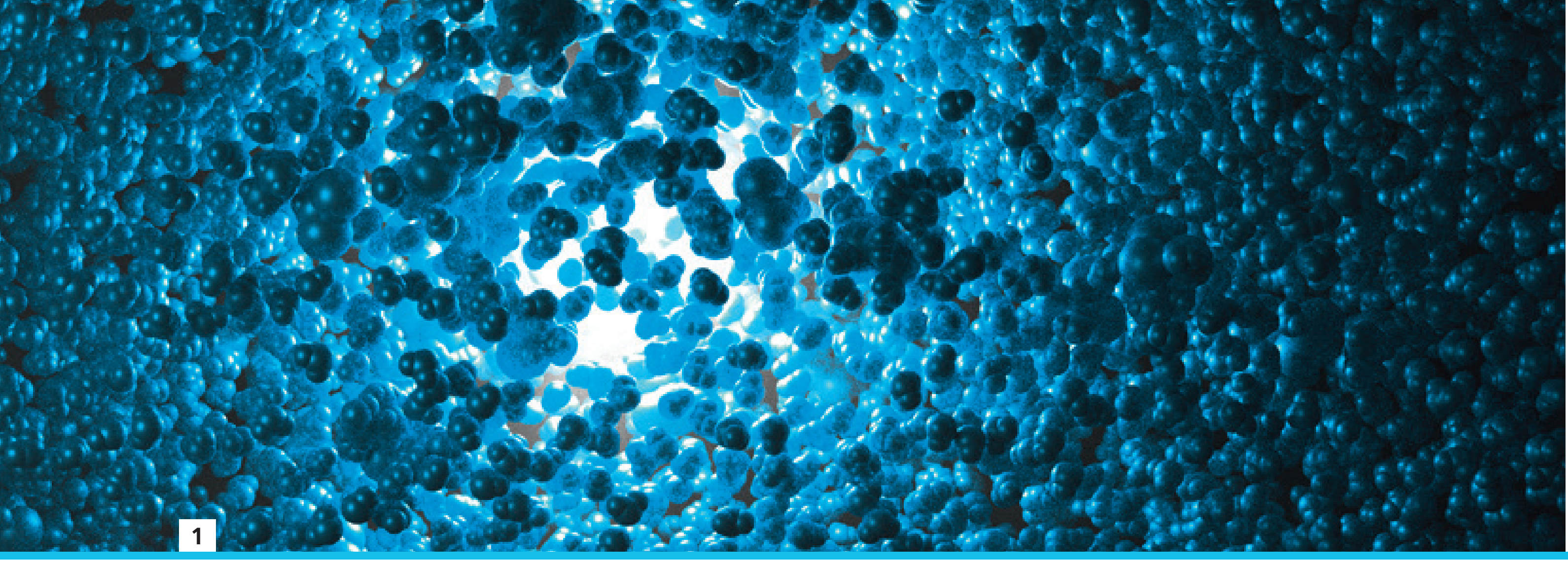
Project ES-FLEX-INFRA

The project ES-FLEX-INFRA is intended to enable energy suppliers and service providers to investigate, evaluate and ultimately operate load shifts and integration of storage facilities in urban infrastructure. Topics of the project are

- the use of previously unused heat (waste heat, rivers) with heat pumps and heat storage tanks or heat networks,
- the use of surplus electricity to generate methane (power-to-gas) and simultaneous use of the high amount of process heat through co-generation,
- the use of gas networks or storage facilities for the extraction and injection of methane and the utilization of methane in co-generation processes,
- the use of surplus electricity for electric mobility or via power-to-gas in vehicles powered by natural gas.

ES-FLEX-INFRA is funded by the European Commission. The project started in June 2016 and will be finished by the end of the year 2019.

1 Efficient energy networks are of great importance for industrialized countries.
2 Surplus energy from wind turbines can be used to generate hydrogen.
3 The graphical user interface of the software MYNTS facilitates user input for the simulation and optimization of complex networks.



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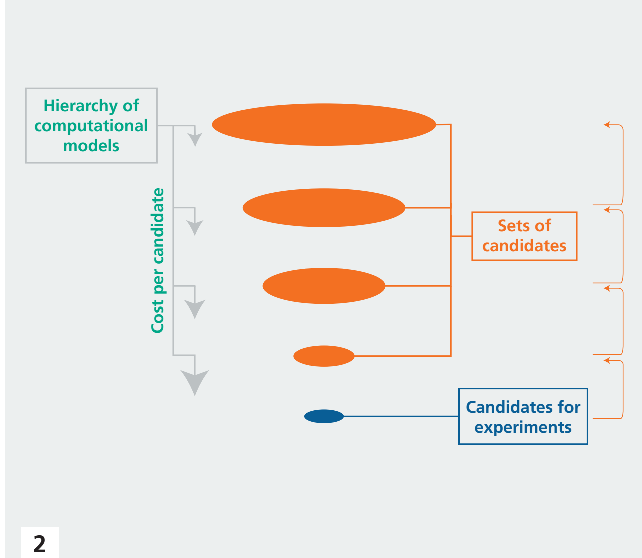

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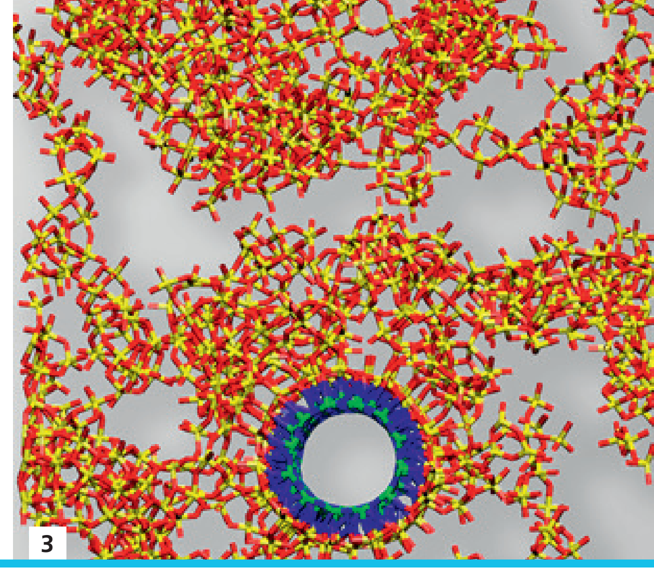

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VIRTUAL MATERIAL DESIGN

The development of innovative materials is a key technology for many applications in the fields of environment, energy, health, mobility, safety and communication. In order to successfully advance new developments, it is necessary to combine mathematical methods and scientific and engineering knowledge with modern data-driven approaches.

The development of highly specialized materials and molecules requires a detailed understanding of their properties, from the atomic level to the visible macroscopic behavior. To understand all aspects of a material's behavior, temporal and spatial multiscale models are needed. One goal of the department of *Virtual Material Design* (VMD) is to generate and investigate new materials and molecules in the computer as a virtual laboratory. This approach promises to replace laboratory experiments with virtual experiments in the computer and thus substantially reduce development costs. In addition, completely new materials can be found and processes in the manufacturing process can be optimized.

Software package Tremolo-X

In order to solve concrete problems, VMD combines its deep knowledge in applied mathematics, empirical data and customized software. The core software package of the business unit is Tremolo-X, a massively parallel software package for highly efficient numerical simulation in molecular dynamics. Tremolo-X is also the numerical back end of the atomistic simulation toolkit QuantumATK (ATK) marketed by Synopsys.

A unique feature of the ATK software package is that atomistic methods from density field theory (DFT) to force field methods can be used and coupled via a software framework. To our knowledge, this is the only software solution that allows, for example, the simulation of electron-phonon coupling, which plays a major role in the development of miniaturized electronic devices. Here quantum mechanical methods (DFT) are coupled with force field methods (Tremolo-X/ATK-FF). Another unique feature of ATK is that this software package includes methods for modeling surfaces and interfaces, materials and molecules as well as methods for simulating processes on long time scales.

Furthermore, Tremolo-X/ATK-FF includes nearly all potential models for solid state systems and also a large number of potential models for molecular systems. In particular, almost all available parameterizations are supplied directly.

CONTACT

HEAD OF BUSINESS AREA
Dr. Jan Hamaekers
Phone +49 2241 14-2463
jan.hamaekers@scai.fraunhofer.de

www.scai.fraunhofer.de/en/vmd

The range of services offered by the business unit extends from Tremolo-X through computer-aided prediction of material properties and chemical processes to data-driven virtual material and process design. In addition, the business unit offers the development of special software tools, the processing of special questions regarding virtual data-driven material design and process optimization using mathematical, statistical and numerical methods.

New field of data-driven research and development

Besides theory, experiment and measurement – computational sciences have established themselves as a new field in research and development over the last decades. The large amount of newly-generated data from experiments and simulations together with new techniques of data analysis and machine learning have opened the field of data-driven research and development.

An important application is the use of modern data analysis and machine learning to develop efficient models for predicting the properties and performance of materials. These models can be used by means of high-dimensional optimization for the efficient design of materials, molecules or processes.

Here, VMD develops similarity measures and kernels which are appropriate for the analysis of the chemical and materials space and uses feature extraction and dimensionality reduction techniques to extract and develop simple models for underlying complex physical processes.

Another development relates to so-called graybox models. They combine so-called whitebox models, which take the exact physical description of a specific modeled systems into account, and blackbox models, which treat input data with generic data analysis methods.

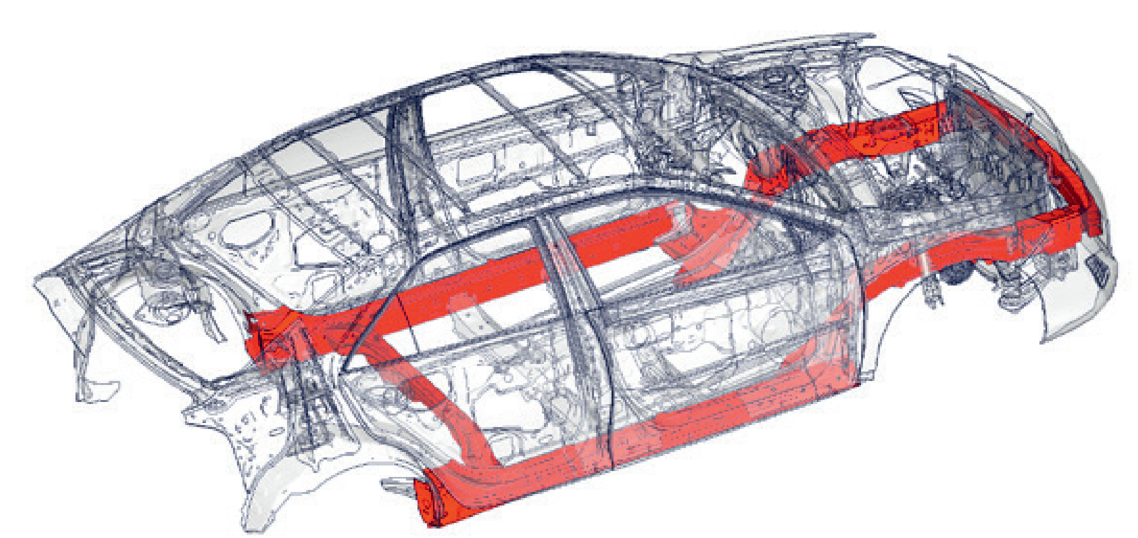
Project MultiModel

The growth and processing of materials is an integral part of chemical and electronic engineering. As nanoscale technologies become more and more important, atomic-scale precision is required in industrial processes, which is difficult and costly to obtain by experimental trial and error.

In the MultiModel project, QuantumWise, AQcomputare and Fraunhofer SCAI have developed a software package which enables atomic-scale simulations of materials growth, atomic diffusion and materials reliability. By incorporating time scalability into multi-scale modeling techniques, the simulation of the dynamics for the long timescales in these phenomena has become feasible.

MultiModel was funded by the *German Federal Ministry of Education and Research* (BMBF), under the Eurostars project E!9389 MultiModel. The project started in June 2015 and ended in May 2018.

1 Insights in condensed phase reactions: amine-catalyzed hydrogen-deuterium exchange.
2 Graphical user interface of the software package Tremolo-X.
3 Boron nitride nanotubes in a silica matrix; representation of reinforced nanomaterials with Tremolo-X.



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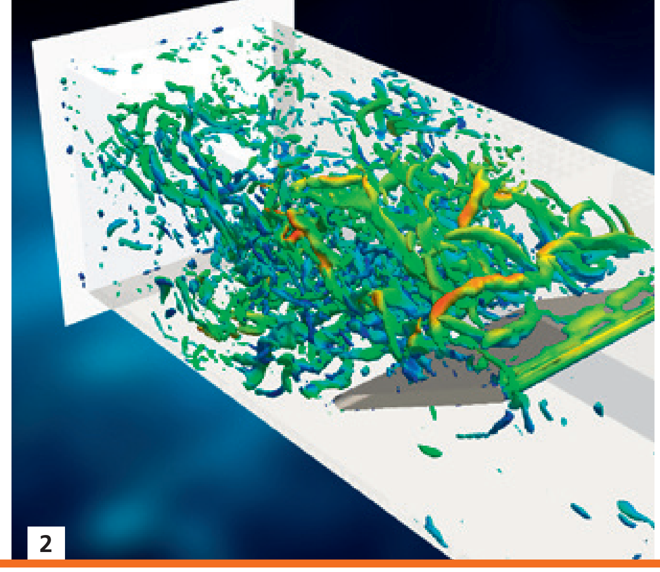

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NUMERICAL DATA-DRIVEN PREDICTION

The general interest in data-driven approaches for science and industrial engineering has increased rapidly. This stems from the combined development and use of efficient data analysis algorithms, large amounts of data from sensors, and numerical simulations. Using machine learning algorithms, the aim is to gain insights from the data, with the eventual goal to assist or to automate decision-making and process control.

The business area *Numerical Data-Driven Prediction* (NDV) focuses on the handling of complex data from physical-technical applications, in particular in order to meet the challenges of industry 4.0. NDV combines mathematics, machine learning, and engineering knowledge to develop robust, scalable and domain-adapted data analysis concepts and methods. Applications can be found in the virtual product development based on computer aided engineering, in condition monitoring including predictive maintenance, or in the realization of digital twins.

The research in the business area is based on mathematical principles and aims in particular to integrate and use existing domain knowledge. The scientific focus is on numerical methods for high-dimensional problems and on the development of domain-specific data representations and similarity measures. The work comprises efficient processing and analysis of large and complex data sets, for example time series or numerical simulation results, the quantification of uncertainties, and contributions to transfer learning. In addition, NDV offers its customers highly developed tools for robust design.

As the work in the field of machine learning research in industry 4.0 is multidisciplinary, NDV offers competencies in mathematics, computer science, engineering and physics.

Software ModelCompare

ModelCompare is a plug-in for finite element pre- and post-processing tools. It provides a simple and direct comparison of two similarly discretized finite element models and calculates differences of the models regarding geometry (grid), material properties or thickness. The software identifies the differences based on the geometry described by the mesh. It uses specialized mapping techniques that result in extremely short run times. ModelCompare is a quick-look tool simplifying the virtual product development process.

CONTACT

HEAD OF BUSINESS AREA
Prof. Dr. Jochen Garcke
Phone +49 2241 14-2286
jochen.garcke@scai.fraunhofer.de

www.scai.fraunhofer.de/en/ndv

Project MADESI – avoiding damage by using machine learning methods to detect anomalies at an early stage

The analysis of sensor data from machines, factories, or buildings makes it possible to detect unusual conditions at an early stage and thus to avoid damage. For this purpose, available data is searched for anomalies. To detect such anomalies by machine learning methods, however, the system first needs a stable learning phase in which it becomes familiar with all possible normal states. In the case of wind turbines or bridges, this is difficult to achieve since they are exposed to highly fluctuating wind conditions. Moreover, only a few data are usually available for anomalous events. As a result, the system cannot categorize those events. However, this would be important in order to recognize how dangerous the respective deviations from the norm are. Exactly these two problems are to be solved in the project "Machine Learning Procedures for Stochastic-Deterministic Multi-Sensor Signals" (MADESI). The three-year project runs from October 2018 to the end of September 2021 and is funded by the „IKT 2020 – Research for Innovation" program of the *German Federal Ministry of Education and Research* (BMBF).

Project EXCELLERAT – new analysis methods improve the evaluation of complex engineering data

A further increase in the performance of supercomputers is expected over the next few years. So-called exascale computers can then deliver more accurate simulation results than ever. NDV develops efficient data analysis methods for the much larger amounts of data generated in this way. Engineers will benefit from the new methods which will provide detailed insights into the complex technical interrelationships.

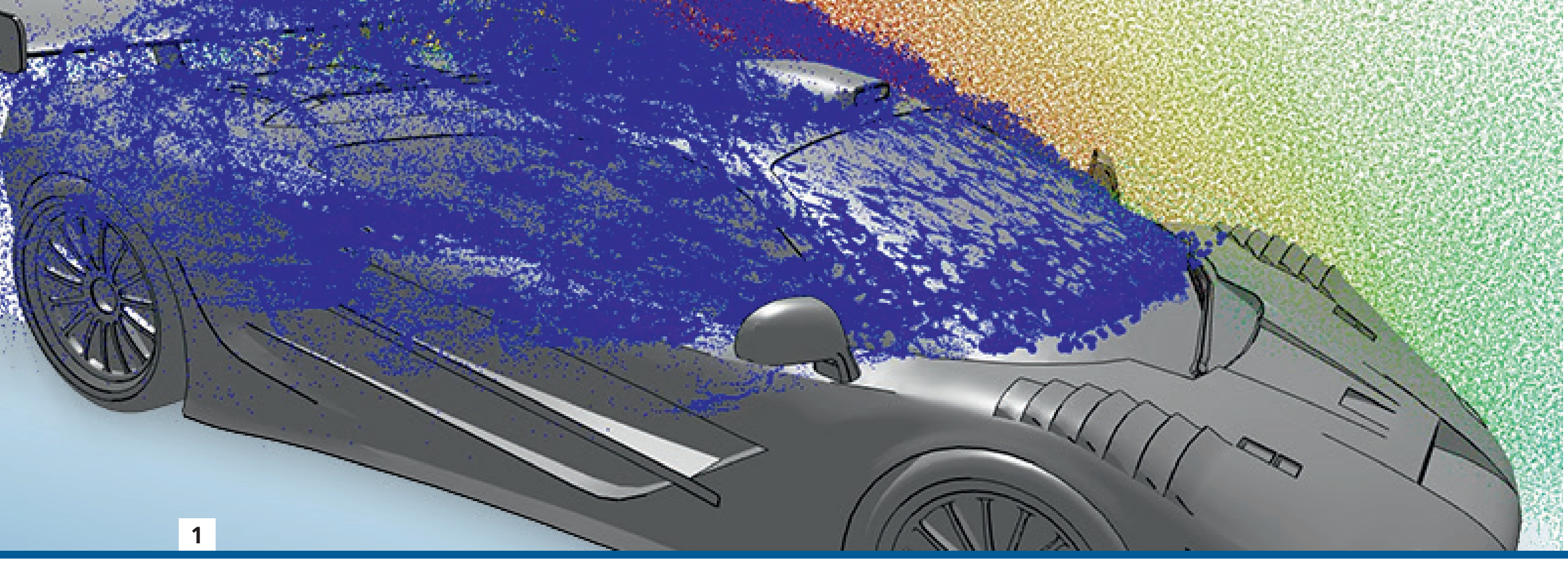
One approach is to carry out data analysis already during the simulation, which minimizes memory requirements and computing time and allows even huge amounts of data to be analyzed efficiently. NDV concentrates on methods for the comparative analysis of simulation data. By automatically comparing the data, engineers can see at a glance how, for example, a modified component shape affects the flow behavior and thus the noise level of an air conditioning system.

EXCELLERAT is funded by the European Commission in the program "Horizon 2020". The project started in December 2018 and will be finished by the end of November 2021.

EVOLOPRO – learning from biology

The great vision of Industry 4.0 is the automatic adaptation of production processes to rapidly changing requirements. The aim of the Fraunhofer flagship project EVOLOPRO is to get closer to this vision. As part of the Fraunhofer „Biological Transformation" initiative, seven institutes jointly research how the transfer of developmental and evolutionary biological principles to transformable digital twins can lend adaptability to man-made production processes. Transfer and multi-task learning play a major role here. Biology is a great inspiration and provides important impulses for the further development of methods. EVOLOPRO runs from January 2019 to the end of the year 2022.

1 ModelCompare compares and visualizes the thickness differences of two car chassis.
2 Project EXCELLERAT: high-resolution simulation of the air flow in a car air conditioning system.
3 Biology inspires the development of methods for automatic production processes in EVOLOPRO.



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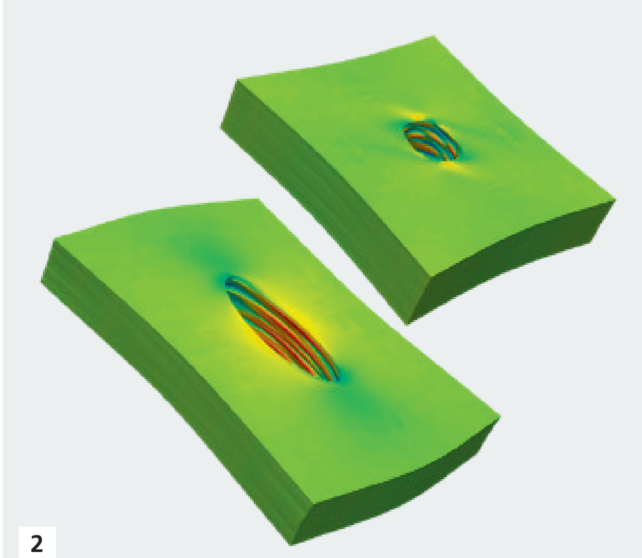

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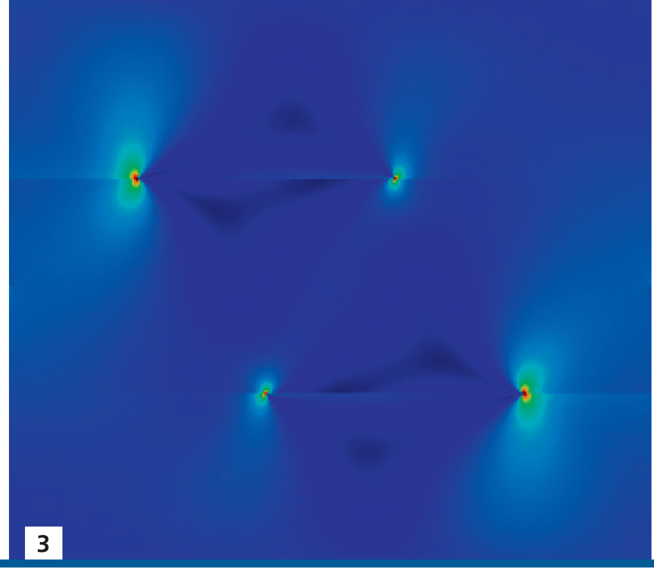

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MESHFREE MULTISCALE METHODS

The prediction of material failure and fracture behavior of large components plays a crucial role in many industrial sectors. Examples are the lifetime predictions of dams, of railway tires, or of aircraft. MESHFREE methods are a suitable approach for such applications.

The business area *Meshfree Multiscale Methods* develops new efficient multi-scale algorithms, for example particle-based multiscale methods or the generalization of finite element methods. These modern methods are suitable for solving problems in which large changes of geometry and changes of topology occur – for example, large deformations or free surfaces. Since no consistent global mesh generation is necessary in these cases, these methods are superior compared to classical mesh-based methods.

The topics of the business area cover the development and implementation of efficient software especially for the design of optimal problem-adapted basis functions and their integration into commercial finite element (FE) packages. One focus is the development of the partition of unity method – a meshfree generalization of the FE method. It supports the direct use of problem-dependent enrichment functions. These application-specific basis functions may be given analytically or only as numerical or experimental data. Overall, this approach provides a much better approximation with fewer degrees of freedom.

PUMA – rapid enriched simulation application development

The PUMA software toolkit allows engineers to quickly implement simulation applications using generalized FE techniques based on the partition of unity method (PUM). Compared to classical FE methods, a PUM can directly utilize user insight, domain-specific information and physics-based basis functions in order improve the approximation properties of the model and to reduce the computational cost. PUMA thus allows for the rapid evaluation of novel models. Benefits of PUMA are:

- PUMA enables the user to quickly implement simulations using generalized FE techniques.
- PUMA easily utilizes user insight, domain-specific information and physics-based basis functions.
- PUMA allows a rapid evaluation of novel models.
- PUMA is particularly suitable for fracture mechanics problems.

Using a multi-layered architecture, PUMA hides the internal methodological and implementation complexity from the user. The PaUnT module contains the computational core of the framework and provides platform independence, computational efficiency, and the possibility to interact with scientific third party libraries.

PUMA provides a Python interface which provides easy access to the higher level functionality of PaUnT.

On the application level, the user implements the simulation application with the help of this interface, which allows to control all aspects of the method, but does not require the user to be aware of all details of the PUM or its implementation within the computational core of PUMA.

MESHFREE – simulation tool for complex geometries and physics

In common simulation workflows, the preprocessing step of grid generation and grid adaption is time consuming and leads to high costs in product development. For this purpose, SCAI and the *Fraunhofer Institute for Industrial Mathematics ITWM* in Kaiserslautern have developed the software package MESHFREE for the meshfree simulation of flow and continuum mechanical problems. With MESHFREE, it is possible to simulate coating, extrusion, forming, homogenizing, injection, kneading, pressing or stirring processes. Such processes are important, for example, in food technology.

MESHFREE discretizes the simulation area by a flexible point cloud. This kind of discretization is especially suitable for simulations with free surfaces or moving geometries.

The software is based on a general material model, i.e., a universal model for fluids and solids. This generality allows complex material behavior to be modeled and treated using the same numerical methodology, regardless of whether the medium is liquid or solid. The specification of the material properties such as viscosity or elasticity in the form of a shear modulus is sufficient to compute the behavior of the medium.

Since MESHFREE does not require any computational meshes, the software is very flexible in organizing the compute points; mesh generation and the time-consuming adaptation of the network topology in highly dynamic processes – such as flows with free surfaces or fast-moving geometry elements – become dispensable.

The software combines the finite point set method (FPM, by Fraunhofer ITWM) for the solution of the conservation equations for mass, momentum and energy with efficient algorithms for solving linear systems of equations (SAMG, by Fraunhofer SCAI). The user exports the geometry directly from common CAD tools and uses them for the simulation.

CONTACT

HEAD OF BUSINESS AREA
Prof. Dr. Marc Alexander Schweitzer
Phone +49 2241 14-2037
marc.alexander.schweitzer@scai.fraunhofer.de

www.scai.fraunhofer.de/ /en/mmm

1 McLaren F1 at 60km/h in heavy rain.
2 Two physics-based displacement basis functions for laminated orthotropic plates. Color shows dilatational strain on the deformed plate.
3 Layered composite plate with multiple delaminations. Color shows the von Mises stress distribution.

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COMPUTATIONAL FINANCE

Computational Finance is an interdisciplinary branch of scientific computing. The main goal is to determine the risks generated by financial products as accurately as possible. Application areas are the evaluation and the trading of securities, stocks, and bonds and the determination of sensitivities and hedging strategies, risk assessment, asset-liability management, as well as investment decisions and strategic corporate planning. Current challenges are increasingly complex financial products, market models with multiple sources of uncertainty and the simultaneous management of assets and liabilities as optimization problems.

SCAI's business area *Computational Finance* develops efficient and robust numerical algorithms and implements them on parallel high-performance computing systems. Current areas of research are:

- Dimension-adaptive sparse grid quadrature
- Multilevel quasi-Monte-Carlo simulation
- Machine learning: deep learning, tensor methods, generalized support vector machines, transfer learning, reinforcement learning, nonlinear dimensionality reduction

These techniques allow calculations with high accuracy while substantially reducing computation times. The aim of the department is to develop a faster and qualitatively better analysis of financial data for predictions and, consequently, for well-founded investment decisions. Typical applications for machine learning methods are, for example, investment predictions, risk management, and algorithmic trading. We describe three examples in detail.

Machine learning for banks and insurance companies

Today, machine learning plays an important role in the optimization of financial services. Machine learning usually refers to stochastic methods in which an algorithm learns from many different but representative data sets. The financial services industry often has very large data sets, such as financial transactions, customers, companies and stock markets. Machine learning techniques are particularly well-suited for analyzing these large volumes of data and for deriving predictions and recommendations. Learning algorithms develop a complex model from the sample data. This model can then be applied to other, similar data to gain valuable and proper predictions.

CONTACT

HEAD OF BUSINESS AREA
Prof. Dr. Michael Griebel
Phone +49 2241 14-2544
michael.griebel@scai.fraunhofer.de

www.scai.fraunhofer.de/en/cf

Integration of novel data sources

Machine learning also plays an increasingly important role in the development of trading strategies. In addition to classic macroeconomic indicators and correlations with other asset classes, new types of data, such as sentiment indicators based on social media posts, are increasingly being incorporated into model training. As a result, the number of data channels considered is constantly growing. This development increases the chance of finding new relationships in the market ahead of other competitors.

Typically, the data in financial applications are high-dimensional. One way to deal with the resulting so-called curse of the dimension is to pre-filter the data appropriately, possibly combined with methods of dimension reduction. The aim is to improve the signal-to-noise ratio of the data in order to reduce the susceptibility to over-fitting. Here, SCAI develops new methods and approaches, also on behalf of partners from the financial sector.

Machine learning supports sustainable and ethical investments

More and more investors wish to invest their money in companies that meet certain criteria for environmental, social and corporate governance (ESG). To this end, machine learning helps to evaluate the performance and sustainability of globally listed companies according to such ESG-defined criteria. Only high-performance shares of companies that can demonstrate certain standards regarding their environmental and social behavior as well as responsible corporate governance are then taken into account.

Together with Arabesque Asset Management Ltd, Fraunhofer SCAI is developing innovative mathematical methods for machine learning processes that can be used to determine complex ESG-compliant equities – and thus to assemble a high-performance portfolio. In addition, the procedures allow predictions about the future potential of the respective shares and assets. The results provide precise investment recommendations for institutional investors.

1 Computational finance helps with the analysis of complex financial products.
2 Sustainability and ethical criteria play an important role in investment decisions.
3 Machine learning allows for predictions from financial data and social media posts.

THE FRAUNHOFER-GESELLSCHAFT

Research of practical utility lies at the heart of all activities pursued by the Fraunhofer-Gesellschaft. Founded in 1949, the research organization undertakes applied research that drives economic development and serves the wider benefit of society. Its services are solicited by customers and contractual partners in industry, the service sector and the public administration.

At present, the Fraunhofer-Gesellschaft maintains 72 institutes and research units. The majority of the more than 26,600 staff are qualified scientists and engineers, who work with an annual research budget of 2.6 billion euros. Of this sum, 2.2 billion euros is generated through contract research. Around 70 percent of the Fraunhofer-Gesellschaft's research revenue is derived from contracts with industry and from publicly financed research projects. Around 30 percent is contributed by the German federal and state governments in the form of base funding, enabling the institutes to work ahead on solutions to problems that will not become acutely relevant to industry and society until five or ten years from now.

International collaborations with excellent research partners and innovative companies around the world ensure direct access to fields of the greatest importance to present and future scientific progress and economic development.

With its clearly defined mission of application-oriented research and its focus on key technologies of relevance to the future, the Fraunhofer-Gesellschaft plays a prominent role in the German and European innovation process. Applied research has a knock-on effect that extends beyond the direct benefits perceived by the customer: Through their research and development work, the Fraunhofer Institutes help to reinforce the competitive strength of the economy in their local region, and throughout Germany and Europe. They do so by promoting innovation, strengthening the technological base, improving the acceptance of new technologies, and helping to train the urgently needed future generation of scientists and engineers.

As an employer, the Fraunhofer-Gesellschaft offers its staff the opportunity to develop the professional and personal skills that will allow them to take up positions of responsibility within their institute, at universities, in industry and in society. Students who choose to work on projects at the Fraunhofer Institutes have excellent perspectives of starting and developing a career in industry by virtue of the practical training and experience they have acquired.

The Fraunhofer-Gesellschaft is a recognized non-profit organization that takes its name from Joseph von Fraunhofer (1787–1826), the illustrious Munich researcher, inventor and entrepreneur.

Fraunhofer SCAI is a member of the following groups and alliances:

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  www.iuk.fraunhofer.de
- **Fraunhofer Cloud Computing Alliance**
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- **Fraunhofer Big Data and Artificial Intelligence Alliance**
  www.bigdata.fraunhofer.de
- **Fraunhofer Numerical Simulation of Products, Processes Alliance**
  www.nusim.fraunhofer.de

RESEARCH AND TEACHING

Institute for Numerical Simulation (INS), University of Bonn

The INS is a mathematical research institute at the *University of Bonn* with a focus on scientific computing as well as numerical analysis and numerical simulation. The institute sees itself as a bridge between mathematics and computer science. In its research work, the INS develops tools for numerical simulation in natural and engineering sciences, geosciences, medicine, life sciences, and computational finance.

A part of SCAI´s Department of Virtual Material Design has been located at the INS since June 2010 and is headed by Dr. Jan Hamaekers. Moreover, Prof. Dr. Jochen Garcke, Department of Numerical Data-Driven Prediction, and Prof. Dr. Marc Alexander Schweitzer, Department of Numerical Software, also lead working groups at the INS.
www.ins.uni-bonn.de

Bonn-Aachen International Center for Information Technology (B-IT)

B-IT is jointly operated by four universities and research institutions, namely the *University of Bonn, RWTH Aachen University*, the *University of Applied Sciences Bonn Rhein-Sieg*, and the Fraunhofer-Gesellschaft. SCAI´s Department of Bioinformatics, led by Prof. Dr. Martin Hofmann-Apitius, participates in the international Master Programme in Life Science Informatics.
www.b-it-center.de

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

The cooperation with the *Bonn-Rhein-Sieg University of Applied Sciences* has developed steadily. The relations with the *Faculty of Mechanical and Electrical Engineering* and with the *Faculty of Computer Science* are maintained through a joint research seminar on "Numerical Simulation" and the integration of graduate 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 is developing positively. In the summer term 2019, Dr. Jan Hamaekers holds a course on "Deep Learning on Graphs".

1 Headquarters of the Fraunhofer-Gesellschaft in Munich.
2 Joseph von Fraunhofer (1787 – 1826)
3 The Main Building of the University of Bonn.

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Contact
Fraunhofer Institute for Algorithms
and Scientific Computing SCAI
Schloss Birlinghoven
53754 Sankt Augustin

Phone +49 2241 14-2500
Fax +49 2241 14-2460

info@scai.fraunhofer.de
www.scai.fraunhofer.de

Director
Prof. Dr. Michael Griebel
Phone +49 2241 14-2500
michael.griebel@scai.fraunhofer.de

Editors
Diplom-Journalist Michael Krapp, Dr. Anton Schüller

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Carina Steinborn

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