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FRAUNHOFER INSTITUTE FOR ALGORITHMS AND SCIENTIFIC COMPUTING SCAI

2011 / 12
ANNUAL REPORT

Cover:
Simulation results from the
Department of Virtual Material Design:
Electronic structure of Gallium
Arsenide (GaAs).

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PREFACE

Dear reader,

The Fraunhofer Institute for Algorithms and Scientific Computing SCAI conducts research in the field of numerical simulation for product and business process development. Hundreds of companies worldwide rely on our innovative software products for:

- optimal cutting and packing,
- multiphysics problems,
- the solution of large linear systems,
- network simulations,
- data compression,
- nanotechnology simulations,
- financial engineering,
- and for text and image mining.

Fraunhofer SCAI continued to grow in 2011 with about 42 percent revenues coming from industry. This indicates both that our products satisfy the need of the market and that our partners value our contributions in numerous projects. We have also increased our marketing and sales efforts through our spin-off "scapos AG".

The positive development of the institute motivates us to explore new market opportunities and to increase our efforts to develop new scientific approaches as well as software solutions for future industrial applications. In 2011 we have created three new and innovative business units with themes that we believe will have a high impact in the near future.

First, we established the new Department of High Performance Analytics which is led by Dr. Tanja Clees. She and the members of her group work on the analysis, simulation and optimization of networks and cooperate with partners and customers from areas such as microelectronics, mobility, energy and the engineering industry. Moreover, their newly developed software *MYNTS* is of great interest for the operators of electricity, gas and water distribution networks.

Secondly, we created a new Department of Numerical Data-Driven Prediction. The head of the group is Prof. Dr. Jochen Garcke. His background is in fast numerical techniques for data analysis and he is an expert in the technical trend prediction, e.g. of foreign exchange rates and related time-series data. Future work will include the development of efficient parallel methods for the prediction of the behavior of systems based on automatically collected current and historical data. One application for such new algorithms is in recommendation engines for online shops.

Finally, we established the new group Computational Finance which is led by Prof. Dr. Thomas Gerstner. He and his team develop efficient and robust numerical algorithms to accurately estimate the risks that financial instruments generate. Customers will be banks, insurance firms and risk management departments of companies. The application areas include, among others, the pricing and trading of financial securities, risk assessment, asset-liability management, investment decisions and corporate strategic planning.

With this report we invite you to get to know more about our research, our products and our services.

Prof. Dr. Michael Griebel

Advisory board meeting on May 23, 2012 at Schloss Birlinghoven. The picture shows from left: Dr. Guy Lonsdale, Dr. Jan Hamaekers, Clemens-August Thole, Dr. Birgit Geier, Prof. Dr. Thomas Gerstner, Dr. Tanja Clees, Dr. Bernd Thomas, Prof. Dr. Jochen Garcke, Dr. Johannes Linden, Prof. Dr. Dr. h.c. Norbert Szyperski, Prof. Dr. rer. nat. Michael Schäfer, Prof. Dr. Ulrich Trottenberg, Dr. Juliane Fluck, Dr. Alexander Kurz, Prof. Dr. Michael Griebel, Prof. Dr. Thomas Lengauer, Dr. Claus Axel Müller, Carl Vogt, Stephan Springstubbe

Directors	Prof. Dr. Michael Griebel Prof. Dr. Ulrich Trottenberg (until February 29, 2012)
Research Departments	
Simulation Engineering	Dr. Johannes Linden
Numerical Software	Clemens-August Thole
Bioinformatics	Prof. Dr. M. Hofmann-Apitius
Optimization	Dr. Ralf Heckmann
Virtual Material Design	Dr. Jan Hamaekers
High Performance Analytics	Dr. Tanja Clees
Computational Finance	Prof. Dr. Thomas Gerstner
Numerical Data-Driven Prediction	Prof. Dr. Jochen Garcke
Central services	
Planning and Controlling	Carl Vogt
Marketing and Communications	Michael Krapp
IT-Services	Horst Schwichtenberg
Branch Lab Bonn	Dr. Jan Hamaekers
Branch Lab Cologne	Clemens-August Thole

Advisory Board

Dr. Bernd Thomas, chairman, *Continental AG*
Prof. Dr. Dr. h.c. Norbert Szyperski*, *InterScience GmbH, University of Cologne*
Prof. Dr. Hans-Joachim Bungartz, *TU München*
Dr. Birgit Geier, *Fraunhofer-Gesellschaft*
Touraj Gholami*, *BMW AG*
Dr. Daniel Keesman*, *August Faller KG*
Prof. Dr. Dr. h.c. Tassilo Küpper*, *University of Cologne*
Prof. Dr. Dr. Thomas Lengauer*, *Max-Planck-Institut für Informatik*
Dr. Bernd Mlekusch, *Audi AG*
Dr. Claus Axel Müller, *Gauss Centre for Supercomputing e. V.*
Dr. Stefan Reimann-Andersen
Prof. Dr. Michael Schäfer, *TU Darmstadt*
Ulrich Schüller, *Federal Ministry of Education and Research*
Dr. Klaus Tschira, *Klaus Tschira Stiftung gGmbH*

** until May, 2012*

Spin-Off

In order to strengthen marketing and sales of its products, the Fraunhofer Institute for Algorithms and Scientific Computing SCAI initiated the launch of scapos AG in 2009; the Fraunhofer-Gesellschaft is one of the scapos shareholders. The company also offers its services to all Fraunhofer Institutes and other research organizations.

scapos AG
Schloss Birlinghoven
53754 Sankt Augustin
www.scapos.com

Financing and Expenditure

In 2011, approximately 42 percent of the overall budget of the Fraunhofer Institute SCAI came from revenues from industry – mostly arising from software licenses. This is above the average of Fraunhofer Institutes.

The top-selling software products of SCAI are the *AutoNester* group of products (automatic placement of markers on fabric and other materials), *PackAssistant* (optimized packaging of components in transport containers), *MpCCI* (enabling co-simulation with leading industrial simulation codes), *SAMG* (library for highly efficient numerical solution of large sparse matrix problems) and *FEMZIP* (compression of numerical simulation results).

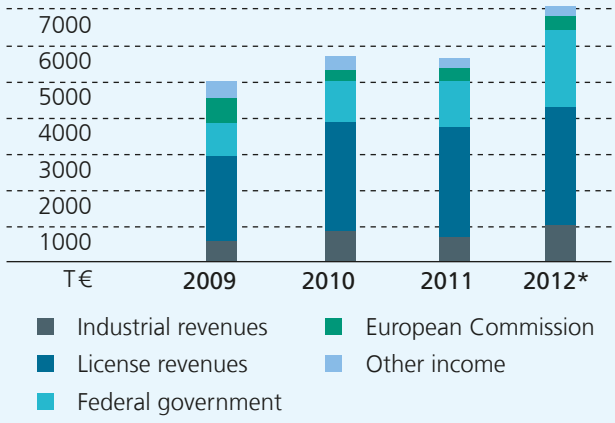
For 2012, the aim is to exceed the value of four million euros turnover from industry. After two successful quarters in 2012, 60 percent of the 3.3 million Euro from license sales, necessary to achieve that target, is already secured.

Overall expenses have remained relatively constant over the last few years. Personnel expenses are the main cost factor, comprising about 70 percent of the overall costs.

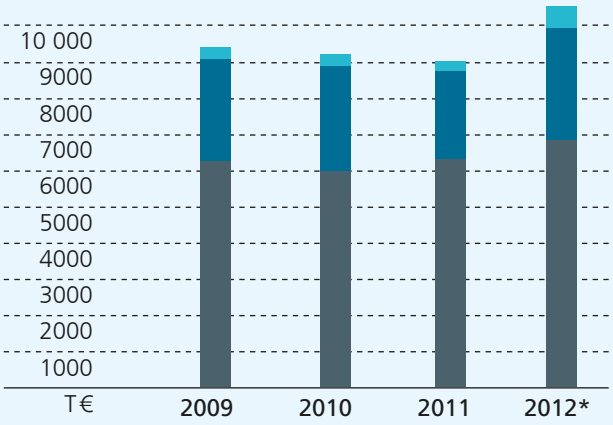
Human resources

At the end of 2011, the institute's staff consisted of 135 employees, including 25 Ph.D. students as well as 25 graduate students and student assistants, which come mainly from the University of Bonn, the University of Cologne and the Bonn-Rhein-Sieg University of Applied Sciences. Furthermore, the institute trained three apprentices as IT specialists and one as a media designer. In the near future, we expect a significant growth of the institute, in particular with a strengthening of the link to the University of Bonn.

Income (from licenses and contract research activities)

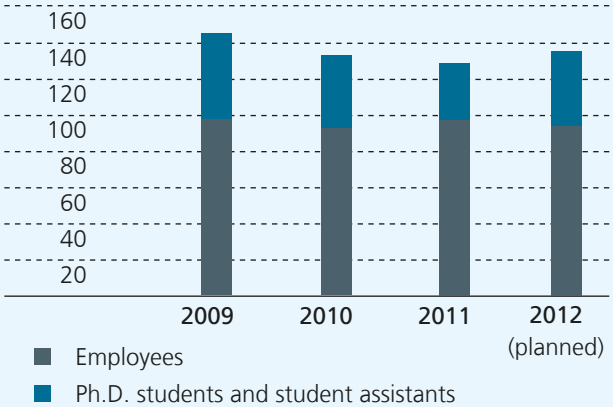


Expenditure



**Forecast based on the first two quarters of 2012*

Human resources



Branch lab at the Institute for Numerical Simulation (INS), University of Bonn

The Institute for Numerical Simulation at the University of Bonn is devoted to the design and implementation of computational tools for scientific applications. At the INS, novel numerical techniques for the simulation of, e.g. processes in chemistry, physics, biology, engineering and economics are developed.

The director of Fraunhofer SCAI, Prof. Dr. Michael Griebel, is also the acting managing director of the INS. The research topics of SCAI's branch lab include multiscale modeling and numerical simulation in materials science, and the numerical treatment of high-dimensional problems. A part of SCAI's Department of Virtual Material Design is located at the INS.

Prof. Dr. Jochen Garcke, head of SCAI's Department of Numerical Data-Driven Prediction, also teaches and conducts research at the university, for example in the area of efficient numerical methods for high-dimensional problems. *www.ins.uni-bonn.de*

Branch lab at the Mathematical Institute, University of Cologne

Since 2007, Fraunhofer SCAI has operated a branch lab at the University of Cologne. The lab consolidates the research of the Departments of Numerical Software (NUSO) and High Performance Analytics (HPA). NUSO's topics include the development of methods and software for the analysis, the evaluation and the compression of simulation results. HPA's research areas comprise network analysis and simulation, graph mining, and robust design for production processes and industrial products. Teaching at the university is closely related to the focus of the branch lab. SCAI's former institute director Prof. Dr. Trottenberg held the chair for applied mathematics/scientific computing at the university. *www.mi.uni-koeln.de*

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

The B-IT is a joint institution formed by the University of Bonn, the RWTH Aachen University, the Bonn-Rhein-Sieg University of Applied Sciences, and the Fraunhofer Institute Centre Schloss Birlinghoven. The Department of Bioinformatics at Fraunhofer SCAI contributes to the international master program "Life Science Informatics" (LSI). The Department, headed by Prof. Dr. Martin Hofmann-Apitius, is substantially involved in the conception of LSI's teaching program. *www.b-it-center.de*

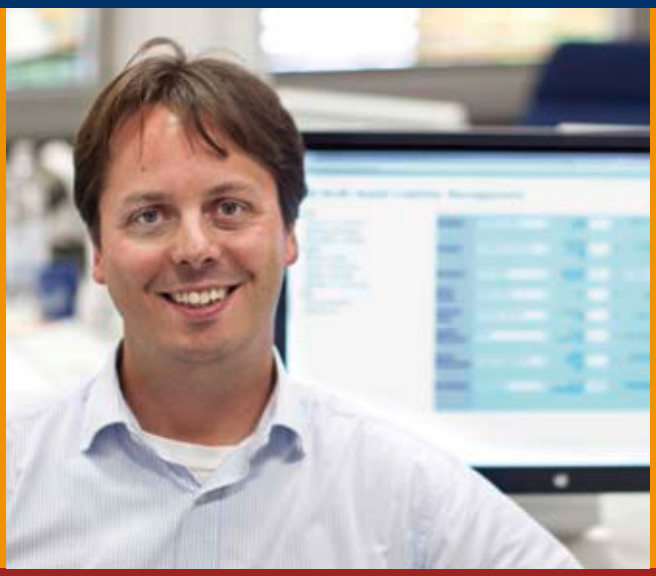
SCAILIGHTS 2011/2012

Researchers in the field of optimization win renowned prize

Researchers from SCAI's Department of Optimization received the German Innovation Prize for Climate and the Environment (IKU) in the category "Environmentally-friendly products and services". The award is donated by the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety (BMU) and the Federation of German Industries (BDI). The researchers developed optimization software, including 3D planning for transport, loading and storage devices, resulting in the optimal utilization of materials and space in resource-intensive sectors. The jury, chaired by Professor Klaus Töpfer, honored innovations which contribute to protecting both the climate and the environment.

Computational Finance aims to estimate the risks that financial instruments generate

Fraunhofer SCAI established a new department named "Computational Finance". The head of the department, Dr. Thomas Gerstner, is Professor of "Computational Finance" at the Institute of Mathematics at the Johann Wolfgang Goethe University in Frankfurt/Main.
The research area of the department is the development of efficient and robust numerical algorithms for financial applications including the pricing and trading of financial securities. Gerstner and his group aim to estimate as accurately as possible the risks that financial instruments generate.



Applied Mathematics inspires students at the "Nacht der Technik" in Cologne

For the third time, Fraunhofer SCAI presented the work of the institute at the "Nacht der Technik" in Cologne. Organized by the Association of German Engineers (VDI), the event attracted around 5 000 visitors interested in the various aspects of technology being developed in the city of Cologne in June 2011. Dr. Tanja Clees, head of the new Department of High Performance Analytics, presented the work of her research group in the field of network analysis and robust design. Many students visited the SCAI stand, located in the University of Applied Sciences in Köln-Deutz, to gather information on the research and educational training opportunities of the institute.

International experts in the field of automotive simulation visit Schloss Birlinghoven

Experts in the field of computer simulation in the automotive industry took part in a workshop held at Schloss Birlinghoven in October 2011, organized by SCAI's spin-off scapos AG and CEI GmbH. The central topics were software tools that support the deployment and integration of the software *OpenFOAM* into the automotive industry's working procedures. Researchers at SCAI gave several talks: Dr. Klaus Stüben demonstrated the software *SAMG*, Klaus Wolf showed the use of multi-physics simulations in process chains and Matthias Rettenmeier put forward the compression of simulation results with *FEMZIP*.

Mathematical methods for the prediction of foreign exchange rates

The new department of Prof. Dr. Jochen Garcke (University of Bonn and Fraunhofer SCAI) is dedicated to numerical methods for data-driven prediction. The aim is to make useful predictions for the future behavior of systems based on automatically collected current and historical data. Data-driven predictions have relevance in many application domains. Examples are technical trend prediction for foreign exchange rates and other financial products, and recommendation engines for online shops. The scientific focus is the research and development of efficient numerical methods for high-dimensional problems.

Fraunhofer SCAI and Microsoft bring HPC computing to the cloud

In the area of High Performance Computing (HPC) companies feel tremendous pressure to innovate and yet at the same time to reduce costs. Heterogeneous IT environments pose new challenges for system management and the interoperability of IT systems is crucial for competitiveness. In the cloud, companies can cost-effectively access numerical simulation applications. A white paper from Fraunhofer SCAI shows how Linux and Windows systems can play together in HPC environments and in the cloud, thereby facilitating service-oriented architectures. This is the result of a close partnership between Microsoft Research and SCAI.

Svenja Schulze gathered information about SCAI's packaging software *PackAssistant*

Thousands of companies worldwide appreciate the quality of packaging solutions by SCAI's Software *PackAssistant*. The Minister of Innovation, Science and Research of the German State of North Rhine-Westphalia, Svenja Schulze, was able to convince herself of the quality of the software during her visit on 25 May 2011. She manually tried to find the best packaging solution for a set of complex shaped components. In only a few seconds the software *PackAssistant* offered an even better arrangement solution. The Minister was impressed and asked Dr. Ralf Heckmann, head of the Department of Optimization, to explain the functions of the software to her. The software saves time and money through optimal container utilization.

“HIERARCHICAL, PARALLEL, DISCRETE AND CHAOTIC PROCESSES”

Scientific Colloquium in honor of Ulrich Trottenberg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Friends, colleagues and longtime companions attended the scientific colloquium held on May 22nd, 2012 in Königswinter in honor of Professor Dr. Ulrich Trottenberg. The title of the colloquium “Hierarchical, parallel, discrete and chaotic processes” might also be taken as a motto of Ulrich Trottenberg’s outstanding scientific career. Renowned scientists paid tribute to his numerous achievements – particularly in numerical mathematics and supercomputing – with entertaining lectures.

Dr. Alexander Kurz, Senior Vice President Personnel and Legal Affairs of the Fraunhofer-Gesellschaft, honored Prof. Trottenberg with the Fraunhofer Medal for his outstanding service to Fraunhofer. In 1992, after his successful career as founder and CEO of Suprenum GmbH and then Pallas GmbH, Trottenberg took over the position as director of the GMD Institute SCAI and subsequently the Fraunhofer Institute for Algorithms and Scientific Computing SCAI.

Since 1984, Trottenberg has held the Chair of Applied Mathematics/Scientific Computing at the Mathematical Institute of the University of Cologne. After his retirement as director of SCAI, he remains Chairman of the Supervisory Board of scapos AG – a spin-off company he initiated to support marketing and sales of the institute’s software products.

Ulrich Trottenberg will continue to improve the image of mathematics in society. Above all, he is committed to the development of a new real-life mathematics education strategy targeting both students and teachers.

1 *Dr. Alexander Kurz, Fraunhofer-Gesellschaft, hands out the Fraunhofer Medal to Prof. Dr. Trottenberg.*
2 *Prof. Dr. Cornelis W. Oosterlee, TU Delft.*
3 *Prof. Dr. Heinz-Otto Peitgen, former Director of Fraunhofer MEVIS.*
4 *Prof. Dr. Dieter Prätzel-Wolters, Director of Fraunhofer ITWM, Kaiserslautern.*
5 *Linde and Ulrich Trottenberg.*
6 *Professor Oliver McBryan, PhD, University of Colorado, Boulder.*

SELECTED PRODUCTS

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 wasted material. **www.scai.fraunhofer.de/autonester**
AUTO COMPACTOR automatic compact arrangement	Compaction of 2D-nests	*AutoCompactor* is a software used for the compaction of two-dimensional nests. It compacts markers generated by humans or automatic nesting software. The software is intended to enhance the nesting functionality of *AutoNester* by an improved compaction algorithm. **www.scai.fraunhofer.de/compactor**
CUT PLANNER automatic cut planning	Automatic cut order planning	*CutPlanner* is a software package for use in the textile manufacturing industry for automatic cut order planning. *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/cutplanner**
PACK Assistant	Optimized 3D packing design	*PackAssistant* is the leading software in the field of optimizing packing configurations of identical parts into containers. With *PackAssistant* the exact 3D arrangement of parts with complex shapes can be calculated and displayed as early as in their design phase. **www.packassistant.de**
MpCCI	Coupling of simulation programs	The *MpCCI* Coupling Environment links simulation programs, thereby solving multidisciplinary problems. The software supports the leading industrial simulation tools. Companies use *MpCCI* to solve difficult multiphysics problems to the benefit of product design and optimization. **www.mpcci.de**
	Coupling of FEM software	The *MpCCI Mapper* supports complex simulation workflows and process chains involving multiple FEM packages. The software handles data interpolation and data conversion between the codes. Examples include codes for metal forming, heat treatment, and crash simulations. **www.scai.fraunhofer.de/mapper**
FEMZIP	Compression tool for simulation results	*FEMZIP* is a software for the compression of simulation results. The size of data files is typically reduced by a factor of 10. Multiple versions can compress data formats in the fields of crash simulation, Noise, Vibration and Harshness (NVH) and Computational Fluid Dynamics (CFD). **www.scai.fraunhofer.de/femzip**
DIFFCrash	Analysis of simulation data	*DIFFCRASH* is a software package for the stability analysis of crash simulations. Physical bifurcations in automobile design and numerical instabilities in simulation packages often cause extremely sensitive dependencies of simulation results on even the smallest model changes. *DIFFCRASH* localizes these critical structural areas and offers suggestions for improvements to obtain greater stability. **www.scai.fraunhofer.de/diffcrash**

SAMG Algebraic Multigrid Methods for Systems	Algebraic multigrid methods for systems	The software package *SAMG* has been developed for the highly efficient, numerical solution of large, sparsely populated matrix problems. Problems of this type can be found in the fields of fluid and structural mechanics, oil reservoir and ground water simulation, process and device simulation, semiconductor physics, and circuit simulation. **www.scai.fraunhofer.de/samg**
DesParO	Data exploration, analysis, and optimization	*DesParO* is a software toolbox for the intuitive exploration, automatic analysis, and optimization of parameterized problems in production processes. *DesParO* can be coupled with all kind of simulation programs or data which stem from physical experiments. **www.scai.fraunhofer.de/desparo**
MYNTS	Simulation and verification of transport networks	*MYNTS* is a multiphysical network simulator which can be used for electrical circuits, gas and energy transport, and water distribution. It models networks as systems of differential-algebraic equations. Users can program subnetworks as well as single special elements. **www.scai.fraunhofer.de/mynts**
ProMiner Recognition and Normalization of Named Entities in Scientific Text	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 derived from ontologies. **www.scai.fraunhofer.de/prominer**
SCAIVIEW	Knowledge discovery in life sciences	*SCAIView* is a knowledge discovery software for the life sciences. It facilitates the rapid identification of aggregated information from large text sources. For this reason it integrates the results of *ProMiner* with the associated text and allows for semantic search. **www.scai.fraunhofer.de/scaiview**
chemoCR chemical compound reconstruction	Automatic recognition of chemical structure depictions	*chemoCR* extracts chemical structural formulas and their chemical structure depictions from scientific literature. The software package converts the structure depictions into a machine-readable format that can be used for computer processing of the information. **www.scai.fraunhofer.de/chemocr**
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 variety of application fields, such as nanotechnology, materials science, biochemistry and biophysics. **www.tremolo-x.com**

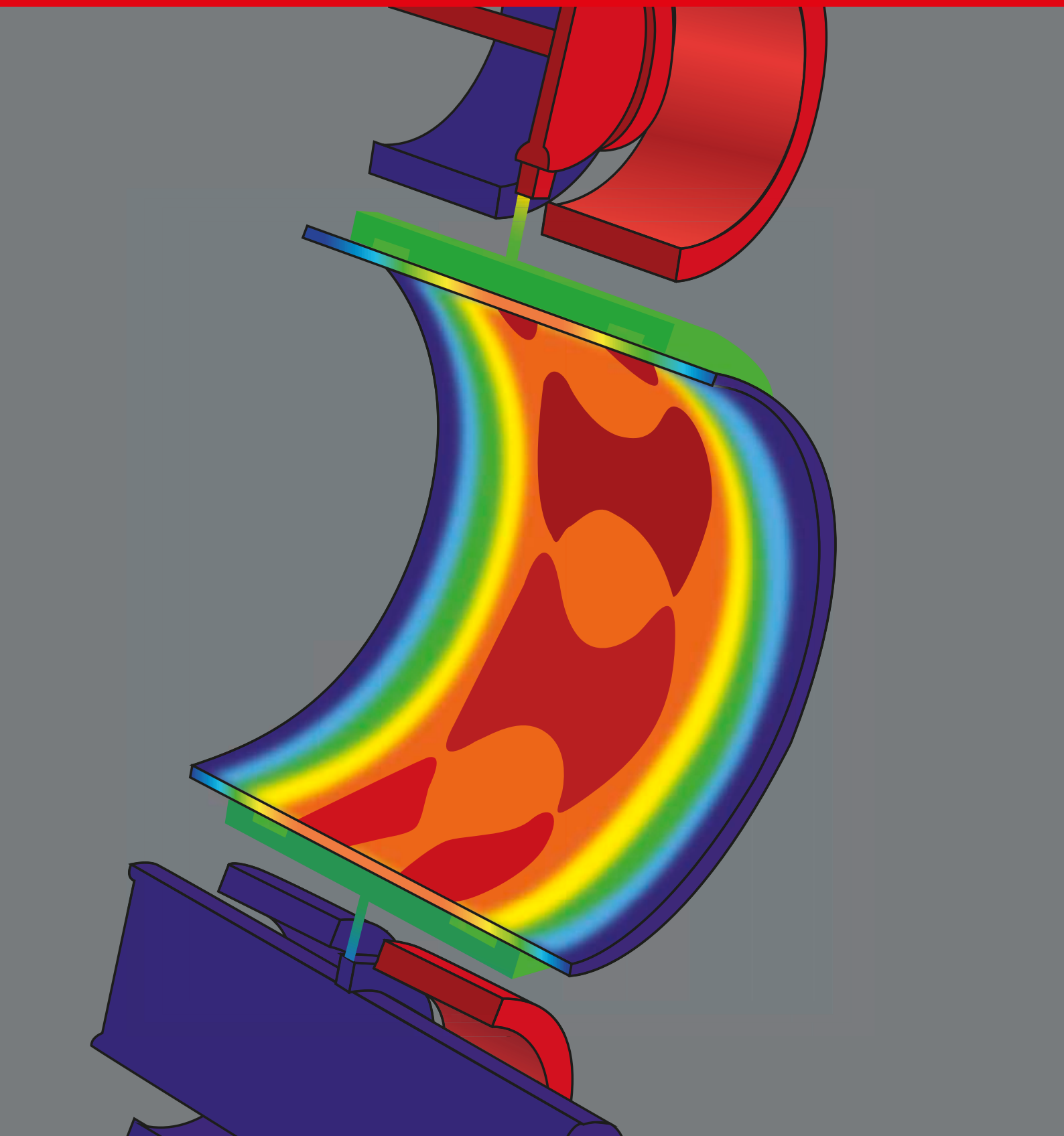
scapos

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

SELECTED PROJECTS

ATOMMODEL	June 2012 to May 2015 Funded by Eurostars/ German Federal Ministry of Education and Research (BMBF)	Electronic components have been miniaturized to such an extent that today single atoms influence their performance and reliability. This is why the electronics industry needs new simulation tools at the atomic scale to improve their products. The objective of the project is to develop efficient methods for the atomistic modeling of new materials in electronics and to implement them in a user-friendly software.
BePhaSys	January 2012 to December 2014 Funded by BMBF	The project develops algorithms and software for the calculation of thermochemical equilibria of multiphase systems with an arbitrary number of system components. Such calculations are used for the prediction of the reaction between chemical substances and the resulting products. The project combines mathematical methods, high performance computing and thermochemical modeling.
BioEquality	June 2010 to August '12 Funded by ZIM/ German Federal Ministry of Economics and Technology (BMWi)	The aim of the project is to improve the safety of biopharmaceuticals which are manufactured using gene technology. Together with industry partners, Fraunhofer SCAI will develop a software for the automated quality analysis of biopharmaceuticals and their equivalents.
Cloud4Health	September 2011 to January 2015 Funded by BMWi	SCAI develops a secure platform for text mining workflows that can easily be deployed in private and public cloud infrastructures. SCAI designs and implements processes and workflows for text mining of medical data, providing the results to users from clinics. This includes setting up and providing the initial cloud Infrastructure as a Service (IaaS) for the projects text mining platform. (www.cloud4health.de)
ComFliTe	January 2009 to March 2012 Funded by BMWi	Numerical simulation has become increasingly important in the design process of aircraft components. Nevertheless, a lot of time is still invested in the testing of prototypes in wind tunnels. For that reason, effort is put into the development of a "numerical wind tunnel" in a virtual flight testing environment to reduce the costs during all stages of the design process.
enhance	April 2011 to October 2013 Funded by BMBF	The project aims for a better integration and simplified usage of heterogeneous computing systems. User-given algorithms are automatically mapped on hetero-geneous architectures including multicore CPUs, GPUs, and new accelerators like FPGAs in an architecture-specific optimized manner. (www.enhance-project.de)
FEMMINER	November 2010 to October 2012 Funded by KMU innovativ/BMBF	SCAI and GNS mbH will develop new data mining methods for the analysis of simulation results in the automotive industry. These methods will be integrated into new software tools supporting simulation engineers in the discovery of branching points in the development history of new products.
GASPI	June 2011 to May 2014 Funded by BMBF	The project addresses a difficult task in the software industry, known as the "Multicore Challenge". The aim is to stimulate the development of programming models and programming languages that lead to new ways for mathematical modeling, algorithms, and their implementation in software. (www.gaspi.de)
Hybrid4HPC	October 2010 to September 2013 Funded by ITEA2/BMBF	The project provides the developers of compute-intensive applications with a hybrid programming environment for heterogeneous computing clusters composed of processors and hardware accelerators. This environment facilitates the development and porting of HPC applications like SCAI's software *SAMG*.(www.h4h-itea2.org)

Neuroallianz	January 2009 to January 2015 Funded by BMBF	In the Neuroallianz Consortium various academic institutions and companies collaborate in strategic research partnerships to develop new therapeutic and diagnostic approaches of neurodegenerative diseases. SCAI contributes a collaborative information technology platform to support data exchange, intelligent data analysis, and disease-centric knowledge discovery for the partners. (www.neuroallianz.de)
FUS	June 2010 to May 2013 Funded by a Fraunhofer Internal Program (MAVO)	The project explores mathematical models and numerical simulations for the biophysical effects of focused ultrasound and its application to tumor treatment in the human abdomen. A demonstrator software for the planning and optimization of the treatment will be developed. (www.simfus.de)
OPTIMIS	June 2010 to May 2013 Funded by the European Commission (EC)	The projekt Optimized Infrastructure Services (OPTIMIS) enables organizations to automatically externalize services and applications to best-execution venues in the hybrid cloud model. SCAI contributes a solution for software licensing and management in clouds and a framework for negotiating and creating service level agreements. (www.optimis-project.eu)
SIMDATA-NL	July 2011 to June 2013 Funded by BMBF	The project aims at the extraction of the effective dimensions in high-dimensional simulation data in the context of automotive design. Linear methods, like principal component analysis, are not sufficient for many applications due to significant nonlinear effects. Therefore, they will be complemented by methods that are able to resolve nonlinear relationships, i.e., by means of sparse grid discretizations.
SOFA	July 2010 to June 2013 Funded by BMBF	In the project, academic and industry partners are working together to find solutions to challenges of the future vehicle development. The aim is to develop methods and software tools for the robust simulation and optimization of coupled multiphysics problems in automotive design. (www.sofa-verbund.de)
+Spaces	January 2010 to September 2012 Funded by the EC	+Spaces targets the use of data from online communities like Facebook, Twitter, and others to support policy making. In these spaces huge numbers of participants can share their opinion in polls, textual debates, or structured role play simulations. SCAI supports the decision making processes by intelligent data analysis services. (www.positivespaces.eu)
Turbo-Keramik	March 2012 to February 2015 Funded by MAVO	Local combined heat and power stations with gas turbines will gain importance as energy source. In order to increase the heat resistance and durability of turbines, the rotor and other parts are made of ceramic materials. SCAI will apply multiphysics simulation methods to optimize the energy efficiency of the system.
EGI-InSPIRE	May 2010 to April 2014 Funded by the EC	EGI establishes a sustainable European grid infrastructure. SCAI is one of the involved service centres in Germany and participates in operating services for the infrastructure. Furthermore, SCAI develops data discovery tools and interfaces for the earth science community. (www.egi.eu)
VERCE	October 2011 to September 2015 Funded by the EC	VERCE supports earthquake research by developing a data-intensive eScience environment. SCAI contributes its experience in distributed infrastructures and service provisioning. (www.verce.eu)
UIMA-HPC	April 2011 to March 2014 Funded by BMBF	The project aims to realize an HPC-based solution for the automated analysis of multi-modal pharmaco-chemical document databases. The text and structure analysis will be based on the Unstructured Information Management Architecture (UIMA). SCAI will develop integrated text and image analysis engines, including annotation engines, and will implement them on HPC systems. (www.uima-hpc.de)
VIPROFORM	February 2012 to July 2014 Funded by KMU innovativ/BMBF	The production of automotive body-parts involves sheet-metal forming via pressing or stamping processes. The core of the software "VIPROFORM" is a database of existing CAD models with the results of already accomplished forming simulations. The aim is to develop mathematical methods and parallelized software that improves the virtual design of robust construction elements.



NUMERICAL SIMULATIONS FOR ENGINEERING AND SCIENCE

Mathematical modeling and numerical simulations are indispensable in nearly all engineering and scientific disciplines. Together with theoretical and experimental research, numerical simulations support engineers in designing new, or optimizing existing technologies and technical devices. This helps scientists to better understand various kinds of processes in nature.

The Department of Simulation Engineering is focused on so-called multiphysics simulations and on developments in High Performance Computing. Our work ranges from mathematical topics and software developments to practical applications in cooperation with our customers in industry and science.

The term multiphysics is to be understood as numerical simulations that combine multiple physical models or multiple physical phenomena. Examples are Fluid-Structure Interactions (FSI), combining Computational Fluid Dynamics (CFD) and finite element calculations, thermal coupling, the simulation of solid conduction and radiation in cooling and heating processes, or the influence of electromagnetic fields on gas flows.

Our central contribution to this field is the software *MpCCI*. It enables the user to directly couple distinct physical models and the corresponding simulation codes. *MpCCI* delivers a complete multiphysics simulation environment based on code coupling, which includes the set-up and control of simulation runs. It also includes the exchange of data among simulation codes, the mapping of computational meshes, highly efficient neighborhood searches in structured and unstructured meshes, and the interpolation of computational quantities. *MpCCI* supports most of the leading commercial simulation codes, e.g. from fluid and structural mechanics. Worldwide, *MpCCI* stands as a brand name for an open and vendor-independent platform for code coupling.

Complementary to our work in numerical simulation, we also address various aspects of high performance and distributed computing. The aim is to enable applications, from industry and academia, to effectively exploit the enormous potential of new heterogeneous computer architectures. Our work includes contributions to optimizing compilers, to new programming paradigms, and to the development of a high performance numerical library for sparse linear algebra, which is often the most crucial part in numerical simulations.

In our Group of Computational Chemical Engineering we are developing algorithms and software for molecular design problems at different length and time scales. The focus of our work is the optimization of force-field parameters for molecular dynamics using data from quantum chemistry simulations or from experiments. Again our aim is to improve the accuracy of simulations, to speed up the modeling process and to make it a bit more automatic.

In all of our working areas, our services include the development of software products with corresponding support and consulting for our customers. In joint research projects we also develop tailored solutions – including physical modeling, computational studies and ready-to-use applications.

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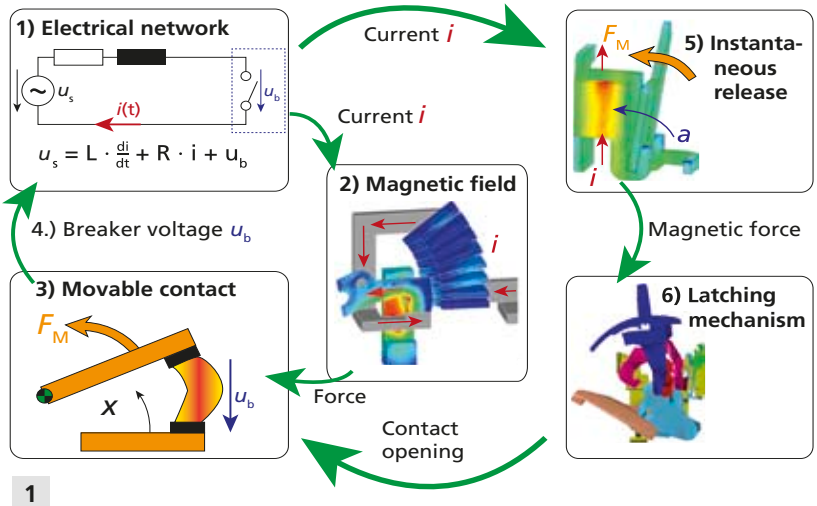
LEFT *Fluid-structure simulation of a compensation chamber in a high-pressure hydraulic pump.*



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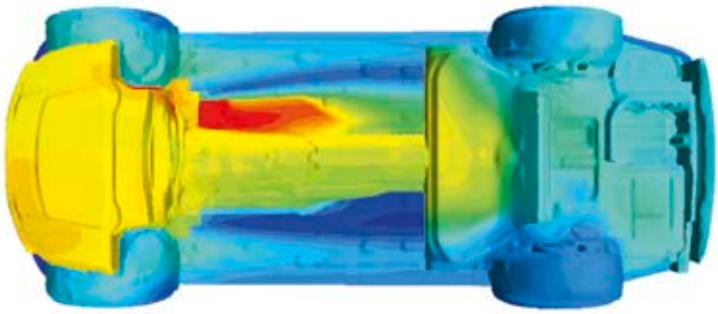

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APPLICATIONS OF THE MpCCI MULTIPHYSICS INTERFACE

Numerical simulation is a widely accepted tool when designing complex technical processes and products. With growing complexity, the requirements for an exact physical modeling increase. A particular challenge is to cover different physical phenomena simultaneously and to combine them into one computational model.

The term multiphysics simulation stands for numerical simulations which couple various physical models. Typical examples are the interaction of fluid flow and structural analysis or fluid-thermal-stress simulations. But instead of completely re-writing the simulation software and the corresponding numerical algorithms for different physical models, one usually follows a so-called partitioned approach. It allows further usage of existing methods and software in each of the related fields combining them by proper interfaces and mapping technologies in an iterative way.

The *MpCCI* Multiphysics Interface offers a unique technology for such coupled or partitioned simulations. It allows the coupling of most of the leading simulation codes in the market and can be used for a wide variety of applications. As an independent developer SCAI collaborates with software vendors including Ansys, CEDRAT, CD adapco, Flowmaster, JSOL, MSC, Numeca, Simulia, and ThermoAnalytics. *MpCCI* provides easy-to-use interfaces to their codes and is also open for specialized codes from industry, research, and academia. The software is available from the institute's spin-off company scapos AG. SCAI supports *MpCCI* users, offers solutions tailored to specific requirements and cooperates in various application projects.

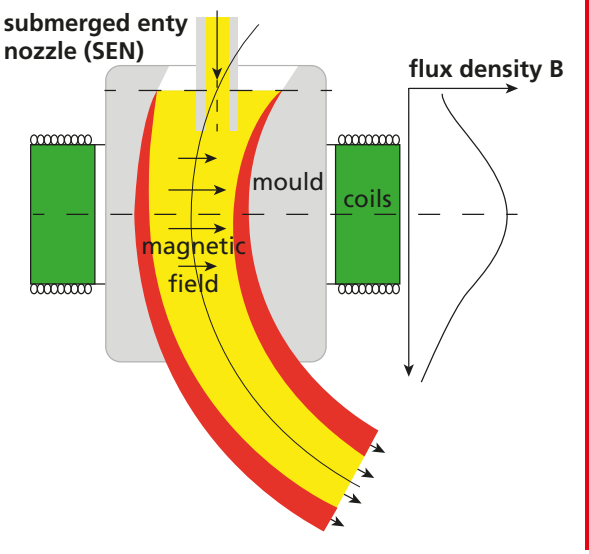
The most popular multiphysics application is certainly the fluid-structure interaction, i.e. the co-simulation of Computational Fluid Dynamics (CFD) and structural analysis for which an example is given in the next article. On the other hand, *MpCCI* is used in a much wider spectrum of applications as we will briefly describe in the following four examples.

Switching arc for a motor protective circuit breaker

In cooperation with Eaton Industries, Bonn, the multiphysics interactions in low voltage electromechanical switching devices were simulated by a coupled iterative approach. Examples of such devices are circuit breakers which monitor if the current exceeds an admissible value and interrupt automatically. *MpCCI* was used for the simulation of the highly complex dynamic behavior of the electric arc moving through the quenching chamber of the device. Numerically, the simulation is based on the Navier-Stokes equations for the gas flow within the chamber coupled with Maxwell's equations for the electromagnetic fields and forces. The finite volume code FLUENT was used for the gas flow, whereas the finite element code ANSYS/EMAG was employed for the electromagnetic part.

Thermal management for automotive vehicles:

When analyzing the thermal behavior of automotive vehicles, the main challenge is to perform realistic simulations which cover the full complexity of a vehicle's geometry and various kinds of heat transport phenomena, for example convection, radiation, and conduction in both the (surrounding) air and the solid bodies. Today, several simulation codes are able to meet



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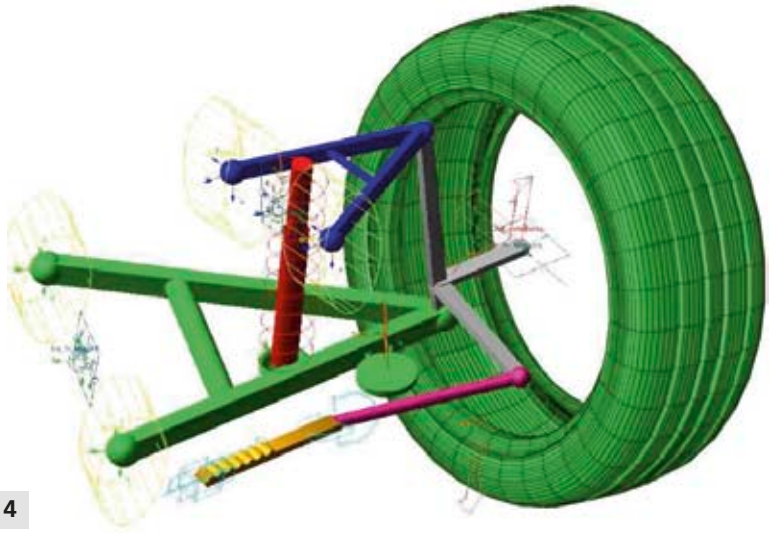

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parts of such requirements. But for each heat transport mechanism the quality of the codes differs significantly in effectiveness and accuracy. In order to cover all or most of the requirements, a coupled approach combining the strengths of different simulation codes is preferable. BMW AG, Munich, has integrated *MpCCI* for the coupling of STAR-CCM+ (from CD adapco) and RadTherm (radiation code from TAI) into its workflows for full vehicle thermal management. BMW uses full car models with more than 45 million CFD elements and nearly one million RadTherm elements on massively parallel clusters. The cooperation with SCAI includes continuous support and the adaptation of the *MpCCI* interfaces to the customer's specific requirements.

Continuous casting of steel with electromagnetic braking and stirring

The simulation of continuous casting of steel is a further example from one of our *MpCCI* customers. Researchers at the Johannes-Kepler-University, Linz, investigate the application of electromagnetic fields to modify the steel flow. Rotating fields are used to excite a rotary motion in the strand, whereas stationary fields are used to break the submerged jets. Numerical simulations gave a detailed insight into the interaction of fluid with the magnetic fields and were used to optimize the production processes. The simulation was based on FLUENT for the liquid steel flow and on ANSYS/EMAG for the electro-magnetic fields. The interaction between both was realized by *MpCCI*'s full volume coupling.

Nonlinear deformation of tires driving through road potholes

MpCCI is in a continuous process of development in order to include new application domains and new simulation codes. An example is the coupling of Multibody Simulation (MBS) with the nonlinear Finite Element Method (FEM). When dealing with flexible bodies, a typical and simplifying approach is to integrate a linear model description into an MBS program using methods like "Craig-Bampton" or others. In many cases such linear models for flexible bodies are not sufficient. This holds, for example, when combining tire models and vehicle dynamics simulations. The simulation code Abaqus from Simulia provides the capability to describe a tire component as a nonlinear model. Via *MpCCI* the coupling of this nonlinear finite element model with the MBS-code MSC.Adams is possible. With such a coupled simulation, deformations and forces of the tire can be considered in conjunction with the complex dynamic boundary conditions provided by the associated multibody system. The effect of the acceleration (from MBS) on the calculated reaction forces (from FEM) can therefore be modeled and simulated with a higher accuracy and reliability compared with a pure MBS-model. The *MpCCI* interface for MSC.Adams enabling the MBS-FEM coupling will be released in the second half of 2012.

1 *Multiphysics interaction in electromechanical switching devices.*
2 *Wall temperature distribution on the underhood of a car.*
3 *Sketch of the casting process (exaggerated strand curvature and mould thickness).*
4 *Coupled model of a suspension system (MBS) and detailed tire model (FEM).*

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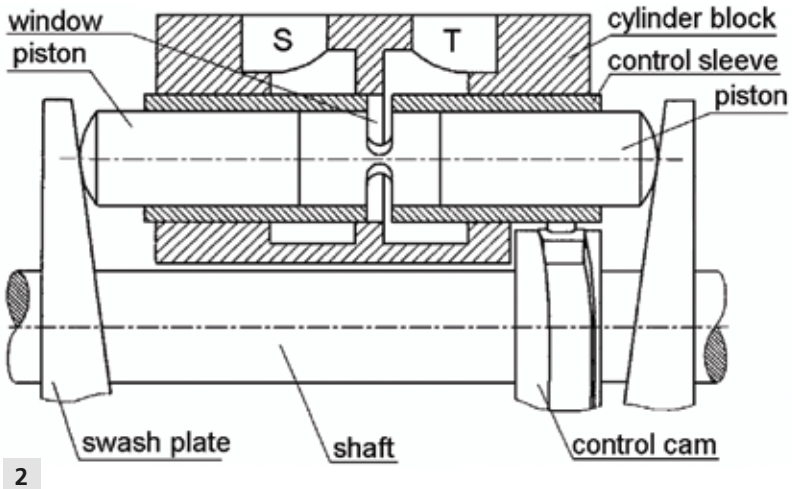

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NEW DESIGN PROCESS FOR AN AXIAL HYDRAULIC PUMP

Axial pumps with cam-driven commutation units – so-called PWK-pumps – emerged as a result of research conducted in the Hydraulics and Pneumatics Department at the Gdansk University of Technology (GUT). In a cooperation with Bandak Engineering (Norway), GUT and the Space Research Center of the Polish Academy of Sciences, Fraunhofer SCAI helps to improve the design of such pumps through the use of fluid-structure modeling.

Axial piston pumps

In axial hydraulic piston pumps, several cylinder chambers are positioned around the rotating shaft of the pump. The shaft rotation and the attached swash plate lead to a piston movement which alternately decreases and increases the fluid volume of the chambers. A window – which is part of the control sleeve or commutating bushing – connects the chamber between the pistons with the low pressure inlet and high pressure outlet channels. The main elements of the pump are shown in Figure 2.

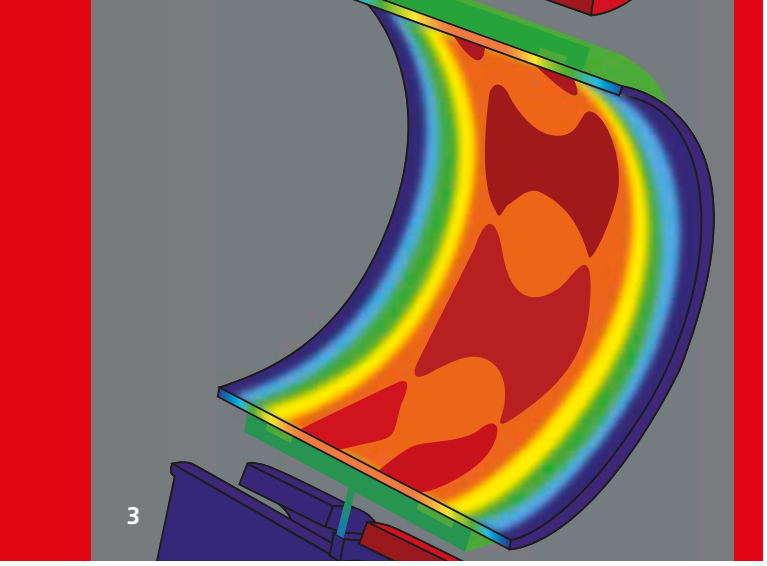
The axial piston pumps with constant displacement show a very good performance with working pressures up to 55 megapascal (MPa), with an overall efficiency of 94 % and good power density. In these types of pumps the pistons always travel the same distance inside the cylinder chamber resulting in a constant amount of output fluid. Furthermore, there are variable displacement pumps, which are used to manage the amount of output fluid. Usually, their piston displacement is controlled with a complicated hydraulic servo-mechanism. Theoretical analysis shows that the displacement of the PWK-pump can be controlled by a low-energy actuator. This is the major advantage of the newly developed pumps because it reduces both the pump's cost and size significantly.

High pressure peaks

First prototypes of the variable displacement PWK-pumps have been built and tested and exhibited good performance. Unfortunately, harmful pressure peaks were observed that could lead to pump damage. During the disconnection of the cylinder chamber from the in- and outlet channels the pressure reaches values that, for a very short time, are more than 20 MPa higher than the average pressure.

To reduce these peaks, the engineers at Gdansk University proposed a compensation chamber. This additional circular chamber – equipped with an elastic wall – is positioned around the shaft. In the compression phase surplus fluid can flow into the chamber; the elastic wall deforms to give the fluid more room. When the pistons retract, the fluid flows back again and leaves the compensation chamber.

First experimental tests showed that the introduction of the compensation chamber reduced the pressure peak value by 50 % without decreasing the pump's efficiency. To find the optimal shape, elasticity and volume of the chamber multiphysics simulations were performed at Fraunhofer SCAI.



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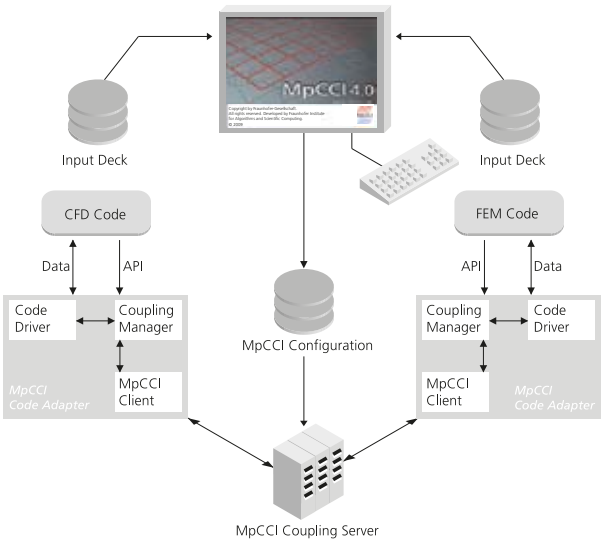

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Coupled computational fluid dynamics and finite element analysis simulations

For setting up the multiphysics simulation, one starts from a complete CAD model of the pump. The first step is then the definition of the Computational Fluid Dynamics (CFD) model and of the Finite Element Model (FEM) for the elastic circular wall of the compensation chamber. For the CFD simulations, due to the customer's requirements, either FLUENT or Star-CCM+ were used while the FEM part was calculated by Abaqus.

The rather complex movement of the piston and the bridge was modeled by user-defined functions in the flow codes. The mesh motion in FLUENT was realized with the dynamic layering method. For STAR-CCM+ a special module had to be developed which provides an efficient remeshing capability.

The "multiphysics" character arises through the coupling of the two models. In the considered case, the elastic wall is subject to pressure forces exerted by the hydraulic oil. The resulting deformation of the wall changes the flow domain and its mesh and, therefore, influences again the pressure and velocity field of the fluid. This is the setup of a classical Fluid-Structure Interaction (FSI). Here, the CFD and FEM codes exchange information relating to that interaction. The pressure forces and shear stresses exerted on the elastic wall of the compensation chamber have to be passed from the flow code to the finite element code. The new nodal positions describing the deformation of the wall have to be sent back to the flow code.

The entire communication between the flow and the finite element code is completely handled by *MpCCI*. This includes the mapping of geometrical and computational quantities, interpolation between meshes of different types and structures, synchronization tasks, and various parameters controlling the iterative numerical processes and the time stepping. *MpCCI* is steered via a graphical user interface which gives full control over the complete multiphysics application, including the flow and the FEM codes.

The results of the multiphysics simulations were in excellent agreement with experimental observations. In particular, the results coincided in a significant better way with the experiments than for simulations based only on CFD.

As a major result, the project identified – from a number of potential compensation chambers employing different layouts – an optimal pump design that maintains high efficiency while minimizing the pressure peaks. Further research will now have to address the integration of cavitation into the CFD model and the important practical aspect of leakage of hydraulic oil through small gaps.

1 *Constant displacement pumps PWK-78 (top) and PWK-27.*

2 *Main elements of PWK-pump. Cross section of one chamber, the shaft and steering elements.*

3 *The compensation chamber and the elastic wall with pressure contours (symmetric model, only one half is simulated).*

4 *MpCCI software architecture.*

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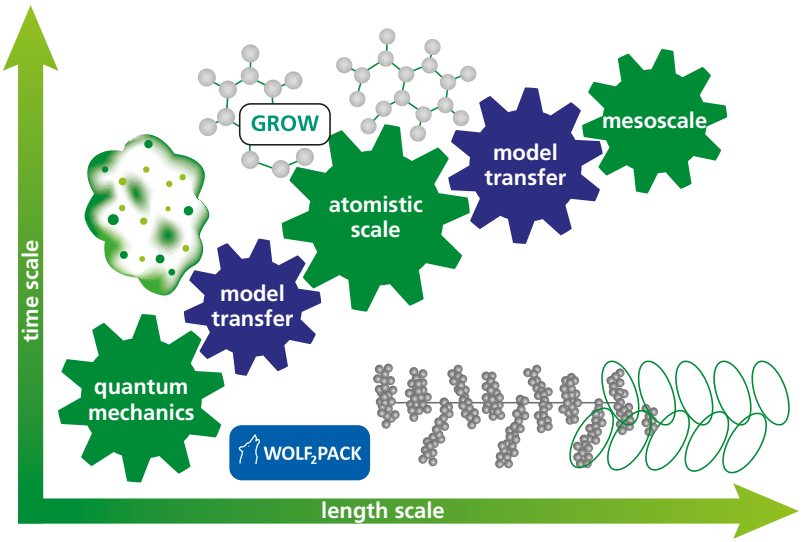

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WORKFLOW-TOOLS FOR MOLECULAR MODELING

A common goal within computational chemistry, whether using Newtonian- or quantum-based methods (QM), is the accurate modeling of physical forces and energetics. Through reliable modeling of the underlying forces, molecular simulations provide atomistic insights into macroscopic experimental observations.

Although there are some commercial developments in the area of computational chemistry, most scientific software packages are written by scientists rather than by software engineers. This is due to the demanding and continuously evolving concepts from physics and chemistry that need to be transferred into proper algorithmic solutions. Our way for enabling our software to evolve is to decouple tasks – in doing so, algorithmic solutions can be introduced in a modular fashion, allowing us to easily identify and update specific tasks as needed. Using this idea, our group has developed several independent software tools for molecular simulations. Figure 1 shows how they address various inter-linked resolutions of molecular modeling to solve one of the primary goals of our research: To develop accurate and reliable molecular parameters and models in a reasonable time and as error-free as possible.

1 *Current evolving software packages developed at Fraunhofer SCAI and how they fit into the multiscale modeling approach of computational chemistry.*

For intramolecular interactions, we have created a scientific "workflow for force-field optimization package" (*Wolf*$_2$*Pack*) that incorporates our approach for transferring knowledge gained from QM to Newtonian-based models. We define a scientific workflow as a series of independent steps that are linked together according to the data flow and the dependencies between them. For intermolecular interactions we developed a systematic optimization workflow, based on efficient gradient-based numerical algorithms called *GROW*. *GROW* is a modular tool kit of programs and scripts. It is a generic implementation and can be easily extended by other developers. Both programs facilitate: a) the development and optimization of molecular parameters for a given simulation engine, b) the transfer of parameters from one software package to another, and c) the testing of the parameters using a standard test suite and protocol via a semi-automated iterative parameterization process.

In combination, the joint efforts of scientists and software engineers at SCAI greatly enhance the task of molecular modeling through superior software tools. Their modular structure not only simplifies the addition of new functions and maintenance, but more importantly accelerates the modeling process and makes it more robust. Users will therefore benefit in terms of both time and resources due to our software and services.

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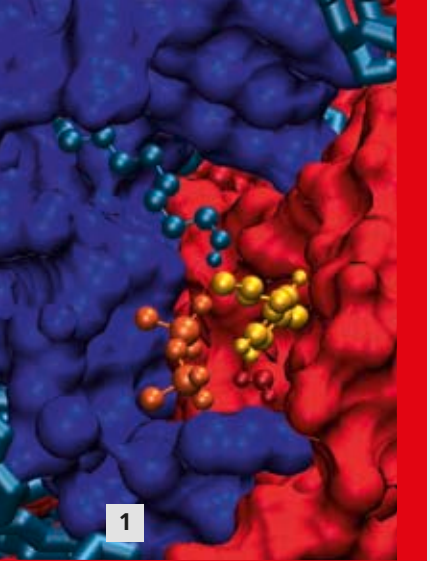

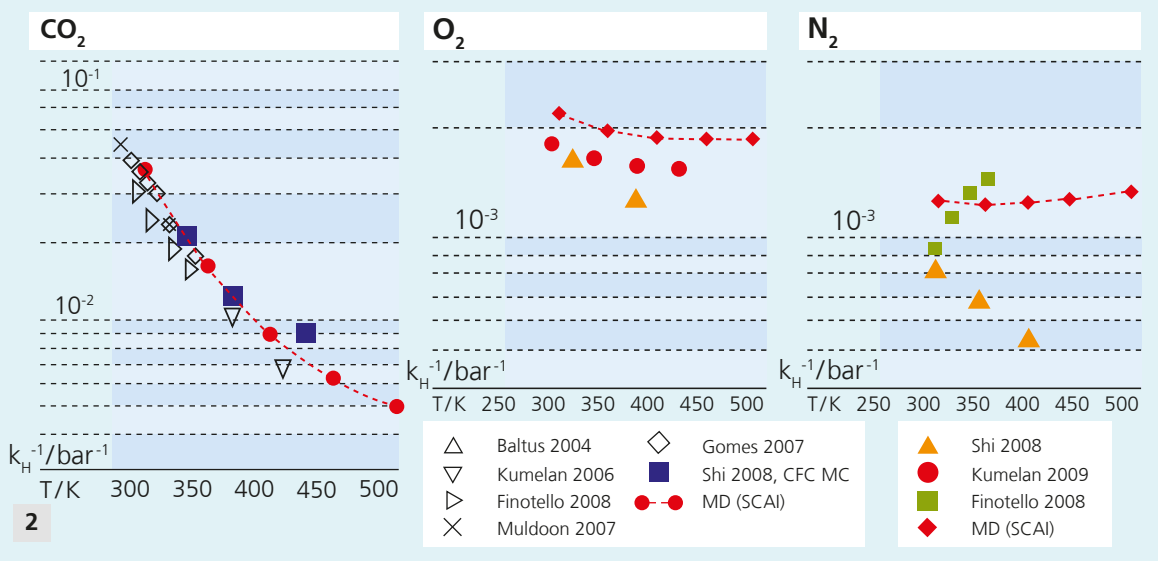

SOFT MATERIALS WITH TAILOR-MADE PROPERTIES

Ionic Liquids (ILs) represent a unique class of materials. They can be regarded as designer solvents because they consist purely of ions. By altering the ion combinations, their properties can be designed as needed. ILs practically do not evaporate, they have a high electrical conductivity and viscosity and are able to dissolve a broad range of substances. Utilizing our own software tools *Wolf$_2$Pack* and *GROW* (see previous page), our group has developed a customized computer model to reliably simulate properties of ILs, with the aim to save time and reduce costs for developing new solvents.

Computational modeling is well-suited to the design of ionic liquids. An IL can be roughly divided into three parts: The anion, the cation head and the cation tail. All parts contribute to the properties of the IL and can be altered independently. Their effect on the IL properties is not entirely independent, but one can still look at each part in order to adjust the IL properties in a required direction. This is true in chemical synthesis and in the computer. The molecular dynamics simulation method, which SCAI uses, can be seen as a construction kit. One builds the desired IL in the computer, parameterizes the ion interactions with an experimental database and then calculates relevant physicochemical properties like the viscosity or the solubility of gases. Furthermore, it is possible to computationally mix ILs with each other or with other chemical compounds. This enables SCAI to optimize IL properties not only by changing the IL itself, but also to find mixtures with optimal properties.

1 *Ionic liquid ion pair at the interface between water and octanol.*

2 *Solubility of CO_2, O_2 and N_2 in [C_6 MIM] [NT f_2] as a function of temperature.*

Customer benefits

Fraunhofer SCAI uses state-of-the-art molecular modeling, which includes quantum chemical calculations. The models gain their reliability through validation with experimental databases. The simulations are able to quantitatively predict important properties of ionic liquids: As can be seen in Figure 2, the simulated solubility of CO_2 exactly reproduces experimental results. In the case of O_2 and N_2 solubilities, measurements from laboratory experiments strongly disagree with each other. Here our simulations can even be used to validate experimental data. As a benefit of the simulation process, customers are provided with important thermodynamic and dynamic data (see Figure 2). The results can be used, for instance, to optimize technical processes involving ionic liquids as lubricants, electrolytes, or thermofluids.

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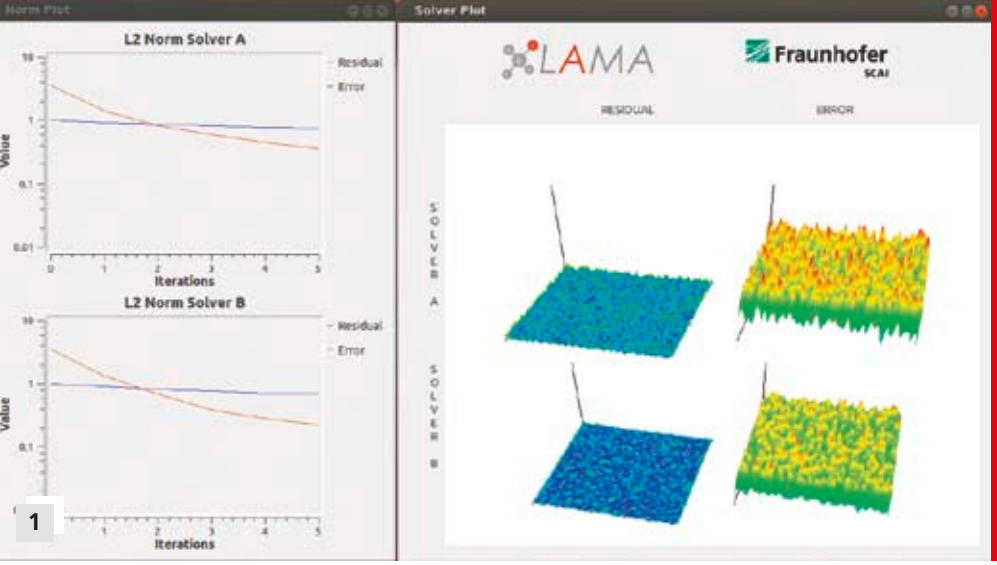


1

```
void solveCG( Vector& x,
              const Matrix& A,
              const Vector& b )
{
    Vector r = b - A * x;
    Vector p = r;
    double rho = r * r;
    ...
    for ( int i = 0; i < nIterations; i++ )
    {
        Vector q = A * p;
        double alpha = rho / ( p * q );
        x = x + alpha * p;
        r = r - alpha * q;
        ...
    }
}
```

2

LIBRARY FOR ACCELERATED MATH APPLICATIONS

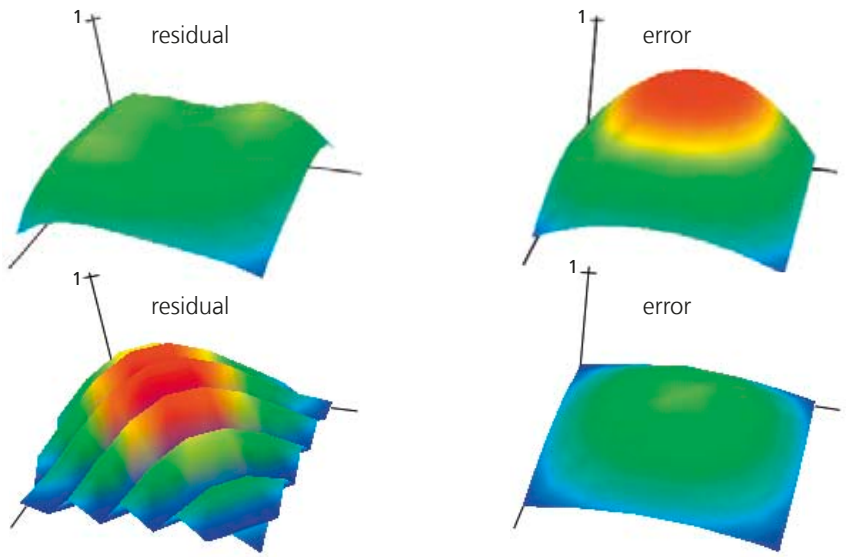
LAMA, the Library for Accelerated Math Applications, is a framework for building efficient, extensible and flexible solvers for sparse linear systems in application domains that involve – sparse and dense – numerical linear algebra. It supports shared and distributed memory compute architectures, including accelerators, through an easy to use interface.

LAMA is an open source C++ library for building efficient and flexible applications that require sparse and dense linear algebra functionality. *LAMA* follows two main design goals: efficiency and extensibility. Although widely extensible and easy to use, *LAMA*'s performance is comparable with other linear algebra libraries that focus only on a single type of target hardware.

Additionally, *LAMA*'s design enables its use on future hardware architectures with optimal performance due to its inherent data structure layout that can be easily extended to support novel and even experimental hardware setups. *LAMA* includes unique communication features, which allow, in many cases, to completely hide the data transfer between compute components within a node and between nodes.

LAMA provides an easy to use and flexible interface with an intuitive semantic. This is achieved by employing a domain specific language to formulate linear algebra algorithms almost in a textbook syntax. For example, a residuum calculation can be formulated directly by `r = y – A * x`, where x and y are vector class instances and A is a matrix instance. An underlying storage class implementation allows for an efficient usage of different types of hardware systems and handles the necessary conversions between them. Figure 2 shows as example an implementation for the well-known Conjugate Gradient (CG) algorithm using *LAMA*.

The *LAMA* interface hides the complexity of distributed and shared memory computers and accelerators – e.g. Graphics Processing Units (GPUs) – without sacrificing efficiency by employing the C++ template technology. Therefore, the mathematical formulation of a given problem is handled independently of implementation details. This approach has a huge advantage for application developers. They can now concentrate on the problem they want to solve. With *LAMA*, the tedious and error prone work of handling distributed and accelerator memory models as well as explicitly programming communication belongs to the past.



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LAMA targets systems that range from desktops and small compute clusters to supercomputing systems. Thus, special attention is paid to the parallel scalability and the serial performance of *LAMA*, facilitating an efficient execution on all of these systems. Currently, *LAMA* supports the application programming interface Open Multiprocessing (OpenMP) to exploit multicore processors, the Compute Unified Device Architecture (CUDA) and the Open Computing Language (OpenCL) to exploit accelerators like GPUs and the Message Passing Interface (MPI) to handle distributed memory systems. A high performance communication layer is being developed that supports different Partitioned Global Address Space (PGAS) implementations in a resilient fashion. Within *LAMA* the OpenMP, CUDA, and OpenCL implementations can be freely combined at run time to achieve the best performance for a given problem size and targeted hardware architecture. In addition to this flexibility, *LAMA* supports the sparse matrix formats CSR, ELLPACK and JDS enabling the best performing data structure to be chosen for each individual problem and available hardware. *LAMA* can be easily extended by new data structures for sparse matrices, if this is needed to achieve optimal performance on special hardware or for problems with unique features.

Besides its Basic Linear Algebra Subprograms (BLAS) functionality for sparse and dense types, *LAMA* is augmented by a solver framework layer for linear systems of equations. This solver framework allows very flexible combinations of available numerical solvers. Hence, highly efficient algorithms for treating large systems can be constructed easily. In an inter-department collaboration, this framework has been used to build an Algebraic Multigrid Method (AMG) for distributed memory systems with GPU accelerators.

LAMA is available under the MIT License, a free software license originating at the Massachusetts Institute of Technology, which allows its straightforward integration into commercial software.

SCAI offers customization of *LAMA*, training on its usage and help with the integration of *LAMA* into customer software.

1 *Visualization of the effects of using different numerical solvers on the same problem, implemented in LAMA.*
2 *A conjugate gradient solver integrated in LAMA´s text-book like syntax.*
3 *Residual and error states for a LAMA-implemented Jacobi solver compared with a conjugate gradient solver after 25 iteration steps for a two-dimensional five-point Poisson problem.*

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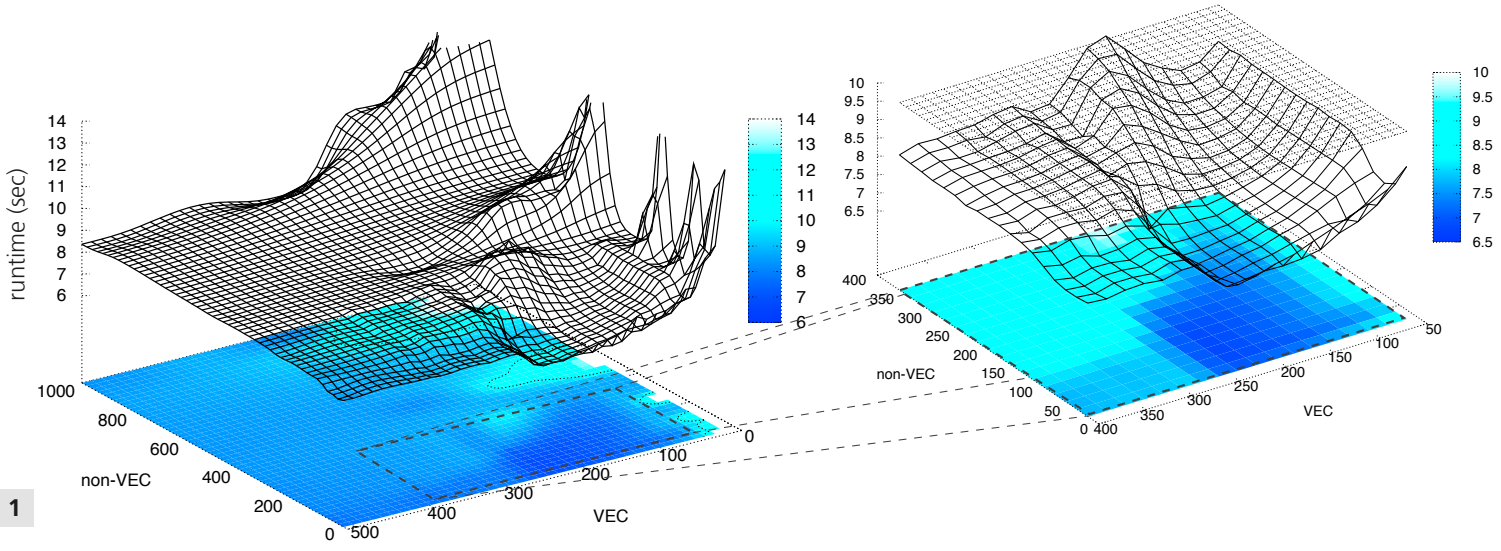

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OPTIMIZING COMPILERS FOR MULTICORE ARCHITECTURES

Multicore hardware architectures are omnipresent. Nevertheless, many applications are unable to use the full power of these workhorses. The reason is simple: the programs have not been designed with parallelism in mind. With its activities for compiler optimization, SCAI focuses on the (semi-)automatic parallelization and memory access optimization of suitable parts of otherwise serially running applications.

Enabling academic and commercial applications for heterogeneous computing architectures will be a key task in the coming years. Automating this task requires improvements of today's compilers. Furthermore, facing the multicore challenge means thinking about new programming concepts and paradigms. The ease of programming will determine success or failure of novel hardware architectures. Moreover, only applications which efficiently use today's and tomorrow's multicore chips and hardware accelerators will prevail on the competitive market.

1 *Resulting runtime of different code transformations.*

For several decades small vector processing units have been present in conventional CPUs. But even today, compilers are unable to automatically make the most efficient use of them. Also for Graphics Processing Units (GPUs), which work similarly, significant manual tuning of code is necessary to exploit their full computational potential.

The HPC group at SCAI develops a (semi-)automatic transformation and optimization engine for source code, which supports many of today's compute architectures. The core of such a source-to-source compilation infrastructure is a mathematical framework built around methods from linear algebra, integer programming, discrete mathematics, and graph theory.

For supporting the Single Instruction, Multiple Data (SIMD) vector extensions in current CPUs, code is transformed by optimizing the cache access patterns and register usage. Valid transformations are automatically applied in order to get optimal performance on a given hardware infrastructure. Introducing this source-to-source compilation significantly improves the performance over non-transformed code.

The project ENHANCE (enabling heterogeneous hardware acceleration using novel programming and scheduling models), funded by the German Federal Ministry of Education and Research, allows for the extension of this compiler framework to other novel compute architectures.

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SOLUTIONS FOR FUTURE SOFTWARE SERVICES

IT-Services (IT-S) is a cross-disciplinary department, servicing the IT infrastructural needs of SCAI's personnel. It is also actively engaged in national and European research projects that arise from the Information and Communication Technology (ICT) sector. The department operates several compute clusters with varying hardware, software and operating systems, including Microsoft Windows HPC based clusters and GPU clusters. The clusters are partly operated under cloud middleware to support HPC cloud services.

Within SCAI, IT-S paved the way for service provisioning for external customers based on the Software as a Service (SaaS) model utilizing the Microsoft HPC Platform on top of its own resources. To support this sales model, a generic SaaS solution including all business processes with accounting and billing was developed. In an early adopter program, the Microsoft HPC cluster solution was extended using Azure cloud nodes. The newest developments, supported by Microsoft, are focused on service provisioning through the Microsoft Azure platform.

In the project Cloud4Health, funded by the German Federal Ministry of Economics and Technology, IT-S operates the underlying secure cloud environment, which is also offered as a service to other interested parties.

IT-S is one of the German regional operating centers for the NGI-DE, the national grid initiative as part of the sustainable European Grid Infrastructure (EGI). IT-S has a successful history in providing support and services for the community in earth science informatics. In the project EGI-InSPIRE, funded by the European Commission (EC), IT-S is responsible for the earth science community by providing services for data access outside of the grid infrastructure through the ESA-governed GENESI-DR infrastructure. In the VERCE project, funded by the European Commission, IT-S provides its experience in grid and cluster computing and its know-how in service development and integration on distributed resources. Specifically, it contributes to the shared aim of providing an efficient data-intensive e-Science environment for seismology research.

IT-S is extending its research investments in infrastructure virtualization and cloud computing, using its expertise to provide its customers solutions for next generation software services.

1 *Providing support and services for the community in earth science informatics.*
2 *SCAI operates a modern IT infrastructure to support its customers and project partners.*

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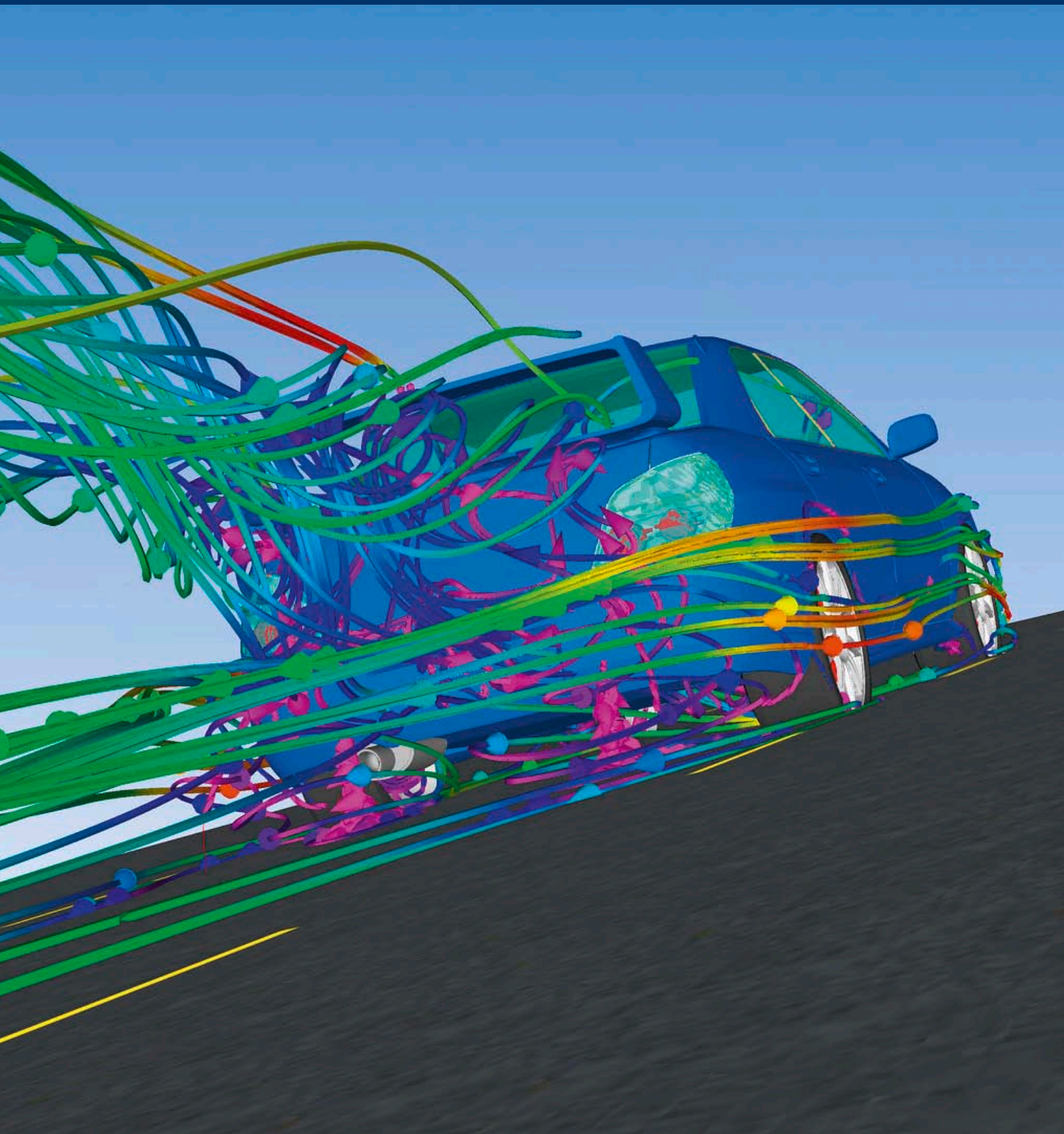

FAST METHODS AND SOFTWARE FOR SIMULATIONS

The use and impact of numerical simulation for virtual product design and understanding product properties are continuously growing. A significant challenge for the future is the combination of interactive simulation and robust design.

The creativity and experience of the engineer determines the quality of a product. Enhancing the engineer's abilities – in terms of achievable product quality and product development time – can be achieved by carrying out numerical simulations interactively and by learning from previous simulations as much as possible.

Here, current numerical simulation often reaches its limits. In particular, the long run-times of large-scale simulations must be substantially reduced. Furthermore, the analysis processes need to be faster and supported much more efficiently. Reducing run-times of numerical simulations is targeted by several activities of the Department of Numerical Software (NUSO):

- *SAMG* solves huge linear systems of equations – usually by far the most time consuming part of a numerical simulation process – exceptionally fast. More precisely, *SAMG* implements an environment to compose state-of-the-art numerical solvers available for all modern computer hardware. Besides parallel distributed and multicore architectures, recent developments also aim at the efficient exploitation of multiple GPU cards.
- Based on a set of simulation results, high-dimensional data reduction methods can be used for interpolation of simulation results instead of re-computing. This has been implemented in the context of *DIFFCRASH* for robust design purposes, and for the interactive selection and evaluation for bifurcation candidates in crash simulation models.

A further major topic is the improvement of the analysis of simulation results:

- Data compression of simulation results helps to save archive space, it reduces transfer times, and reduces times for loading simulation results into post-processors. Here, *FEMZIP* is a well-established SCAI tool for compression of crash and structural simulation results. Recent developments include the application to CFD and novel approaches for the compression of highly refined finite elements grids.
- Learning from previous designs and their impact on the performance is important for future designs. *FEMMINER* is a joint development of GNS mbH and SCAI on mining simulation data bases, which are growing exponentially at major companies. *FEMMINER* allows to interactively find variations of parts used in the designs and to evaluate the redesign impact on the model's overall performance. Instead of just evaluating available metadata, *FEMMINER* takes geometries and the whole set of simulation results into account. It also applies high-dimensional data reduction methods to derive intrinsic metadata information from the designs and the results. This enables a very fast overview to be obtained on past developments and to assess their impact on the performance of the design.

High-dimensional data reduction algorithms based, for example, on Principle Components Analysis and its nonlinear variants, are an active research field in NUSO. The simulation of process chains in manufacturing, the analysis of robust design and bifucation in crash, the analysis of medical applications (such as the ultra sound treatment of liver cancer), and the compression of sets of simulation results are other applications of this mathematical approach in NUSO.

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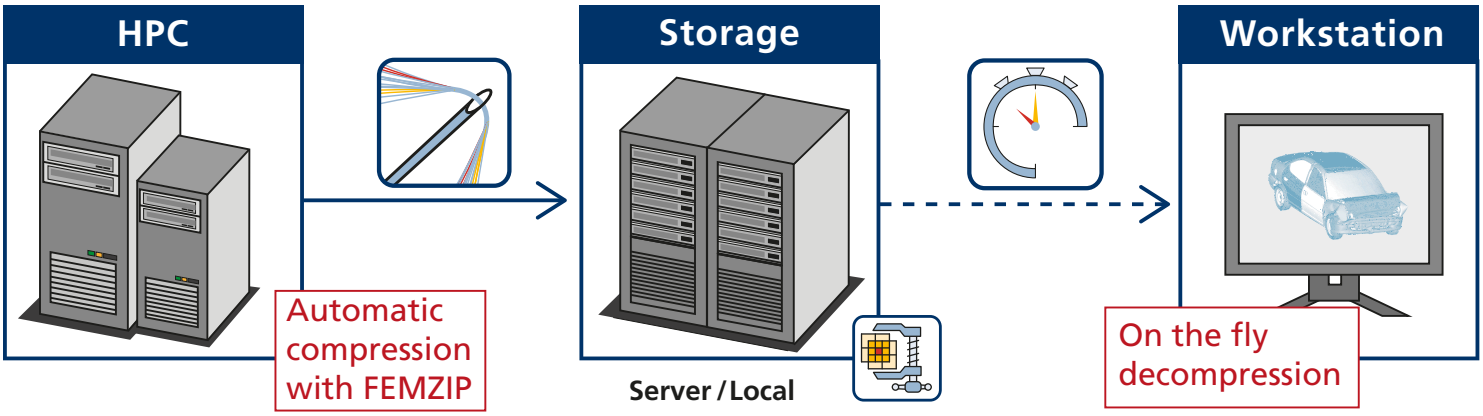
LEFT *Computational fluid dynamics simulation of vorticity around a car model.*



1

COMPRESSION OF SIMULATION DATA

FEMZIP tools are specialized for the compression of simulation results. There are multiple versions suitable for various data formats in the fields of crash simulation, simulation of Noise, Vibration, and Harshness (NVH) and simulation of Computational Fluid Dynamics (CFD) .

Computer simulations, as commonly used for product development in various industries, generate a vast and growing amount of data. The growth in data is a result of larger, more detailed models and an increase in the volume of simulations performed to improve engineering design. Simulation data has to be analyzed, exchanged among engineers and archived for future reference and re-analysis. Network connections and storage space can become bottlenecks in workflows used by engineers. With *FEMZIP*, these bottlenecks can be eliminated. *FEMZIP* data compression tools are specifically designed for the compression of simulation results and can thus achieve high compression factors. The significant reduction in data volume that can be achieved with *FEMZIP* data compression leads to the following benefits:

Reduced Archive Size

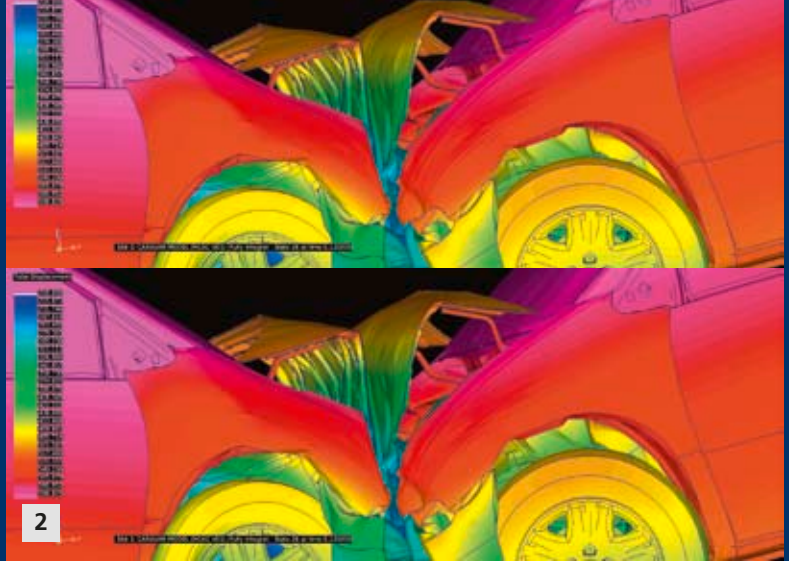
If all simulation data is compressed, only a fraction of the storage is required. Storage and backup capacities can hold more simulation results. Hence, costs for the expansion of storage and of archive infrastructure can be avoided.

Shorter Data Transfer Times

Transferring data across computer networks can be very time consuming. Transmission speeds are limited by the available network bandwidth. Since compressed simulation results require significantly less storage, they can be transmitted in a fraction of the time required for transferring uncompressed results.

Quicker Data Loading

Reading data into post processors can be a time consuming task as well. If data storage is provided on file servers, compressed data can be read directly into post processors significantly quicker due to the faster data transfer. In some cases load times can even be improved when reading from a local hard drive.



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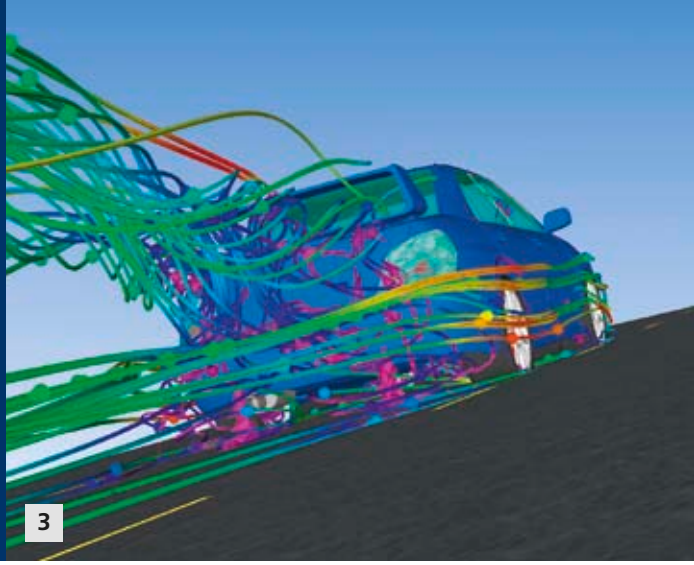

3

FEMZIP is based on a lossy compression scheme that exploits the fact that the 32- or 64-bit floating point representation used to store simulation results is often too precise. Unnecessary information is eliminated from the data to increase compression factors. The loss is controlled by the user by means of precision settings specified for the geometry and for each variable contained in the simulation results. This so-called quantization is combined with specialized mathematical methods to approximate solution values. The differences between the approximation and the quantized values are encoded by utilizing standard encoding techniques. *FEMZIP* compression and decompression is designed to be integrated into existing workflows, such that the engineer is not required to compress or decompress the data manually.

This approach has shown to be very suitable for use in industry and *FEMZIP* products for crash simulations have become very popular. Crash simulations are a standard Computer Aided Engineering (CAE) application in the automotive industry and today, most car manufacturers worldwide make use of *FEMZIP* compression to reduce the volume of simulation data. Solutions for result files from PAM-CRASH, LS-DYNA and Radioss are supported by *FEMZIP* products. The support for Radioss was added recently with the introduction of *FEMZIP*-R. In addition to crash simulation data, *FEMZIP* products have also been developed to compress data from noise vibration harshness simulations generated by NASTRAN and Radioss in the OP2 format.

Currently, a new set of *FEMZIP* versions is in development to further expand the range of supported simulation data and to provide new technologies. They will become available in 2012 and add the support for data from Computational Fluid Dynamics (CFD) to the portfolio. The complexity of CFD problems often requires a fine spatial discretization that is represented by very large volumetric grids. As a result, data sets with tens, if not hundreds, of gigabytes are generated and data compression must be employed. The *FEMZIP* group at Fraunhofer SCAI has developed an entirely new software architecture that is specially designed for the compression of extremely large amounts of simulation data. It utilizes a parallel structure to exploit the resources of today's multicore workstations and supports an efficient memory management. In addition, newly developed compression techniques for CFD data were added to achieve high compression factors and adapt *FEMZIP* to the special requirements of CFD applications.

1 *Engineers can maintain their workflows – FEMZIP is designed to be integrated into existing processes.*
2 *Visualization of a car to car crash simulation – no difference is noticeable between the original and compressed result file.*
3 *Visualization of a fluid dynamics simulation.*

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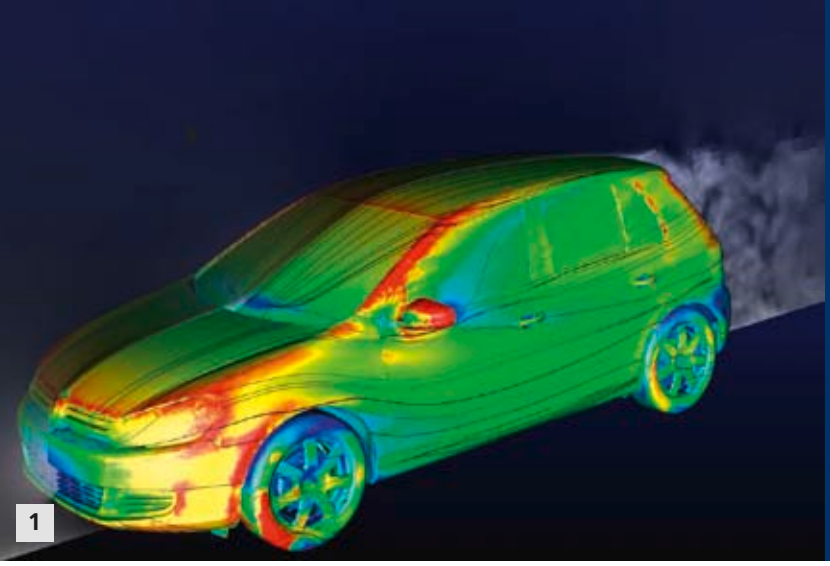

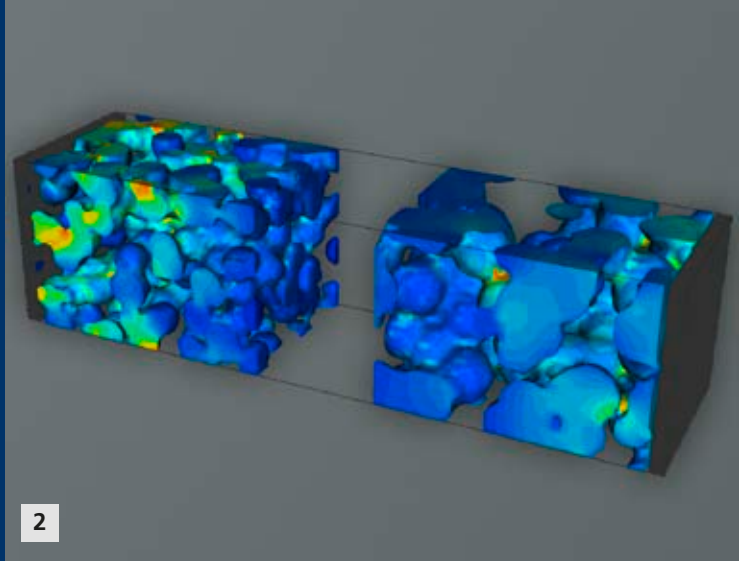

ACCELERATING NUMERICAL SIMULATIONS IN INDUSTRY

Increasing demands in industrial large-scale simulation call for highly efficient linear solvers suitable for solving huge sparse systems of equations. Solvers based on the Algebraic Multigrid (AMG) technique are most promising. Fraunhofer SCAI is continuously developing and generalizing its AMG-based solver package *SAMG*.

Numerical simulation has become an increasingly important technology in industrial design processes. Linear sparse systems of equations with tens to hundreds of millions of unknowns are becoming standard for today's large-scale simulations. Due to its hierarchical approach, *SAMG* is suited for solving such large sets of equations very efficiently. Being a framework rather than a plain solver, *SAMG* can be configured to meet the requirements of specific types of application and/or simulation environments by selecting the most suitable algorithmic components and tuning them for optimal performance. As a matter of fact, there exists no single numerical algorithm that will efficiently work for all possible situations arising in numerical simulation. New applications typically require application-specific investigations and developments aiming at the balance of efficiency, generality and robustness. Hence, there is a strong focus on application-specific optimizations.

The flexibility of the *SAMG* framework has already been successfully proven in the past. *SAMG* has become a well-established tool in various industrial simulation processes, such as the simulation of oil and water reservoirs, fluid dynamics, structural mechanics, casting and molding, semiconductor and devices, and electrochemical plating. "Virtual batteries" is one of the new areas: The simulation of batteries at the microscopic level of electrode particles is used to shorten and simplify the costly experimental development process of lithium-ion batteries. The outstanding efficiency of *SAMG* – in particular, the linear dependency of its computing time on the problem size – was an important step towards making large-scale industrial simulation practicable. This work has been done in cooperation with Fraunhofer ITWM.

An important focus is on the efficient exploitation of modern computer architectures ranging from high performance clusters over multicore machines to commodity GPU cards. Accordingly, there is a range from huge HPC simulations (for example in computational fluid dynamics in automotive and aerospace industry) to commodity applications specifically for small and medium enterprises.

1 *Computational fluid dynamics: flow simulation around a car.*
2 *Battery simulation: electrical current density in anode (left) and cathode (right).*

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1

EXPLOITING THE POWER OF GRAPHICS PROCESSING UNITS

Over the past few years, Graphics Processing Units (GPUs) have gained increased popularity in High Performance Computing (HPC). Fraunhofer SCAI is investigating possibilities of exploiting the power of GPUs to further improve the performance of its solver package *SAMG*.

Growing with the demands of the games industry, the consumer market of graphics cards now offers relatively cheap hardware capable of surpassing, in many respects, the performance of traditional x86 processors. Indeed, for many scientific applications it has already been demonstrated that they benefit from GPUs when used as accelerators. These GPU applications run significantly faster than their pure CPU-counterparts. Therefore, Fraunhofer SCAI is investing effort to exploit the power of GPUs to further improve the performance of *SAMG*, a software package for the solution of sparse linear systems arising in large-scale industrial simulation.

Since the memory bandwidth is usually the performance bottleneck of linear solvers for sparse linear systems, they should especially benefit from the high throughput of GPU architectures. While modern GPU hardware looks theoretically very promising, there are still challenges regarding the best and most practical way to combine numerical and hardware requirements in order to meet industrial needs.

Based on SCAI's high performance library *LAMA* (see page 24) for linear algebra operations, a first version of *SAMG* for GPUs will soon be available. It will be possible to dynamically utilize GPUs for the most expensive *SAMG* components, resulting in a significant increase in performance by factors up to 10. This includes the combination with distributed parallel programming models – e.g. the Message Passing Interface (MPI) – to exploit multiple GPUs.

Ultimately, SCAI aims at a "hybrid" version of *SAMG* ranging from "commodity desktop solutions", available for everyone's office (including GPUs), to large production clusters. A generic interface will make it easy to select resources and corresponding (also heterogeneous) mappings if available: MPI processes (one or several compute nodes), OpenMP threads, accelerators (e.g. one or several GPUs) will cooperate effectively while technical details shall be almost completely hidden from the user.

1 *The power of today's GPUs improves the performance of SCAI's solver package SAMG.*

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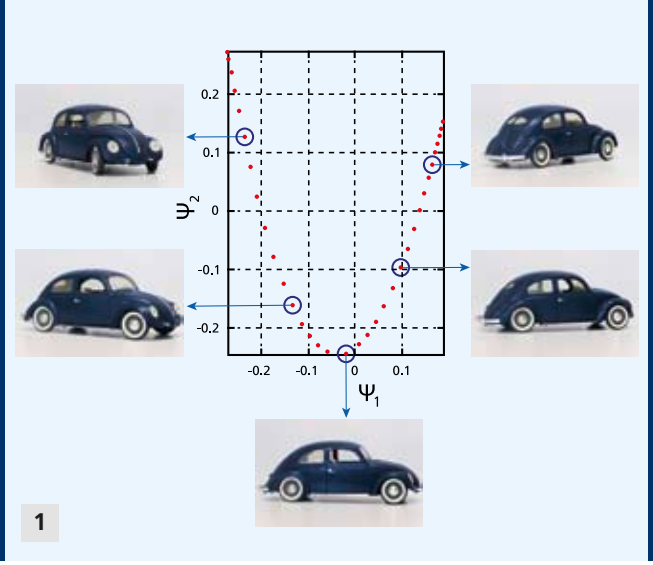

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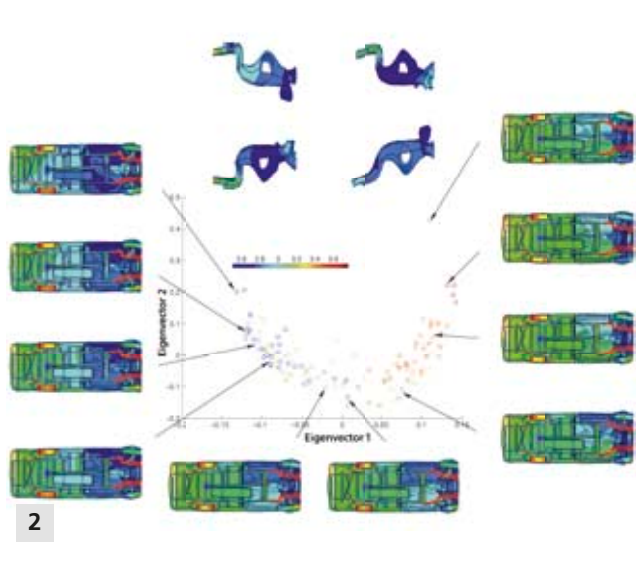


2

DATA MINING TECHNIQUES FOR CAR SIMULATION RESULTS

The demand for improved product creation has led to an exponential growth in the number of large-scale finite element simulations being performed. Data mining techniques that extract the essential variations between designs and simulation results provide a new approach for analyzing product variants stored in huge simulation repositories.

More product variants, the increase in government regulations and the use of stochastic and multidisciplinary optimization cause a drastic increase of the number of numerical simulations performed in the car design process. The availability of this data creates the opportunity to compare thousands of simulation variants, to find optimal design variants (even from previous projects) and to evaluate their impact on the functionality of the car. The huge volume of data (large number of simulations and large data-sizes per simulation) and the diverse content of simulation data are major obstacles that can be overcome by data mining methods based on dimension reduction.

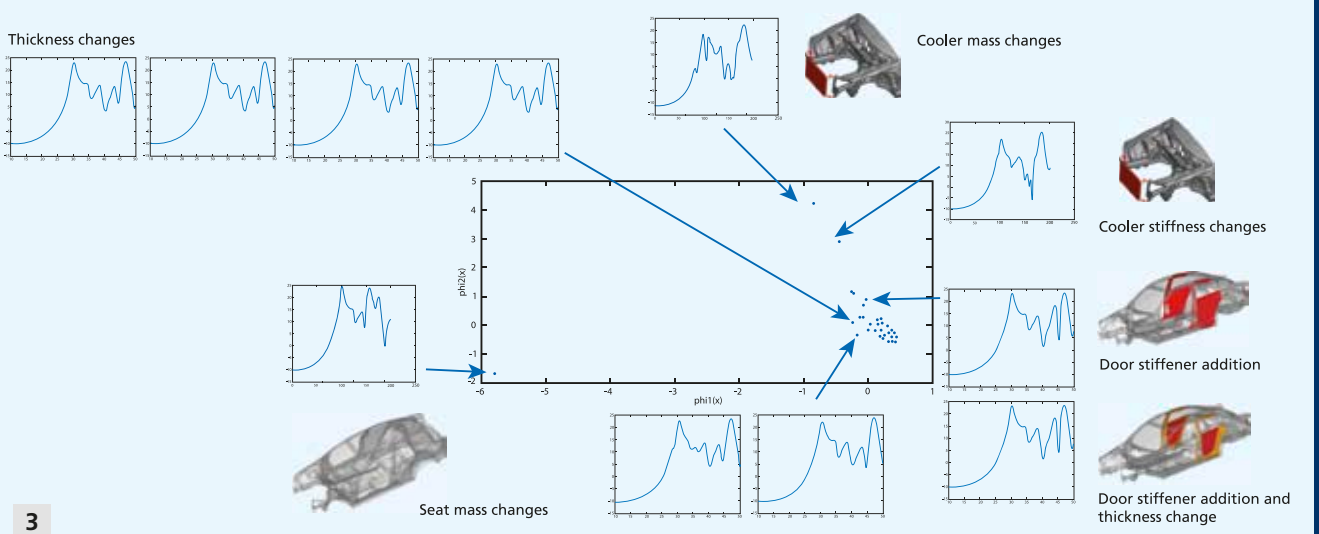
Aspects of the car design process in automotive industry

Our activities in data mining of simulation results focus on two aspects of the virtual product development process:

- In order to find an optimal design while taking specific constraints into account (like safety regulations), many model variants are analyzed in which small modifications in material parameters and geometries are introduced. This is an iterative and time consuming process. Post-processing software tools are able to display the model geometry and the results of the numerical simulation in an intuitive way, but engineering judgment is limited to the analysis of just a few (perhaps at most five) simulations at once.
- The other aspect of the car design process involves the reuse of information from previous projects or development phases. Geometrical shapes and geometrically distributed properties like stresses or deformations, defined on very fine meshes, are the essential information to evaluate. Unfortunately, this information is not accessible for direct database queries because of its size and its missing common structure.

In both application cases, nonlinear dimension reduction methods are used that exploit the high correlation arising from the basic similarities in the models and problems to be solved. The major trends of the differences, which are hidden in the detailed results, are computed and simple parameters provide information about the contribution of each of these trends to the individual geometries or simulation results. A simple illustration of this idea can be given by considering several pictures of a car that has been rotated around one axis (see Figure 1). After application of a nonlinear dimension reduction to adjust the images consisting of pixel values via the so-called Multidimensional Scaling (MDS) method, we are able to extract dependency on the rotation angle and represent all images in a parametric way.

Each circle in the MDS plot (see Figure 1 and its explanation) represents a snapshot of the car and the major parameter resulting from the mathematical analysis turns out to be just the rotation angle.



3 **Analysis with models from the EC-funded project SIMDAT**

Applying nonlinear dimension reduction methods

Figure 2 shows the application of these methods to vehicle crash simulation. The deformations of a set of parts at the front of a car are extracted from 132 simulations and nonlinear reduction methods are applied to these data sets. Here, each point corresponds to one of these 132 simulation results. Its position in the graph is given by the contribution of the two major deformation modes to the simulation result for this point. The formation of the points is almost a one-dimensional curve, indicating that the results are determined by one major deformation mode. By comparing two extreme results, it can be seen that the behavior of the deformation mode is determined by lower longitudinal rail. The color of each point indicates the thickness of the frontal part of the longitudinal rail and it is obvious that the major mode is highly correlated with this thickness. The example shows that the essence of 132 simulation results can be derived by analyzing the MDS plot and visualizing a very small subset of carefully selected simulation results.

The main objective of Noise, Vibration and Harshness (NVH) simulations of a car is the comfort of the passengers when exposed to car vibrations. Figure 3 shows examples of 32 possible changes (red colored parts) along with the 32 corresponding vibration response curves from such simulations. Our dimension reduction methods generate a MDS plot with a point for each variant that is based on the similarity of the vibration response curves. It shows groups of different curve shapes due to changes in 1) the seat masses, 2) the cooler properties, 3) the lateral structure (at the door) and 4) the part thickness. The MDS plot not only allows for the identification of these groups, it can also be seen that changes in the thickness do not influence the curve significantly (big cluster on the right). Having all 32 curves organized in this way allows the engineer to fast and easily evaluate his designs.

The described development was initiated by a Fraunhofer Challenge Project running from 2009 to 2010 and is continued within the project SIMDATA-NL – funded by the German Federal Ministry of Education and Research (BMBF) – until 2013. The project focuses on the application of efficient mathematical methods for dimension reduction of large data sets. In another project, named FEMMINER (funded by the BMBF from 2010 to 2012), SCAI and the company GNS mbH in Braunschweig implement these methods in GNS's post-processing software environment.

Our expectation is that the new analysis environment will substantially increase the productivity of engineers. Consequently, a faster way to car designs will be possible.

1 The rotation angle of the images is a parameter that can be identified by a reduction method applied to the images. We use a multidimensional scaling technique to assign a location in N-dimensional space to each data, such that neighboring data are more related to each other than distant ones. For sufficiently small N, the resulting locations may be displayed in a graph or 3D visualization.

2 Analysis of a set of crash simulation results using high-dimensional data reduction (testcase calculated using a truck model from the US National Crash Analysis Center).

3 Analysis of a set of NVH simulation results using high-dimensional data reduction (testcase provided by AUDI AG as part of the SIMDAT EU project).

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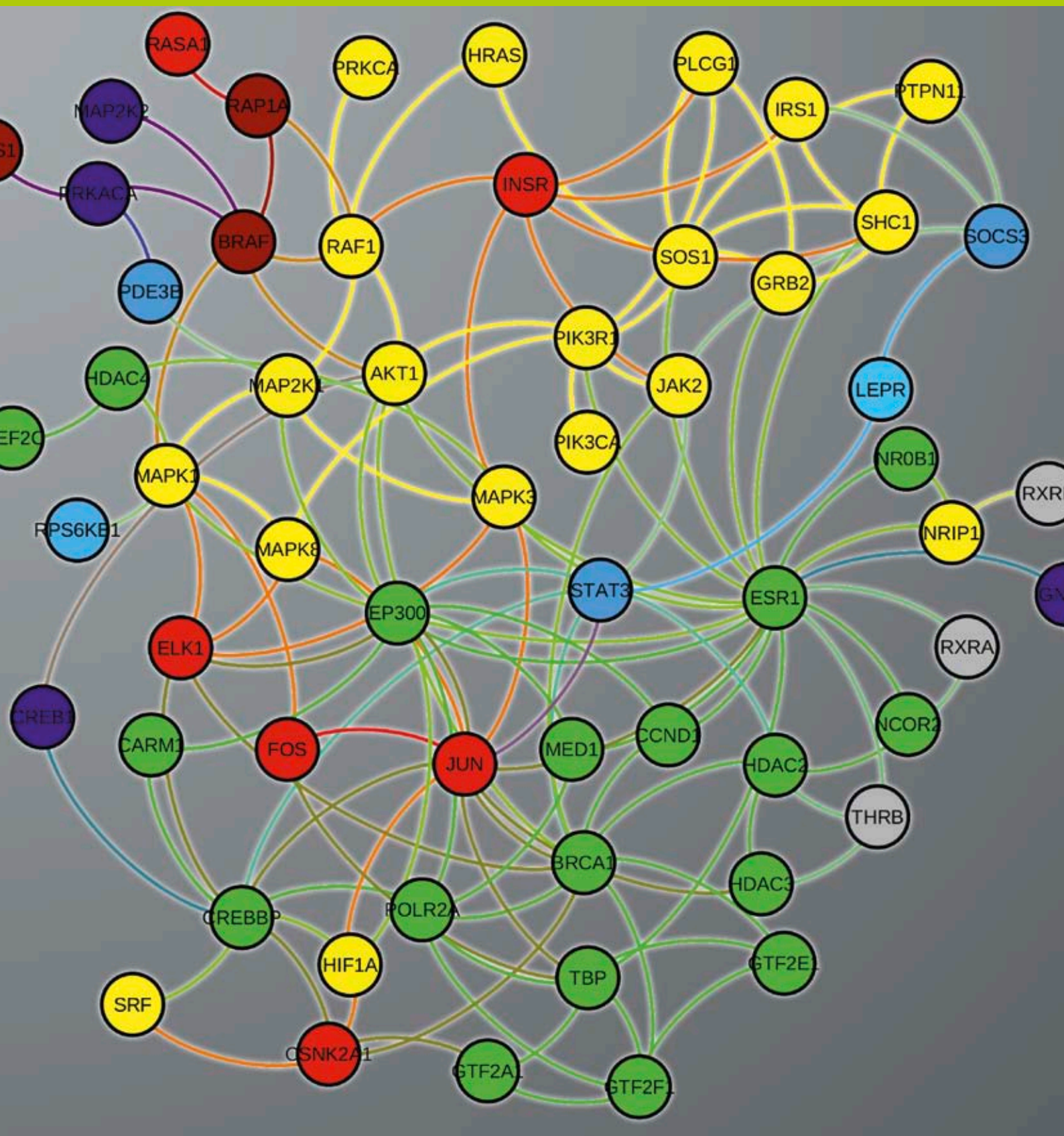
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BRCA1
HDAC3
CREBBP
POLR2A
HIF1A
TBP
GTF2E1
SRF
CSNK2A1
GTF2A1
GTF2F1

BIOINFORMATICS

Technologies developed at the Department of Bioinformatics are in active use in the pharmaceutical and biotechnology industry, as well as in the publishing industry. A perfect blend of products on one side and professional services on the other side help our partners in the pharmaceutical industry to extract valuable information from unstructured information sources. With strong links to both, the commercial and the academic research community, we thrive at maintaining a balance between academic scientific excellence and industrial innovation.

The Department of Bioinformatics is active in research and development in the following areas:

- information extraction from text and images
- disease modeling with a focus on neurodegenerative diseases
- distributed computing with a focus on license management in clouds and grids

The Bioinformatics team works closely with industrial partners – ranging from SMEs to global enterprises – to enhance their competitiveness through mediating knowledge and technology transfer from academic research to industrial application. Our academic affiliation with the Bonn-Aachen International Centre for Information Technology (B-IT) provides us with ample opportunity to do excellent academic research. On the Fraunhofer side, we work closer to application, addressing the real needs of our industrial partners. Our products solve information management problems prevalent in the pharmaceutical, biotechnology and publishing industry:

ProMiner is a software product for the detection of a broad spectrum of biomedical named entities in text, spanning from molecular entities (e.g. gene, protein, disease and drug names) to very complex knowledge representations (e.g. disease ontologies). In 2010 and 2011 we have demonstrated the capabilities of our technologies by reaching top ranking positions in a variety of international benchmarking competitions (TRECCHEM; TRECMED; I2B2 challenge).

The new literature-mining environment *SCAIView* is a simple, web-based engine that allows biologists and clinical researchers to use complicated text mining technology. The user-friendly interface efficiently shields the user from the complexity of the computer science behind this environment.

chemoCR is a software tool that automatically reconstructs chemical information from chemical structure depictions. Although communicating chemical information via images is quite common among chemists, so far computers are unable to read information present in chemical structure depictions. *chemoCR* addresses this problem by reconstructing chemical information from images that contain chemical structure drawings.

Some of our unstructured information mining tools have been successfully used to support our disease modeling activities, which began in 2010. The productive use of information extraction technologies could be demonstrated 'in house' in research activities aimed at modeling neurodegenerative diseases – one of the most challenging areas in modern systems biology.

Finally, a brand-new approach to distributed license management began in 2008 and has been further developed with *elasticLM*. It addresses specific challenges that arise with the distributed use of commercial license software. *elasticLM* will be commercialized in 2012 and will contribute significantly to the overall innovation and revenue of the Department of Bioinformatics.

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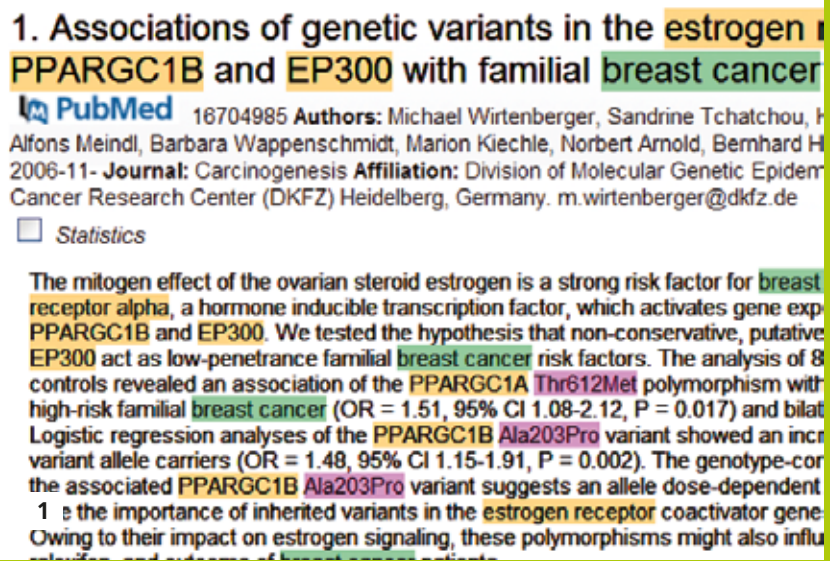
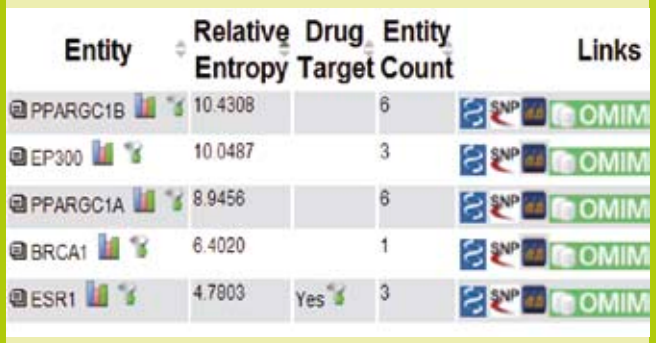
LEFT *A hormonal network underlying dementia and Alzheimer's disease.*





KNOWLEDGE DISCOVERY IN SCIENTIFIC LITERATURE

The software tools *ProMiner* and *SCAIView* provide an advanced solution for knowledge discovery in the biomedical domain. Unstructured text resources, like publications and web-content, are textured and purified for efficient retrieval and visualization of their information content. They are designed to enable biomedical researchers to explore huge amounts of data in a fast, accurate, and user-friendly way.

ProMiner is a highly scalable system for named entity recognition based on large-scale dictionaries, complex thesauri, and even ontologies. *ProMiner* addresses several fundamental issues in named entity recognition within life sciences:

- recognition of biomedical entities and their spelling variants in texts
- mapping of synonyms to reference names and data sources
- context-dependent disambiguation of biomedical termini and resolution of acronyms
- fast and accurate annotations, even on large-scale corpora

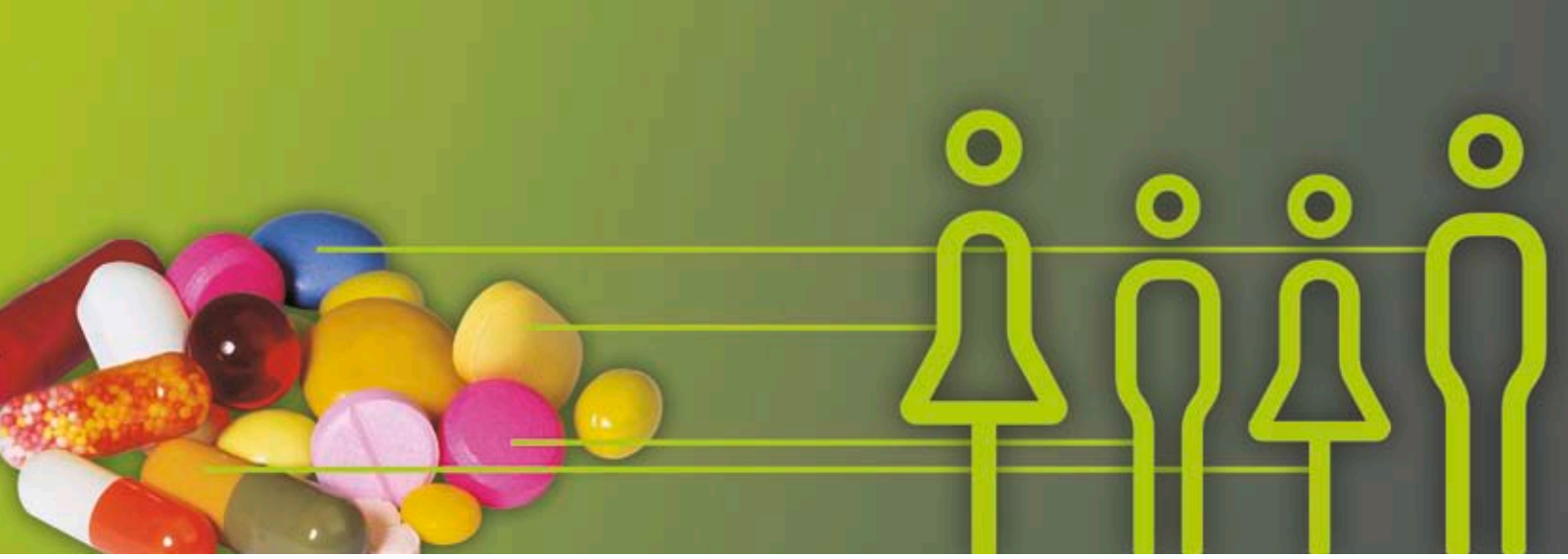
The information retrieval system *SCAIView* allows for semantic searches in large text collections by combining free text searches with the ontological representations of entities derived by *ProMiner*. *SCAIView* gives answers to questions such as "Which genes/proteins are related to a certain disease, pathway or epigenetics?" *SCAIView*'s key features are:

- a user-friendly search environment with a query builder supporting semantic queries with biomedical entities
- fast and accurate search and retrievals, based on the newest technologies of semantic search engines
- visualization and ranking of the most relevant entities and documents
- exportation of the search results in various file formats

Documents are retrieved by precisely formulated questions using ontological representations of biomedical entities. The entities are embedded in searchable hierarchies and span from genes, proteins, accompanied single-nucleotide polymorphisms to chemical compounds and medical terminologies. *SCAIView* supports the selection of suitable entities by an auto completion functionality and a knowledge base for each entity. This includes a description of the entity, structural information, pathways and links to relevant biomedical databases like EntrezGene, dbSNP, KEGG, GO, and DrugBank. *SCAIView* represents the search results by color-coding of the different entity-classes, statistical search results, and various ranking functions.

1 *The highlighted text corresponds to entity classes.*

2 *Found entities can be indexed, ranked, and linked to other data.*



TEXT MINING TECHNIQUES FOR PERSONALIZED MEDICINE

Fraunhofer SCAI develops semantic search strategies for the selection of potential biomarkers for personalized medicine. SCAI deploys information extraction methods to detect adverse effects or failures of medicinal products in scientific literature and electronic health records.

Personalized medicine helps to define patient groups with high drug efficacy and low rates of adverse effects. This is why scientist are looking for biomarkers – for example in the human blood – that indicate the presence or absence of diseases. Biomarkers support the evaluation of efficient drugs, the identification of patient groups or of disease stages.

Before a new drug is approved and marketed, pharmaceutical companies have to identify possible unknown side effects. Apart from published case reports and spontaneous reporting systems, the mining of electronic patient reports helps to detect potential risks of medicinal products much faster. However, mining electronic health records is challenging because of the enormous amount of data and the requirements for data protection.

Examples for current projects include:

- **mining for biomarker information in biomedical literature**
  In a project with industry, Fraunhofer SCAI explored how information about potential biomarkers is expressed in literature and which textual features in addition to disease and gene expressions are relevant for the retrieval of potential biomarker information. A specialized, selective biomarker retrieval terminology has been integrated into *SCAIView*, allowing for the enrichment of biomarker information in a flexible way.
- **automatic identification of drug-related adverse effects in medical case reports**
  In cooperation with a partner from the pharmaceutical industry, we developed a machine learning application for the automatic identification of drug-related adverse effects in medical case reports. The established framework can be used to identify drug safety signals and to establish alert systems to support pharmacovigilance.
- **improving patient care through semantic annotation and mining of health records**
  Electronic health records present challenges for the development of text mining techniques and for data protection. Build on SCAI's *ProMiner* software we developed techniques for named entity recognition that were successfully evaluated by the US initiative "Informatics for Integrating Biology and the Bedside" (I2B2).

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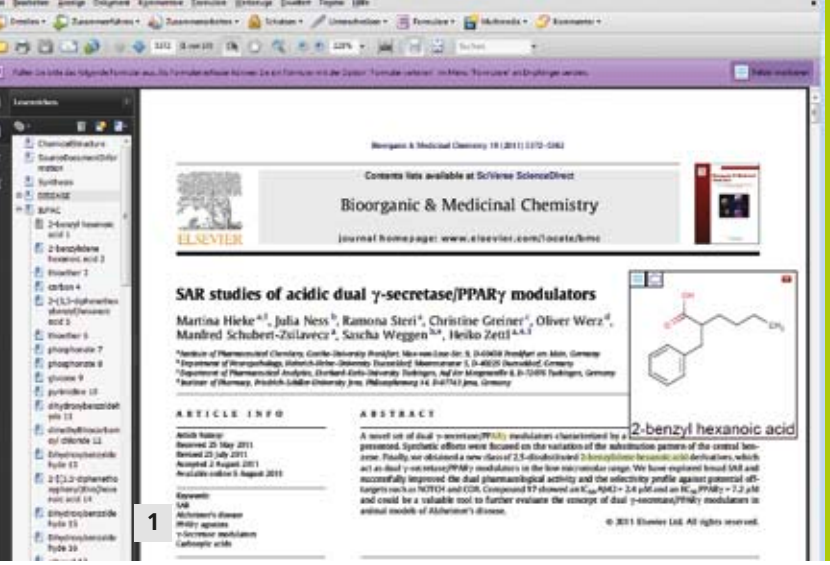

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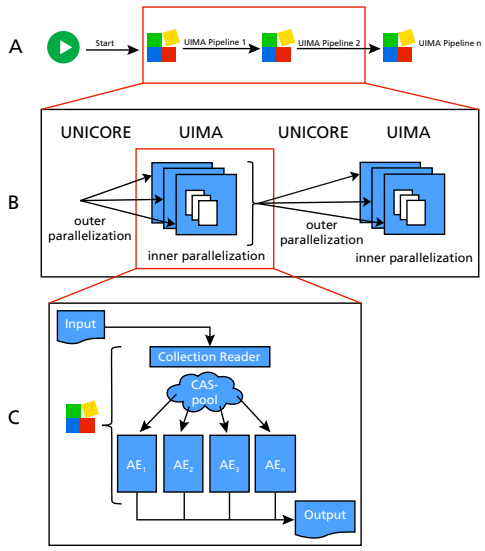

2

EXTRACTING CHEMICAL PATENTS USING HPC

Finding information about annotated chemical reactions for drugs and small compounds is a crucial step for pharmaceutical industries. This data is often presented in the form of unstructured documents (especially patents), and manual extraction of this information is a time- and cost-inefficient effort.

Up to now, the European Patent Office (EPO) hosts about half a million chemical patents containing multi-modal information (image and text) in different languages. Goals of the Unstructured Information Management Architecture (UIMA) project are:

- making patents searchable in terms of structure and full-text search
- providing an 'on demand' service that can scan and prepare thousands of documents in hours, by exploiting available resources in the grid

Because of the enormous amount of data, this can only be realized by using techniques of High Performance Computing (HPC). The UIMA-HPC project aims at a solution for the automated analysis of multi-modal pharmaco-chemical document databases, taking the following patent-search use case as an initial solution design driver:

- pharmaceutical research in legal context (claim extraction)
- pharmaceutical research in scientific context (knowledge extraction)
- chemistry extraction (for example adding jump marks to synthesis description)

The combination of text and structure analysis is an innovative approach. It will be based on an well-tested data analysis architecture. It specifies component interfaces, design patterns and development roles for describing, composing and deploying multi-modal analysis capabilities.

The UIMA-HPC approach centers on workflows for the automated annotation of a document corpus. Each workflow comprises different analysis components within the UIMA. The individual "annotation engines", such as the text mining of a document or the analysis of diagrams within a document based on Optical Character Recognition (OCR), are very complex and computationally demanding. Thus, parallelization at the level of the heterogeneous "node" of a HPC system is highly appropriate – meaning parallelization for deployment on multicore processors and/or on multiple graphics processing units. The HPC system needs sophisticated load balancing algorithms due to the fact that a large quantity of diverse computationally complex documents is used as input. The efficient distribution of independent annotation engines on the compute nodes is realized within an adaptation of the Unicore software system.

1 *Result of the work-flow: UIMA-HPC presents chemical semantic enriched PDF documents providing a molecule index, molecule depictions, and chemical summary.*

2 *Technical solution: The workflow engine of UNICORE starts and manages an extraction workflow for thousands of PDFs. Each workflow consists of small specialized UIMA pipelines. Each pipeline extracts a special type of information (e.g. chemical names in text, chemical depictions, tables).*

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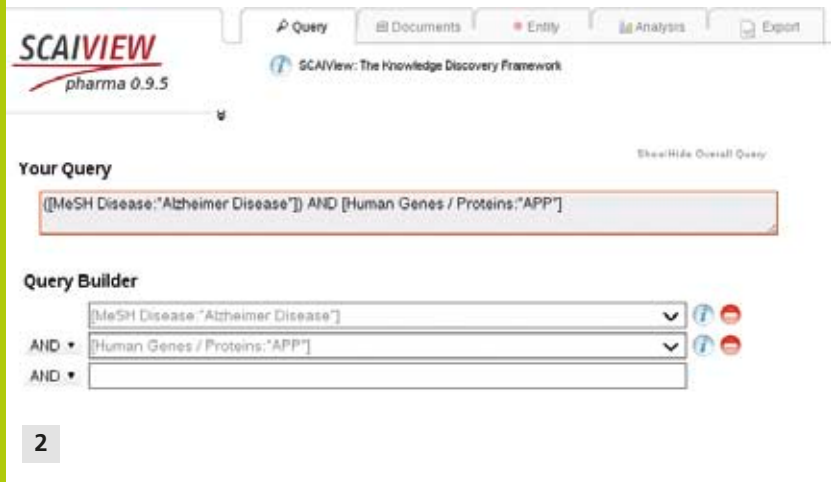

2

NEW WAYS TO COMBAT NEURODEGENERATIVE DISEASES

To provide fresh impetus to Germany's biopharmaceutical research sector, the German Federal Ministry for Education and Research (BMBF) launched a pharmaceutical research initiative entitled "BioPharma: For the Medicine of Tomorrow". Neuroallianz emerged as one of the winning consortia of the tendering process.

The Neuroallianz Consortium has adopted an innovative, strategic partnership model to facilitate collaborative research between both academic institutions and pharmaceutical companies. The goal is to improve diagnosis and therapeutic intervention in neurodegenerative diseases. In 2009 the work began with a focus on epilepsy, Alzheimer's and Parkinson's disease as the core targets.

The consortium is subdivided into several therapeutic, diagnostic and infrastructure projects. As a strategic partner in the Central IT Platform (CIP) infrastructure project, SCAI has developed a joint information technology platform to support collaborative research between the partner organizations. This platform addresses a broad spectrum of functionalities including:

- secure management and exchange of documents and data
- IT support for cross-project collaborative work
- provision of data mining functionality (including "data mining workflows")

The CIP consists of modules that encapsulate specific functionality, e.g. a single-sign-on mechanism and provide failure-free and safe operation of the entire system. The groupware Basic Support for Cooperative Work (BSCW) was adapted to support the collaboration of the project partners and to integrate all components of the system. Specific data mining modules are offered in the form of pre-configured, automatically executed workflows. A module for text mining is based on the semantic search engine *SCAIView*.

Project partners can access a shared workspace containing all functionalities and modules via a web interface. The development of the system has been performed in close cooperation with experts in UCB Pharma. The IT infrastructure meets the safety requirements of the industrial project partners. An additional goal is to develop "in-silico" methods for the identification and validation of new target proteins involved in the mechanism of neurodegenerative diseases.

The provision of this infrastructure to the Neuroallianz consortium will be extended over the lifetime of all projects. Moreover, SCAI and UCB Pharma have initiated another Neuroallianz project for the prediction and discovery of novel biomarkers for neurodegenerative diseases.

1 *Facing the challenge of an ageing population.*
2 *Querying for Alzheimer's disease and the protein "APP" with SCAIView´s pharma search interface.*

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POLICY-MAKING IN POPULAR ONLINE COMMUNITIES

In governmental models, public opinion is often obtained with traditional methods like telephone or street surveys. The dynamicity in society can only be captured with tremendous effort. The EC-funded project +Spaces (dubbed "Positive Spaces") aims at the use of popular online communities in which people literally live: platforms like Facebook, Twitter, Blogger, or Open Wonderland.

Social Networking platforms can be considered as virtual spaces real people literally live in. The focus of +Spaces is to move towards engaging such citizens in virtual spaces ("virtual citizens") in the policy making process. Information and communication technology is allowing for the investigation of governmental proposals and decisions at large scale and for measuring public opinion. The project participants are developing tools to exploit virtual spaces for assessing public thoughts. The outcome is a flexible service-oriented platform with tools adapting to different spaces and analyzing the outcome with different analytical approaches. The main goal is to support policy makers in their decision making process.

Simulating and testing people's opinions and behavior in these virtual spaces is conducted in so-called experiments. A policy maker develops a novel idea and can deploy a poll, a debate, or a role-play simulation to get feedback from the public. A poll supports structured questions, a debate allows for gaining more insight into the ideas and opinions of the population, and a role-play is a structured way of investigating different possible outcomes of a potential policy.

Such experiments can generate a lot of complex data, and the decision making process needs to be supported by intelligent data analysis services. The text mining group of Fraunhofer SCAI develops such a service that provides statistical analysis including automatic topic and sentiment detection, plus visualization of the results. Therefore, the policy maker can concentrate on specific important aspects without being overwhelmed by the sheer amount of unstructured data.

+Spaces is funded by the European Commission. The consortium consists of IBM Haifa (Israel) as the coordinator, the Institute of Communication and Computer Systems at the National Technical University Athens (Greece) as technical manager, the University of Essex (United Kingdom), AtoS (Spain), K. U. Leuven (Belgium), Athens Technology Center (Greece), the Hellenic Parliament (Greece) and Fraunhofer SCAI.

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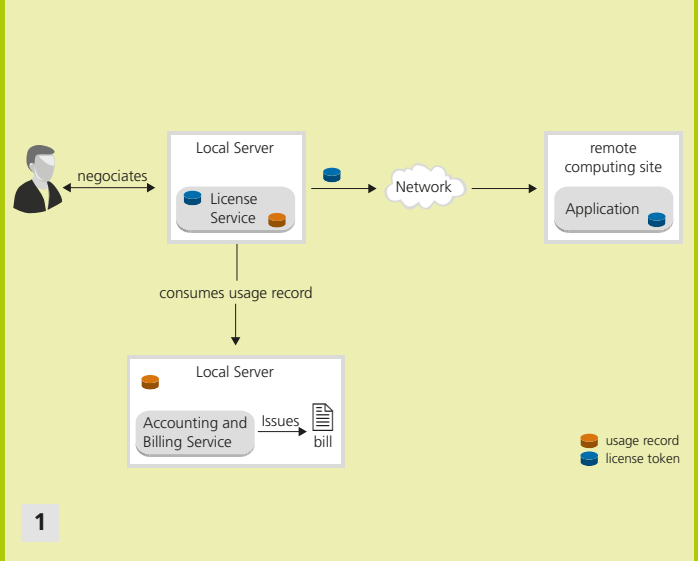

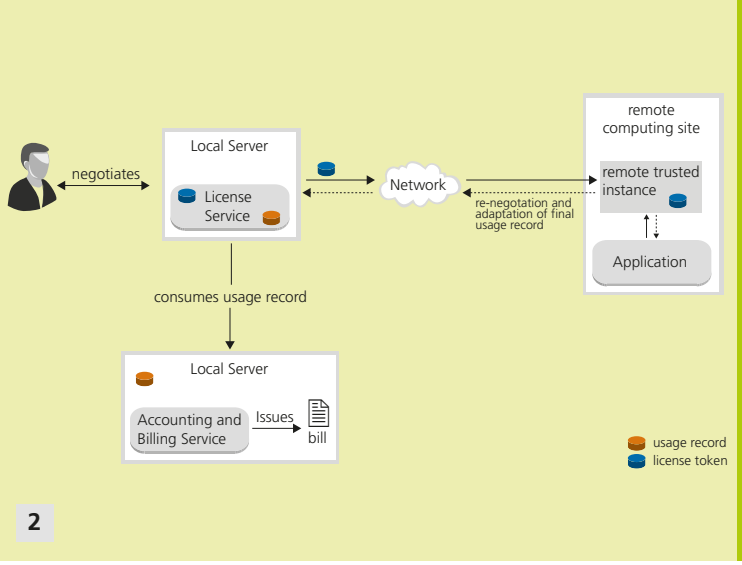

SOFTWARE LICENSING FOR TODAY'S IT INFRASTRUCTURES

In recent years, grid and cloud computing have provided the foundation for the migration from monolithic computation centers to more flexible structures that dynamically integrate external resources. This raises a number of issues regarding new business models and licensing technologies for the independent software vendor.

As a consequence, independent software vendors are challenged by both customers requirements and the evolving technology:

- The way software is used has changed over the years, customers want more flexibility and the acceptance for present business models is decreasing.
- Virtualization of computing resources threatens the current licensing technology. The binding of licenses to properties of the utilized hardware (e.g. CPU identification) gets weak since these properties can be easily defined as part of a virtual environment. As with hardware dongles, floating site licenses are not suitable when resources beyond the customer's administrative domain will be used.

The producers of commercial software must switch to a better license technology that protects their software products. *elasticLM* is Fraunhofer SCAI's response to the challenges of the paradigm change in the provisioning of IT services.

elasticLM is an innovative tool for the generation and management of software licenses for distributed computing infrastructures like grids or clouds, but keeps all its advantages for applications being executed on local resources like workstations or clusters. The built-in policy engine enables a variety of license and business models, including pay-per-use. As a result, *elasticLM* equally protects applications that benefit from using external resources dynamically added to those of the license owner for times of peak demand. For the customer, the use of license-protected applications on external resources is as easy as local use while the level of protection for the Independent Software Vendor (ISV) remains the same.

Besides increased flexibility, customers of ISVs benefit from *elasticLM*'s support for the monitoring of application usage and the creation and recording of software usage records. The records are needed to analyze the software usage as well as for accounting and billing. This functionality is available both for license-protected applications and arbitrary other applications.

1 *Basic Scenario: No bi-directional network available.*

2 *Advanced Scenario: Bi-directional network available.*

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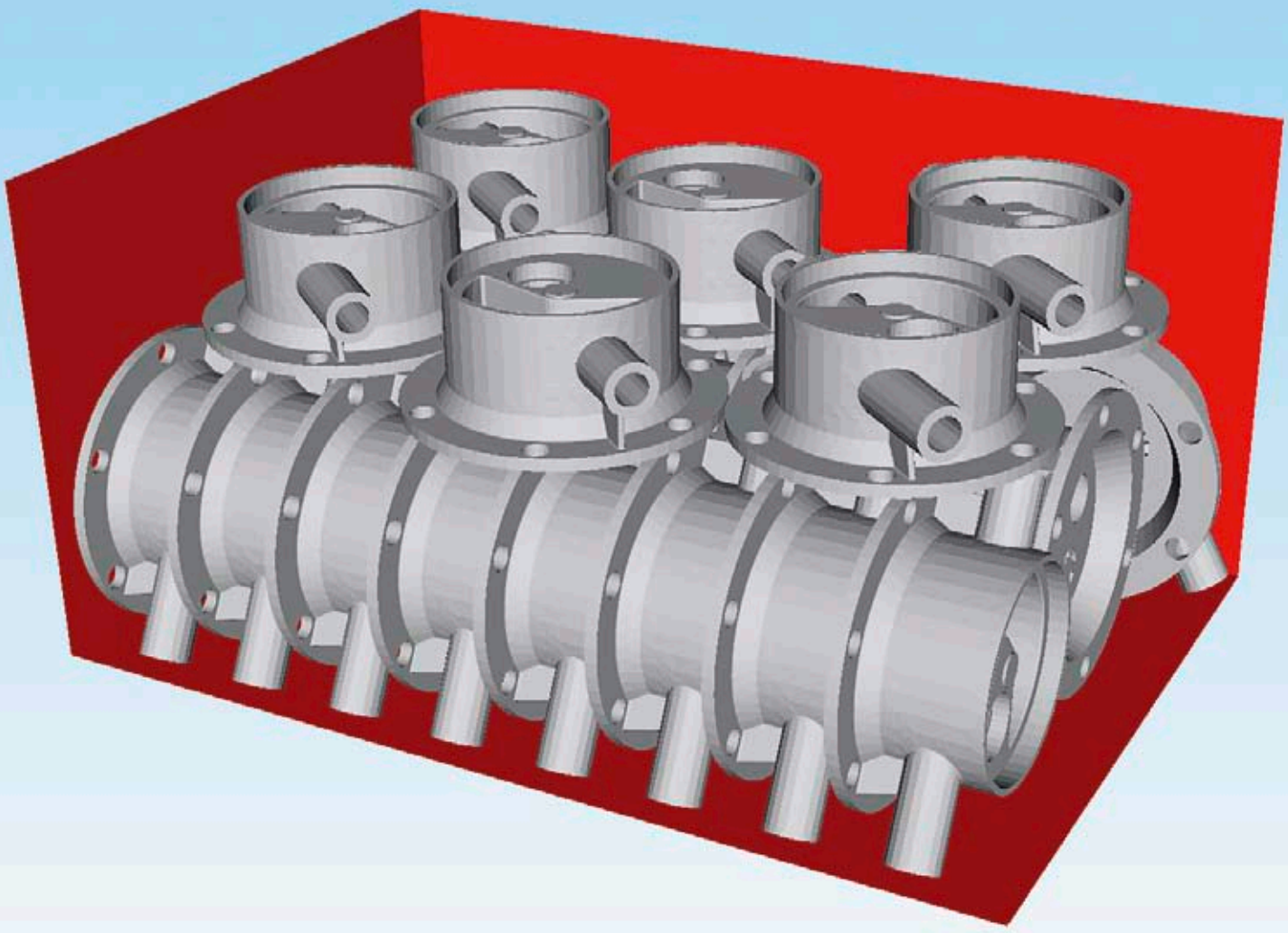

OPTIMIZATION IN LOGISTICS, PRODUCTION AND PLANNING

How can a production line run at its optimal capacity without delaying delivery due to long set-ups? How can storage be optimized so that all components are made available for the production process while at the same time overstocking and delays are avoided? These are questions asked daily in the manufacturing industry. The answers can be provided by the specialists in the Department of Optimization.

In many branches of industry, commerce, and transport, computer-based optimization algorithms can achieve amazing savings in money, resources, and time by addressing:

- **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

Our optimization solutions contribute to climate and environmental protection, which earned us the *Innovationspreis für Klima und Umwelt* (IKU) for our cutting and packing solutions. The space-saving packing of goods reduces freight transport volume, thereby minimizing fuel consumption and pollutant emission. Each tour that can be avoided also decreases noise exposure. By developing optimal nesting patterns, material can be exploited best possible and waste is reduced. Saving material also minimizes the consumption of resources and energy in production and handling processes. This is especially important in the field of energy-consuming manufacturing of metals and composites.

The Department of Optimization acts as a consultant for trading and industrial companies. SCAI has always a sympathetic ear for any kind of problem that seems to be solvable by optimization methods. Among the services SCAI offers to companies are the following:

- **consulting/problem analysis:** evaluation of the solution complexity for a given customer problem
- **specification:** development of mathematical and methodological descriptions for specific problems
- **development of custom-cut solutions:** creation of an optimization software with precise consideration of the problem-specific fundamental and ancillary conditions
- **development and licensing of standard products:** marketing of optimization products – alone or together with partners
- **maintenance:** training and support to guarantee the best possible life cycles of the solutions
- **further development and customization:** long-term support and modification of standard products to individual needs

SCAI has about 20 years of experience in optimization and a large "tool box" of optimization methods at its disposal, which can be utilized when constructing solutions for new problems.

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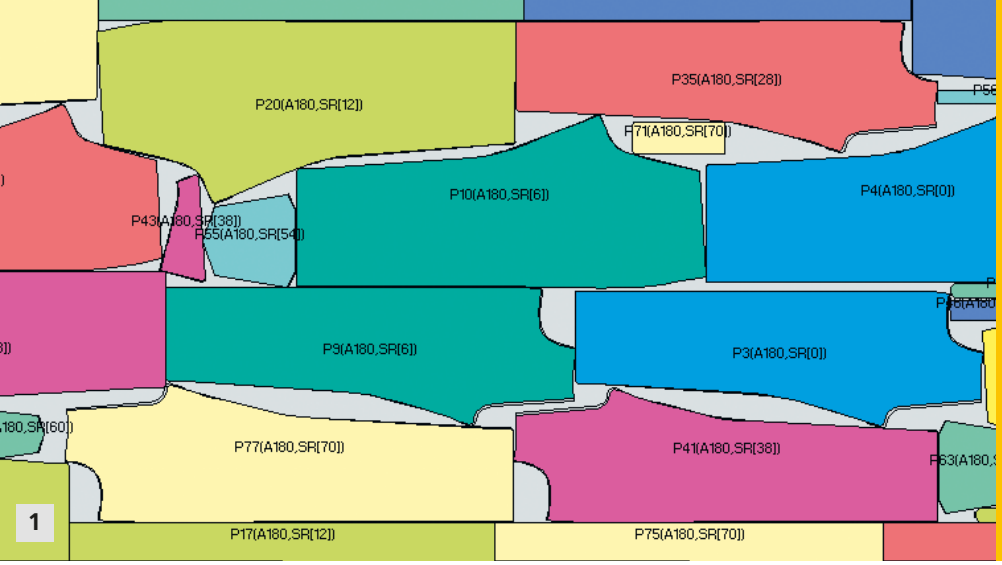
LEFT *SCAI's software PackAssistant optimizes packing configurations of identical parts into containers.*



OPTIMIZING MATERIAL USAGE IN CUTTING PROCESSES

Materials often need to be cut into smaller pieces before manufacturing and assembling to the final product. Raw materials, production, transportation, and storage are becoming increasingly expensive. Companies strive to optimize their logistics and production process to make it more efficient, cheaper, or environmentally friendly. Since material in many business areas is one of the heaviest cost factors, optimal usage of material is the key to remaining competitive. Better material utilization has a direct effect on production cost by using less material, saving resources, and reducing energy consumption in production and logistics.

Fraunhofer SCAI has developed sophisticated optimization algorithms for solving cutting and arrangement problems on two-dimensional materials. The software *AutoNester* can create cutting patterns for a wide variety of materials, including fabric, leather hides, metal and wood plates, or composite materials.

Depending on the application area, several – and often fundamentally different – constraints for generating such cutting patterns have to be considered. *AutoNester* covers the most current constraints needed for practical production purposes. These include more than sixty different settings and options for piece positioning, consideration of cost, material, or production properties.

The underlying algorithms run in a very short time, and meet modern production requirements. The results achieved by our algorithms are often better than the results achieved by humans or other software packages. Material savings of up to 30 percent have been reported by end users. *AutoNester* algorithms are available as an optimization library that is integrated by partners into their software and sold to end users around the world. The software is already in daily production use by several thousand companies.

SCAI's software and algorithms are under continuous development to support more materials and constraints. The institute also produces individual solutions for any kind of cutting problem upon customer demand.

1 *Garment: Cutting pattern for pieces of a garment. Material utilization: 90%. Computing time: 3 minutes.*
2 *Leather: Cutting pattern for a leather hide. Material utilization: 86 % Computing time: 3 minutes.*

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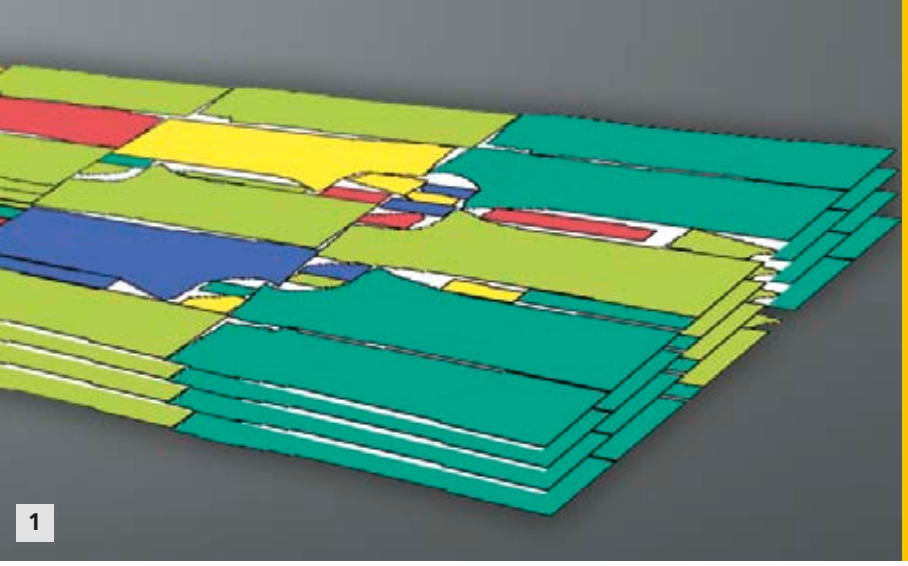

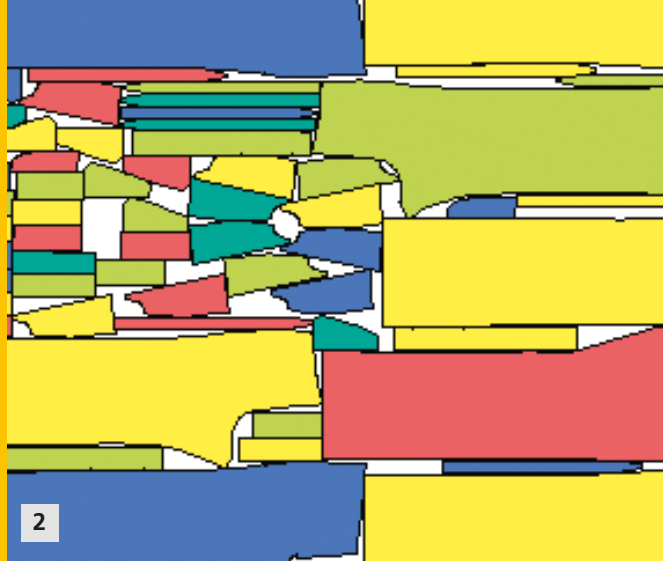

AUTOMATIC CUT PLANNING FOR GARMENT PRODUCTION

CutPlanner extends *AutoNester* by cut order planning. It makes and optimizes cut order plans for an entire customer order. The complexity of this order can include material in several different sizes and different colors. *CutPlanner's* solutions are based on real markers computed by *AutoNester*.

CutPlanner works with the polygonal piece data defined in a CAD system. The textile engineer inputs the data of the available fabric and the desired cut for sizes and shapes. Based on this data, *CutPlanner* calculates a cut order plan – an optimized compilation of more than one set of clothing pieces with different sizes on a fabric panel. Subsequently, *CutPlanner* uses *AutoNester* to create patterns of cloth, so-called markers. It supports several optimization goals: it can minimize the production cost, maximize the yield, and minimize the number of markers used. No further manual intervention is required.

CutPlanner offers several advantages for textile planners:

- It allows them to specify the cost of the cutting process, the cost for spreading plies, or the material loss at the end of the cutting table. *CutPlanner* will take this into account in addition to the net material cost.
- It supports constraints, such as the cutting table maximum length, minimal and maximal ply numbers, or limitations to the available fabric.
- The software informs the user if a slight over- or underproduction would boost the solution's efficiency.
- If good markers or solutions are known, *CutPlanner* can use them to find excellent solutions more rapidly. Furthermore, if an estimated yield is sufficient for customer purposes, *CutPlanner* can deliver very fast approximate results.

The new version of *CutPlanner* is the result of heavy refactoring. It is more than twice as fast as the previous version and reliably solves most input settings.

1 *Cutting the same marker out of an entire ply of fabric saves a lot of time and effort. The colors show different sizes.*
2 *CutPlanner improves the material yield by nesting polygons from mixed bundles.*

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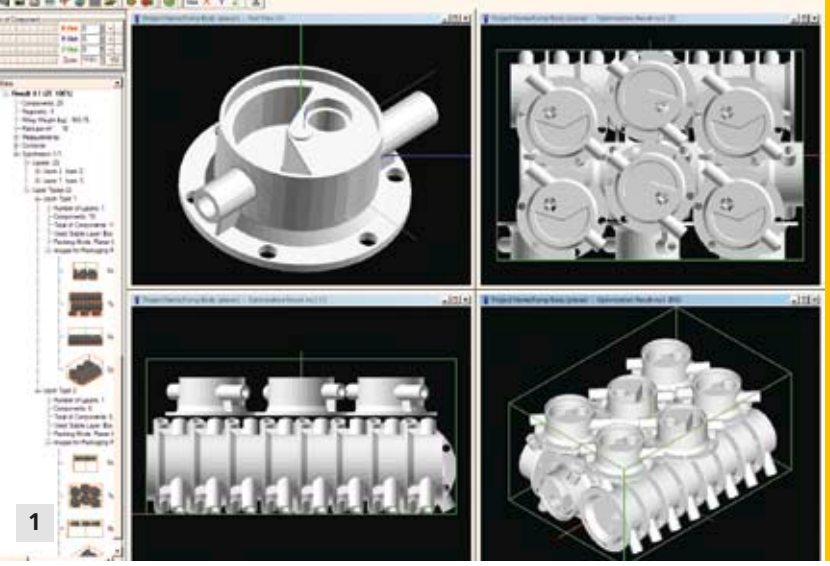

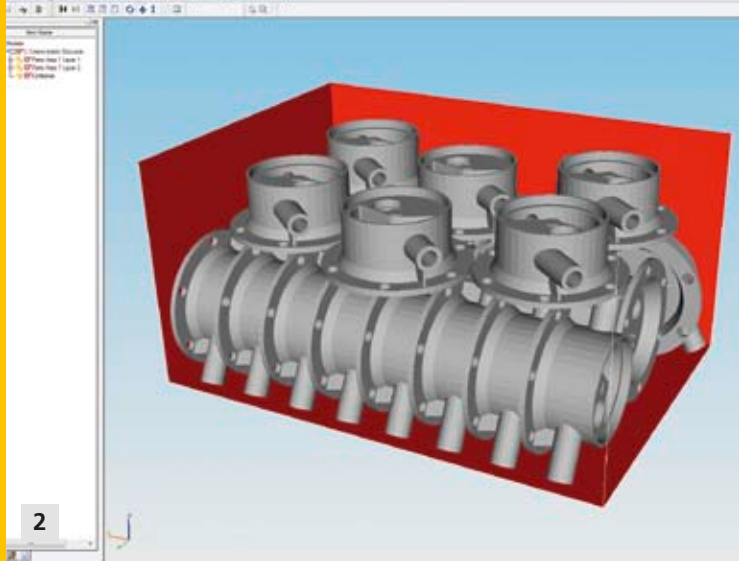

FAST AND EFFICIENT CONTAINER LOAD PLANNING

The development of packaging solutions for the safe and efficient transportation of parts of cars, machinery, or equipment from suppliers to the assembly line was previously an expensive, fiddly job. Now optimization algorithms from Fraunhofer SCAI can calculate the ideal filling of transport boxes with identical parts in a few minutes. The software *PackAssistant* is already in use by numerous manufacturers and suppliers worldwide, especially in the automotive industry. In practice, up to 25 percent more components can be accommodated within the transport boxes.

The software *PackAssistant*, developed by Fraunhofer SCAI, calculates optimized packaging solutions for the safe and space-saving storage of identical components in standard boxes (e.g. mesh stillages). Previous solutions in the packaging industry have been identified with time-consuming and costly packaging experiments. First, prototypes of the components or subassemblies were made. This was followed by numerous attempts with different boxes and different packing methods to determine how the components can be stored as space-efficiently and as well-protected as possible. In the experiments all possible variants also needed to be considered – from packing in layers, through stacked components, or layers with compartments, up to parts that fall off the assembly line directly into the box. Even for experienced designers of packaging solutions, it was hardly possible to find an economical solution within reasonable time.

1 *The user interface of PackAssistant.*
2 *Packaging solution exported into the CAD data format "JT".*

Accurate prediction of the filling of transportation boxes

Now – with *PackAssistant* – entirely virtual packaging tests are possible. The starting point for the calculation is the CAD data of the respective component in the formats JT, STEP, STL or VRML. In contrast to manual packing experiments the filling of transportation boxes can be predicted much more accurately.

The software achieves high packing densities, particularly in the arrangement of components with complex geometries. The unused space between the components is reduced to a minimum by an interlocking of the components. The software calculates the arrangement such that a simple insertion and removal of individual components is guaranteed. The spacing between the components or the compartments and the weight limitations of the boxes can be

3 *With PackAssistant, the production planners at KTM were able to complete an optimal container planning for all 450 parts of the X-Bow sports car.*

considered. Alternative packaging methods and boxes of various sizes can be compared easily with each other. The software can also automatically choose the box with minimum unused space from a list of available box sizes.

The result is shown as an interactive three-dimensional view. It can be exported to a Microsoft Word document as packaging manual. The result can also be exported into various CAD formats. So, for example, the compartment designs obtained can be processed further.

Less transportation costs and shorter planning times in industry

As a development partner for *PackAssistant*, Audi AG has already been working with the software for many years and uses the software's high-speed calculations to facilitate teamwork with its suppliers. The enormous savings – which can be realized through optimal packing of parts in large quantities – is seen in this real-world example of a rear light for an automobile:

Supplier's recommendation	*PackAssistant*'s calculation	Reduction in transportation costs
36	**45**	**57 T€**
parts per container	parts per container	savings per year

In setting up a production facility for series production of the X-Bow sports car, KTM Power Sports AG used the software *PackAssistant* to plan container sizes and packing of 450 parts. Since neither real components nor prototypes were available during the set-up phase, planning was carried out using CAD data for the components. Strategic planning for the containers revolved around the future logistics processes, material flows and the production cycles within the plant.

With *PackAssistant*, it was possible to shorten the times for planning and implementation of new containers by more than 50 percent in comparison to the nine to twelve months which is a standard for the industry. With Fraunhofer SCAI's software, KTM needed only four months. The software enabled a comparison of different packaging types and container models. This way, planners could generate a concept for each individual part before developing standard or special containers.

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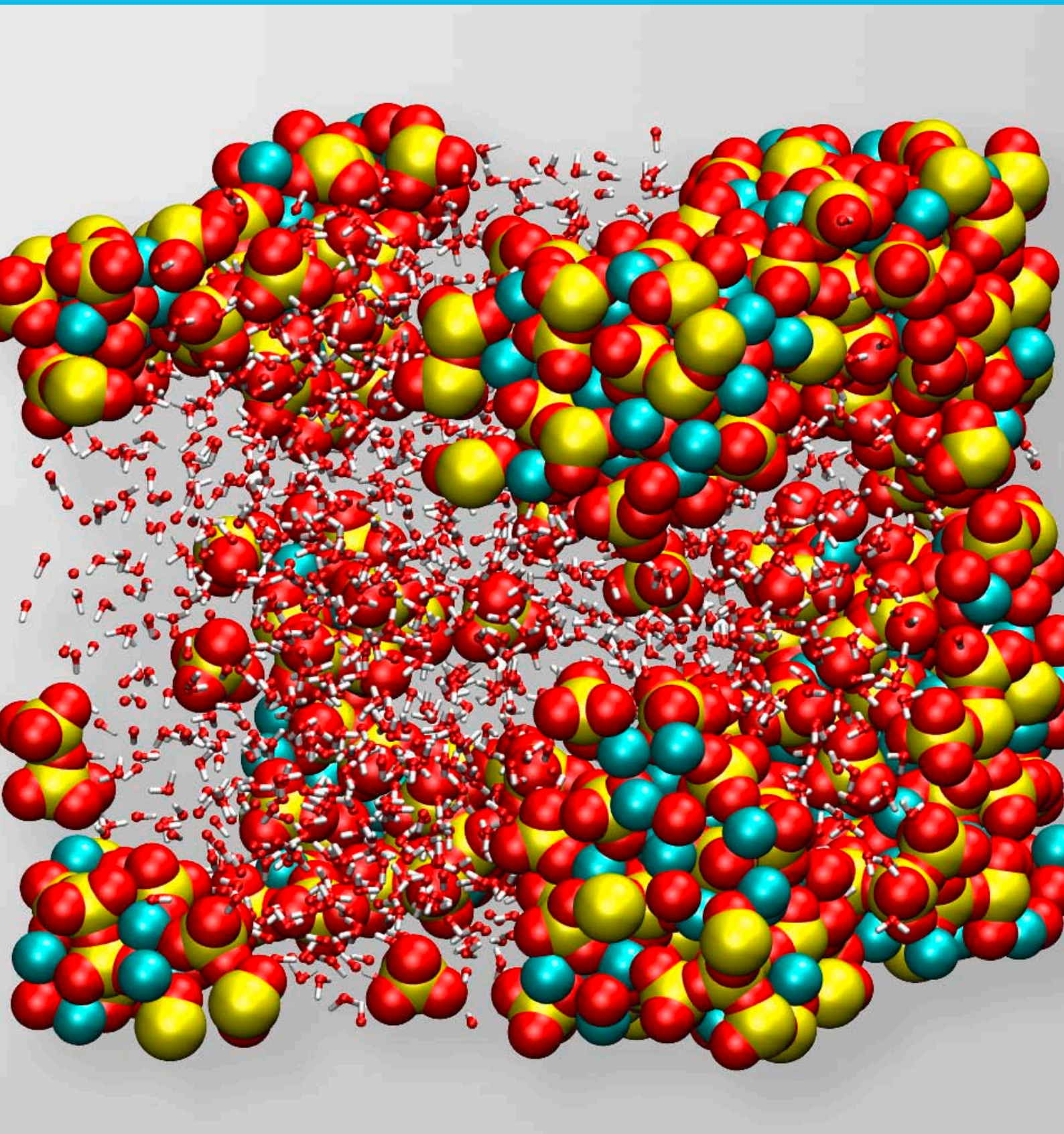

VIRTUAL MATERIAL DESIGN

Many challenges of the 21st century – such as the development of new and improved energy technologies, environmentally friendly technologies, and improved information and communication technologies for health and mobility – will rely on the availability of a new generation of materials. The design and creation of these new materials depends on interdisciplinary fields that incorporate fundamental natural sciences and application oriented engineering. Numerical simulation gives the opportunity to highly speed up the process of designing a new material.

Applied research and development within the Department of Virtual Material Design (VMD) is focused on multiscale modeling and numerical simulation in materials science and nanotechnology. Massively parallel computers are employed to simulate new materials at the nano-, micro- and macroscale using modern multiscale methods in quantum mechanics, molecular dynamics and continuum mechanics. The aim is to use the computational "virtual laboratory" to create and study new innovative materials with specific targeted properties. This way their structure and design can be proposed before they are synthesized in reality. This approach to material design promises to avoid many expensive prototypes and experiments in real world laboratories. Hence, the development costs can be substantially reduced in discovering new and completely novel materials.

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Nanostructured materials exhibit different material properties than their bulk counterparts since their high surface-to-volume ratio results in more surface exposure to nanoparticles and, thus, to more reactive materials. Many new materials are created solely by redesigning the surface structure of existing materials for enhancing properties such as impermeability, heat resistance or anti-bacterial characteristics. Nanoparticles and special nanostructures are also applied to design new innovative materials which, among others, include meta-materials and nano-composite materials.

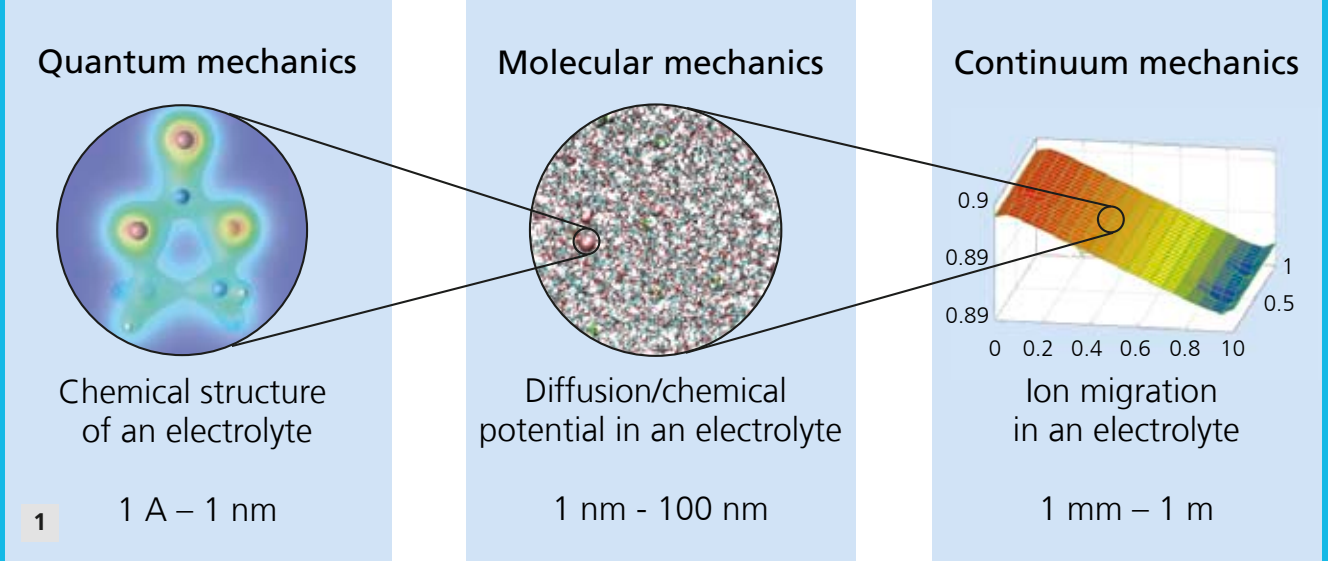
The resulting effective macroscopic properties are mostly a consequence of the detailed structure at the nano and micro scale. At the scale of molecules, atoms and electrons, all physical systems are in principle described by quantum mechanics. Thus, the underlying mathematical model is the Schrödinger equation. However, to simulate one second of behavior of one milliliter of material at the atomic scale, the calculation would take approximately 10^{20} years of computing time on today's largest supercomputers. Therefore, it is necessary to adopt a multiscale approach to model the physical behavior that occurs at different scales in space and time. Hence, mathematical models and numerical simulations must consider the respective scales at which behavior is influenced. In particular, the up-scaling of models has to be done carefully, since quantum effects and microscopic effects have consequences on the macroscopic level.

Fraunhofer SCAI offers individual solutions to our partners and customers in the following areas:

- multiscale modeling and numerical simulation for materials science and nanotechnology
- high performance computing in quantum mechanics, molecular dynamics and continuum mechanics

In particular this includes mathematical modeling, algorithm development, implementation of efficient parallel software packages for materials science and nanotechnology simulation, and customized software.

LEFT *Cementitious C-S-H gel at the nanoscale.*

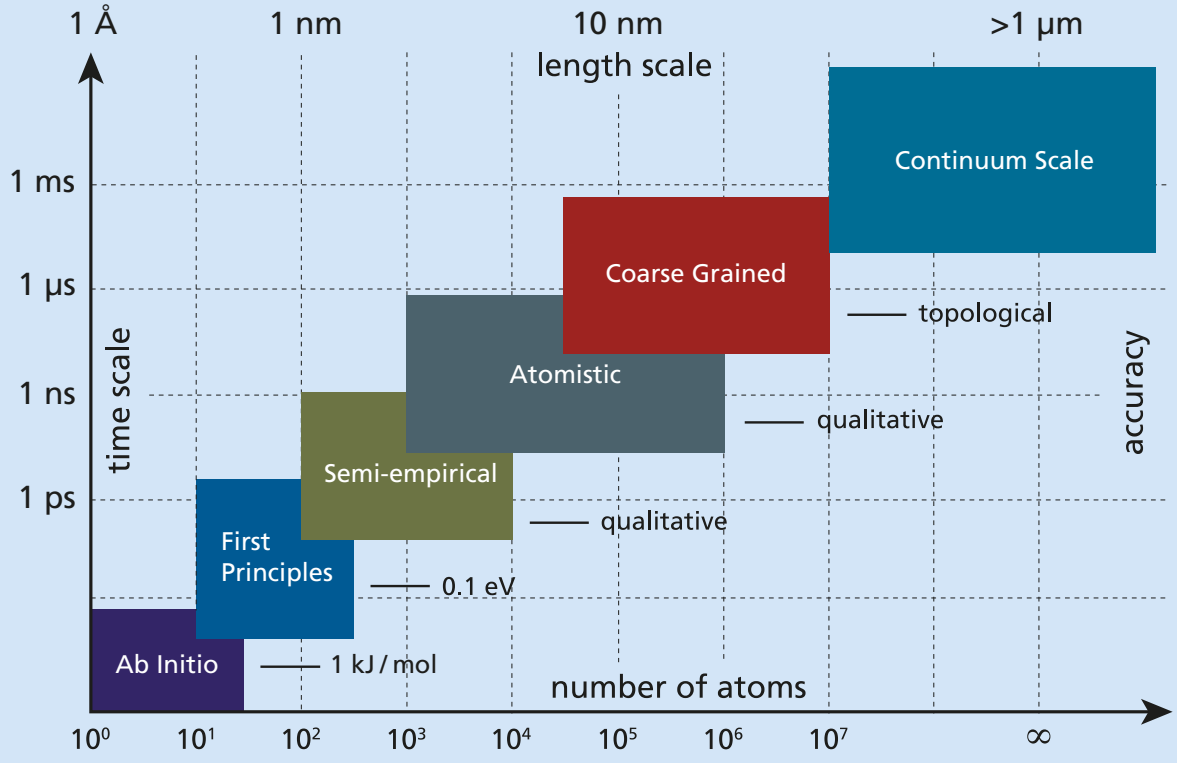


MULTISCALE MODELING

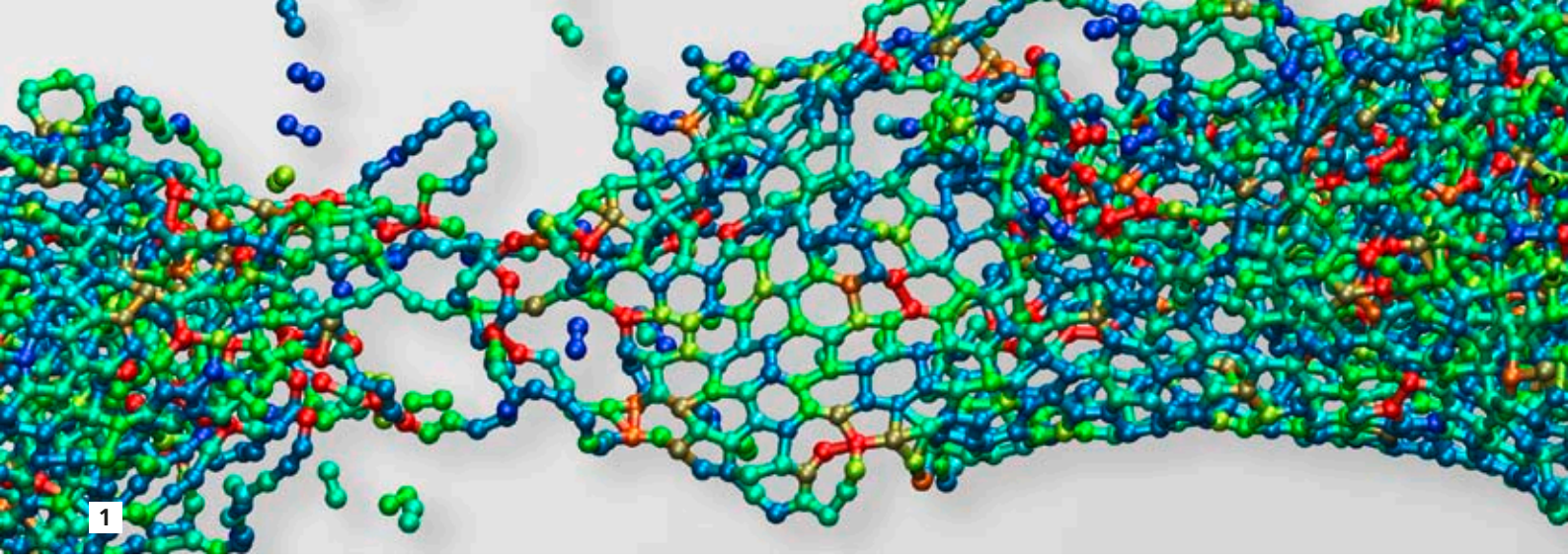
In a multiscale approach different mathematical models for different scales are typically coupled in a vertical or horizontal fashion. The goal of a horizontal coupling method is to locally balance required accuracy and costs (e.g. in QM/MM methods), whereas in the framework of a vertical coupling method, characteristic coefficients are extracted from a finer scale and upscaled towards a coarser scale. In the Department of VMD we follow and apply both approaches.

1 *Multiscale model of an electrolyte in Li-ion batteries.*

LEVELS OF MATHEMATICAL MODELS



- **Ab Initio Methods:** e.g. Quantum Monte Carlo, Coupled Cluster
- **First Principles Methods:** e.g. Density Functional Theory
- **Semi-empirical Methods:** e.g. Tight Binding
- **Atomistic Methods:** e.g. Force Field Molecular Dynamics
- **Coarse Grained Methods:** e.g. Coarse Grained Molecular Dynamics
- **Continuum Scale Methods:** e.g. Continuum Mechanics, Computational Fluid Dynamics



1 *Breaking of a multiwall Carbon Nanotube (CNT).*

SIMULATION OF MOLECULAR DYNAMICS

Tremolo-X is an efficient software package used for the numerical simulation of interactions between atoms and molecules. Since macroscopic material properties are based on the atomistic scale, it provides an environment to design new innovative materials.

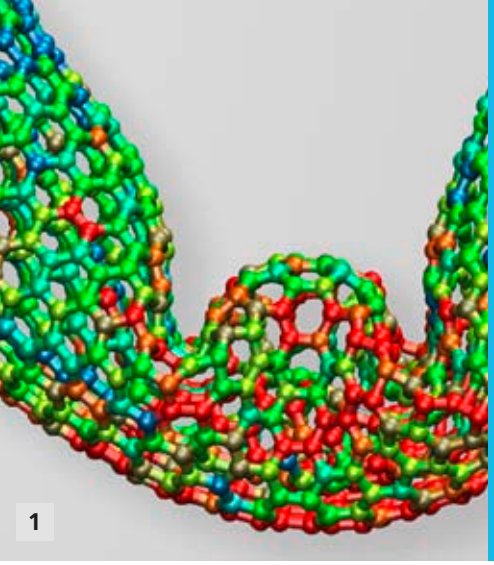
Tremolo-X uses highly efficient state-of-the-art algorithms for the treatment of short- and long-range potentials, where great emphasis has been placed on its parallel implementation and efficiency. All commonly used potential types are included for modeling systems in the areas of material science, nanotechnology and biophysics.

The software has already been successfully applied in many practical projects in different areas. Some examples are given on the next pages.

Tremolo-X also includes *Tremolo-X*-GUI, which is a user-friendly graphical user interface front end. This provides an easy set-up and analysis of numerical experiments.

Features

- user-friendly graphical interface
- parallel version for distributed memory computers (MIMD) with the Message Passing Interface (MPI)
- parallel implementation of reactive many-body potentials of Brenner, Marian, Tersoff, Feuston-Garofalini, Stillinger-Weber and Sutton-Chen
- parallel implementation of fixed bond, angle, dihedral and inversion potentials
- NVE, NVT and NPT ensemble, structural optimization and Dissipative Particle Dynamics (DPD)
- several time integrators and local optimizers: Verlet, multistep like Beeman-Verlet as well as Fletcher-Reeves and Polak-Ribière
- replica exchange methods like Hybrid Monte Carlo and Parallel Tempering
- computation of many derived quantities and measures, e.g. diffusion coefficients, stress-strain diagrams, elastic constants, distribution functions, correlation functions and shortest-path-ring statistics
- fast implementation of short-range potentials via linked-cell method and parallelization by dynamic load-balanced domain decomposition
- fast algorithms for long-range potentials:
  - Particle-Mesh-Ewald with domain decomposition and parallel 3D FFT and parallel multigrid
  - Barnes-Hut/fast multiple methods and parallelization by space-filling curves
- simple extension to new potential types by modularity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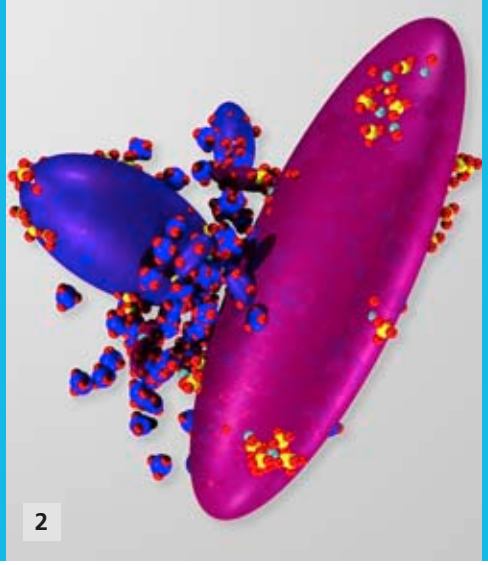
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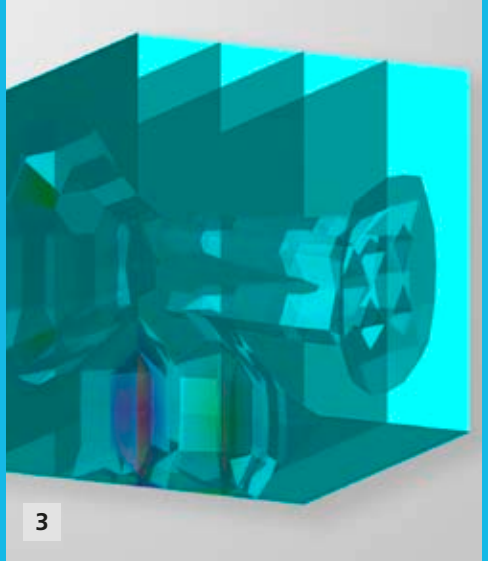
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SELECTED PROJECTS

Numerical simulation tools can be applied to tackle a wide range of challenges that arise in materials science and nanotechnology applications. In the following, we give some examples where we focus on.

Nanomaterials

Nanoparticles exhibit exceptional material properties and thus provide a wide range of possible applications in various areas. Examples are lightweight materials (reinforced nanocomposites, concrete), energy and environmental engineering (batteries, fuel cells, hydrogen storage), electronics (cooling, transistors, field emission display), medicine (sensor technology, drug-delivery), and information and communication technology.

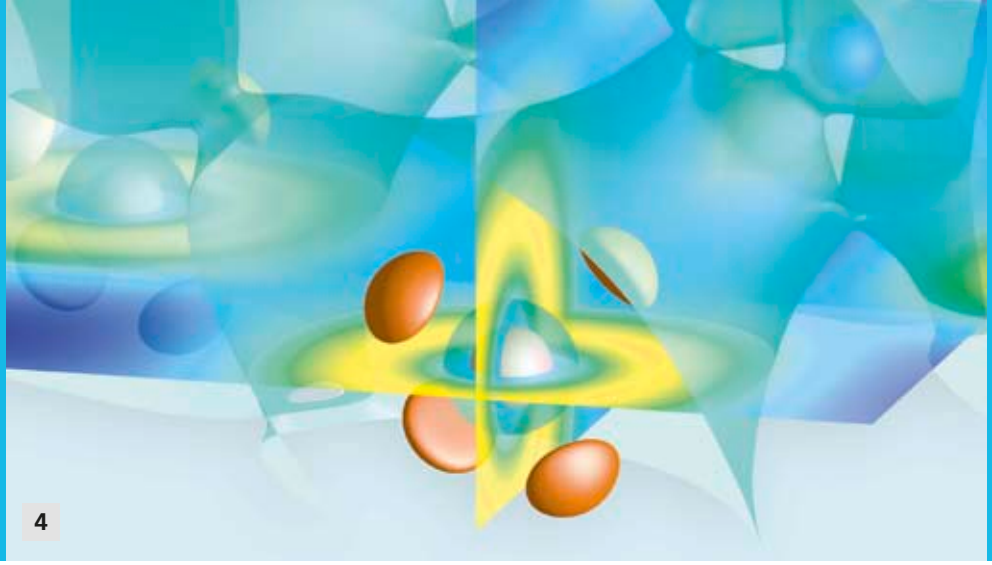
Carbon Nanotubes (CNTs), for example, show outstanding mechanical, thermal and electrical properties. Hence, they are already used in industrial applications for mechanical reinforcement and optimization of electrical conductivity of polymer composite materials. Besides carbon or boron-nitride based nanoparticles (Fullerene, CNTs, graphene, BN-NTs), ceramic and metallic nanoparticles have also been synthesized with remarkable properties. In the context of design and production of nanomaterials, many questions and challenges emerge, such as the homogeneous dispersion of the fibers in a matrix and the optimal nanoscale linkage of the fiber to the base material. The Department of VMD provides several efficient software tools to tackle such problems.

Innovative cementitious materials

Cement and cementitious materials are of paramount importance in today's society. They have widespread use in the construction of bridges, airports, residential and office buildings, and countless other key components of modern infrastructure. However, it is well known that the leeching of ions has a destabilizing effect on those materials. A degeneration process is accelerated by industrial pollution and acid rain that surround urban centers. With this in mind, it may come as a surprise that many fundamental questions relating to cement and cementitious materials have not yet been answered by science. One open issue is that there is no reliable knowledge about their nanostructure. Furthermore, there remains a lack of models describing the progression of ion leeching from the cement matrices. The Department of VMD supplies tools, which tackle these open problems.

Simulation of ion migration

The combined diffusion and convection of ions through different materials is the foundation of a variety of technically interesting processes, ranging from battery operation via concrete degradation to the use of biomembranes. Nonlinear Poisson Nernst Planck (NPNP) is a software package for the numerical simulation of complex ion migration processes induced, for example, by electric fields. NPNP is designed for time-dependent problems, it can treat multiple ion species and can deal with arbitrary geometries.



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Atomic-scale modeling of novel metal-oxides in electronics (ATOMMODEL)

Electronic components have nowadays been downsized to the point where single atoms have an impact on performance and reliability. There is awareness in the electronics industry that new atomistic simulation tools are needed since the currently used models fail. Parameterized potential models can be applied in practice. However, the development of new parameterized potential models is a slow and manual process. In this project, the main aim of the Department of VMD is to develop and implement a new method for the automated generation of reactive potential models and its integration in *Tremolo-X*. The new techniques are based on state-of-the-art numerical methods for high-dimensional approximation and machine learning. In particular, one goal is to develop a self-learning version.

High performance computing

Numerical simulations in quantum mechanics, molecular dynamics and continuum mechanics are highly demanding in terms of computational requirements. To this end, the research in the Department of VMD focuses on the development and implementation of highly efficient and parallel scalable simulation tools for state-of-the-art hardware architectures and high performance computing clusters.

CUDA Research Center

Because of their leading research in numerical simulation using parallel computing, Fraunhofer SCAI and the Institute for Numerical Simulation at the University of Bonn have officially become one of the first German NVIDIA CUDA Research Centers. One focal point is research and development regarding the parallelization of existing simulation codes to run on machines with multiple Graphics Processing Units (GPUs). The second focal point is the development of massively paralleled multi-GPU based software packages for numerical simulation in the natural and engineering sciences. In the Department of VMD the goal is to develop a massively parallel, completely multi-GPU based high performance molecular dynamics software package. To this end, the SCAI software *Tremolo-X* is adapted. SCAI's customers from industry and research institutes will profit from the transfer of knowledge from basic research to practical applications.

1 *Bending of a double walled carbon nanotube.*
2 *A coarse grained model of a cementitious C-S-H gel.*
3 *A concentration profile of a perturbed electrolyte.*
4 *Electronic structure of Gallium Arsenide (GaAs).*
5 *SCAI is involved in one of the first German NVIDIA CUDA Research Centers.*

HIGH PERFORMANCE ANALYTICS

The term High Performance Analytics (HPA) was originally used in the analysis of business processes. In the context of numerical simulation, HPA comprises the highly efficient creation, storage, and analysis of large amounts of data. The aim thereby is to provide new, nontrivial insights into processes, which can be exploited for purposes of steering and optimization.

The work of the Department of HPA focuses on two main areas:

- solutions for parameter-dependent problems

The work in this field includes the development and integration of numerical methods for exploration, statistical analysis, multi-objective optimization, and robust design. The robustness and quality of production processes and products suffers from variations in, among others, material properties, process parameters, and geometry. Analyzing and controlling the effects of these variations helps to find robust optimal settings under realistic conditions. Computer-aided robust design and intuitive exploration of design spaces and simulation results is highly relevant for industry.

Advanced methods developed for such problems have been implemented in the *DesParO* software suite. This toolbox integrates techniques like metamodeling, data mining, statistical methods for clustering and machine learning. Furthermore, *DesParO* includes robust multi-objective optimization methods. This means that optimization is used to enhance the quality of metamodels or to find parameter sets for the resulting metamodels that reflect optimal solutions of the engineering application behind them.

- analysis, simulation, and optimization of networks, circuits, and graphs

The focus of this work lies in the development of the software *MYNTS*, whose purpose is the multiphysical simulation of many kinds of networks. *MYNTS* models networks as systems of differential-algebraic equations and uses state-of-the-art solvers for these problems.

These networks can also be analyzed, manipulated, and visualized by using HPA's new software library *net'O'graph*. Both tools, *MYNTS* and *net'O'graph*, support a broad variety of practical applications ranging from the simulation and optimization of electrical circuits and devices to the transportation of gas, oil, water, and electricity.

The Department of HPA offers technology studies, software licenses, tailored software solutions, and the integration of self-developed software modules into other software products to both academic and industrial partners. Target industries for HPA's software and services portfolio are companies dealing with the transportation of oil, gas, water, and electricity as well as companies in the microelectronics industry, the automotive industry, engineering, and chemistry.

To ensure that HPA's work reflects the state-of-the-art in mathematics and engineering, we cooperate closely with the groups of Prof. Dr. Caren Tischendorf at the Humboldt University of Berlin, and Prof. Dr. Margot Ruschitzka at the University of Applied Sciences in Cologne.

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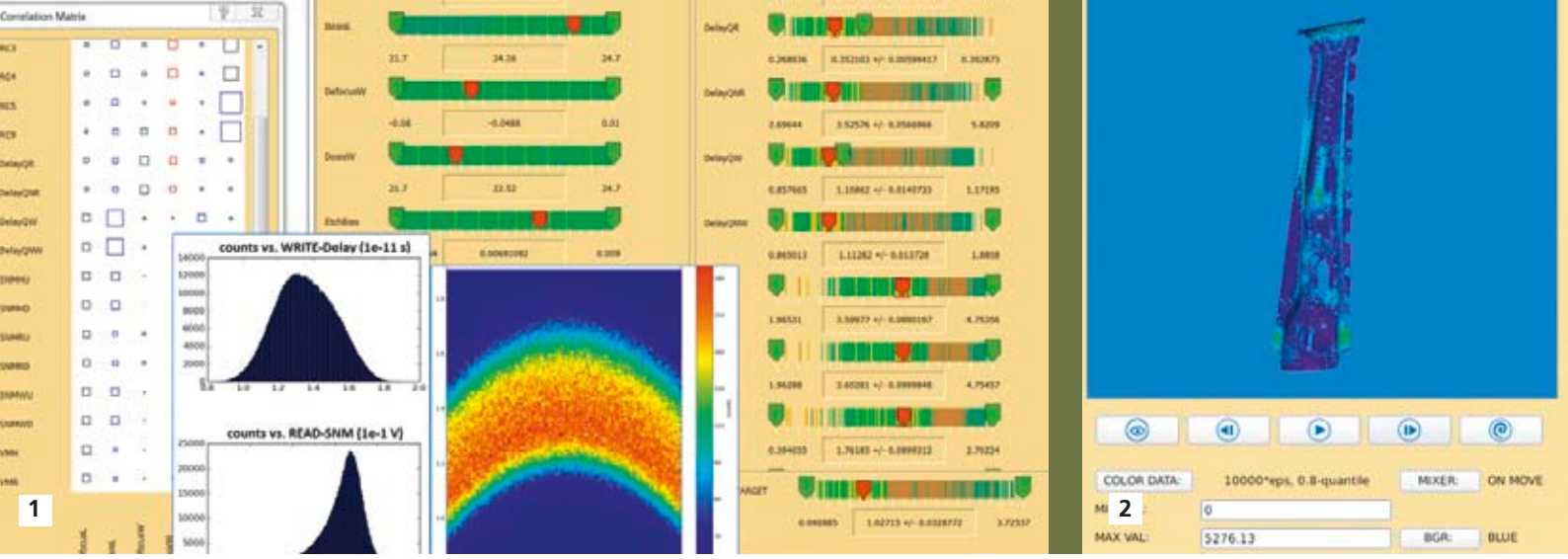
LEFT *Gas pipelines can be simulated and analyzed with SCAI's software MYNTS.*



ANALYZING DATA FROM EXPERIMENTS OR SIMULATIONS

Technical processes and products commonly depend on many parameters. Engineers are interested in configurations of these parameters that will optimize the production process, the product features, and the quality. SCAI's software package *DesParO* offers its users an efficient interactive solution.

DesParO is a software package for the intuitive exploration, statistical analysis, and optimization of parameterized problems. *DesParO* can be coupled with simulation packages or used for analyzing data which stem from physical measurements. In particular, *DesParO* focuses on keeping the number of necessary experiments – simulations or measurements – small since experiments follow a strategic design (Design-of-Experiments, DoE) and can be performed in parallel. *DesParO* is especially useful for time- or resource-intensive simulation runs or for costly measurements.

DesParO's correlation measures, as well as its local tolerance and sensitivity estimation, can handle nonlinearities efficiently. *DesParO* provides an easy-to-use graphical user interface (Figure 1) with sliders for parameters and criteria that allow for interactive, intuitive exploration of dependencies.

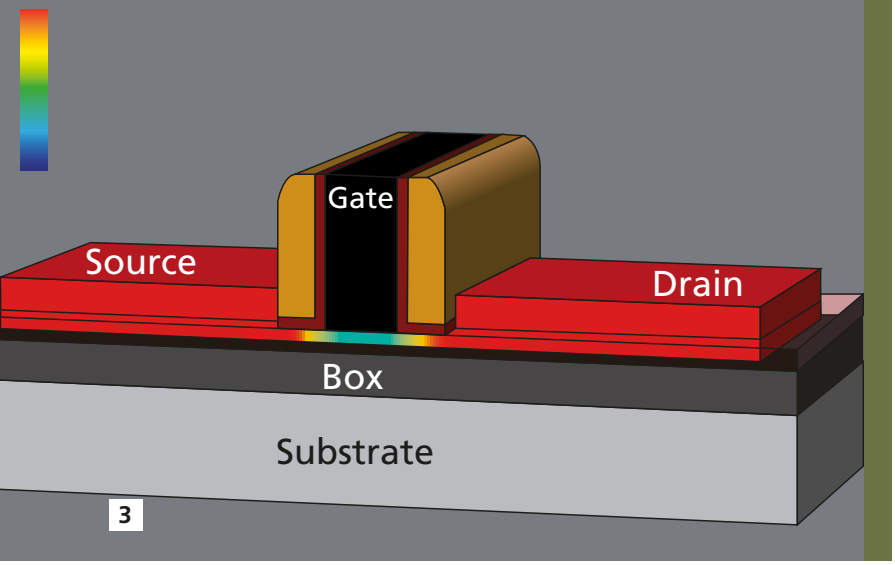
Novel features of *DesParO* include intensive statistical analysis methods. Examples are quantiles, robustness measures, classical histograms, two-dimensional histograms and scatter plots which reflect correlations, dynamic sensitivities, and interpolation of statistical measures on highly resolved grids.

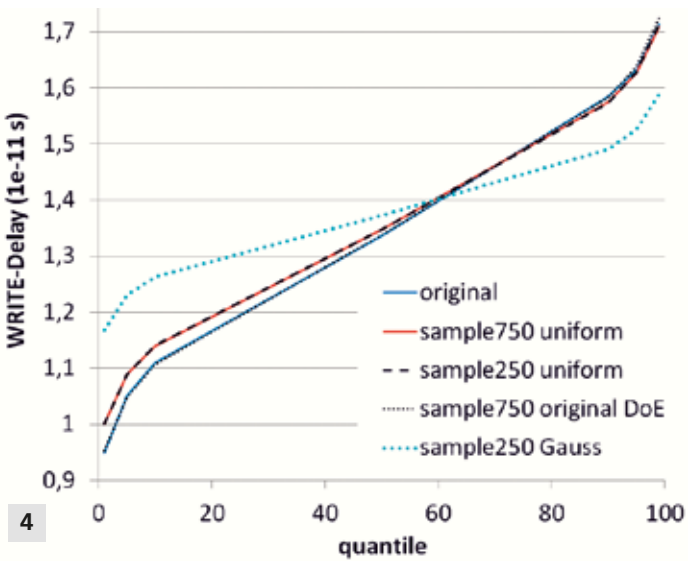
Recently, an adaptive hierarchical metamodel refinement was built into *DesParO*, based on extensions of so-called expected improvement approaches, clustering methods, and decay functions. It enables step-by-step improvement in accuracy in order to keep simulation and evaluation costs even smaller.

DesParO is used in a broad range of applications in the following areas:

- the oil and gas industry (e.g. oil reservoirs: calibration of parameters with respect to oil production rates)
- the microelectronics industry (e.g. lithography; circuit and device simulation analysis)
- the automotive industry (e.g. metal forming, spot welding, crash analysis; entire process chains resulting in robust virtual automotive design)

1 *The graphical user interface of DesParO with some statistical evaluations: correlation matrix (nonlinear effects), classical exemplary and two-dimensional histograms.*
2 *The picture shows DesParO's geometry viewer with results for a crash simulation model of a car's B-pillar.*





3 *Device simulation of a 32 nm transistor.*

4 *Comparison of several DoEs and models shows the metamodel accuracy.*

SIMULATION OF PROCESS VARIATIONS

Fraunhofer SCAI's software *DesParO* was used in an internal Fraunhofer research project to efficiently investigate the impact of several process variations on device performance and accuracy. It has been shown that the results are of high relevance for industry in order to minimize the influence of variations – thereby saving production costs through simulation.

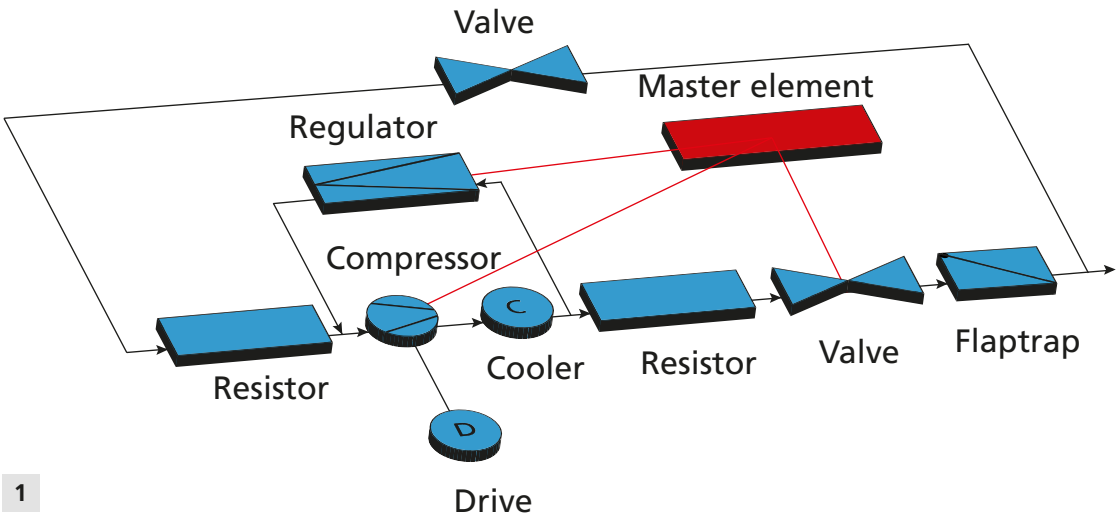
With the transition from micro- to nanoelectronics, the control of production variations cannot keep pace with the reduction of the absolute sizes of semiconductor devices and circuits. Most studies published so far only considered the impact of one or two sources of variability. To overcome these limitations, Fraunhofer SCAI and the Fraunhofer Institute for Integrated Systems and Device Technology (IISB) developed a novel approach. It combines state-of-the-art computer-aided design simulations with *DesParO*´s advanced methods to enable the efficient investigation of the impact of several process variations on device performance. The work was conducted in the internal Fraunhofer research project *Hierarchical Simulation of Nanoelectronic Systems for Control of Process Variations* (HIESPANA) from January 2008 to January 2011.

SCAI studied the impact of six different process variations on a Static Random Access Memory (SRAM) cell built from 32 nm Metal Oxide Semiconductor Field-Effect Transistors (MOSFETs) (see Figure 3). They were originally designed using a standard approach, i.e., a full factorial design, which means that the full set of all mixed variations must be computed. This requires very long computation times since more than a million simulations have to be performed.

In order to drastically reduce the number of simulations needed and to enable the treatment of more sources and types of variations, SCAI enhanced the simulation study by using state-of-the-art Design-of-Experiments (DoE) and response surface techniques (metamodeling) which employ the *DesParO* software. Two metamodels were constructed by sampling the original DoE based on results from the previously performed 1.6 million simulation runs. The metamodels have different numbers of DoE points in order to compare accuracy. Both metamodels – even the one based on only 242 simulations – give accurate results compared with the original data set. Quantiles correspond very well (Figure 4).

Metamodel construction and evaluation is a very efficient overall process: Here, a speedup factor of more than 6500 – compared with the original approach – could be achieved. Moreover, a metamodel allows us to evaluate many what-if-scenarios conveniently. In contrast to applying the classical approach and working with simulation runs directly (here, for 1 million points corresponding to a Gaussian-type or other distributions), we only have to perform model evaluations that are several orders of magnitude faster.

In summary, *DesParO* yields accurate statistical results efficiently, also in the presence of nonlinearities where the misleading impression of the classical Pearson correlation could be corrected: Figure 1 shows the most dominant variations; temperature has a large impact on contact resistances. The efficiency of the overall approach enables the application to real-case industrial applications.



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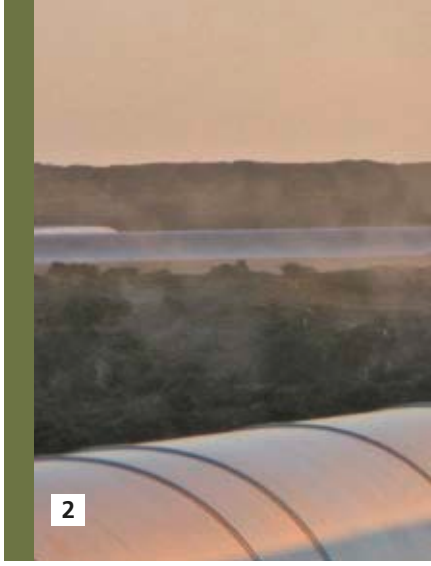

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SIMULATION SOFTWARE FOR NETWORK OPTIMIZATION

Efficient transport networks are of utmost importance for developed countries. Examples of such networks can be found within the infrastructure for the transport of gas, electricity, and water. As is known, three percent of the totally consumed electrical energy is used by water companies – mainly for pumps. This means that even small improvements in pump efficiency will result in significant reductions of energy consumption and costs.

In order to enable and increase the use of renewable energy, the German government supports the modernization and construction of thousands of kilometers of new electricity networks. These "smart grids" will be complex networks that need new strategies for management and operational optimization.

To meet this increasing demand of the market, Fraunhofer SCAI has developed a software called *MYNTS* (Multiphysical Network Simulator). *MYNTS* exploits the fact that networks – from the transport of water, gas and electricity to electrical circuits inside technical devices – can be modeled in a very similar fashion as systems of differential-algebraic equations. Their numerical simulation can be performed based on the same numerical kernels! Resulting from the project HIESPANA (see page 59) and other projects, the software supports different applications ("one for all").

1 *Schematic representation of a compressor station as a subnet for "MYNTS-Gas" with master elements.*

Flexible planning of gas, power and water grids

Since each field of application has its unique features, specialized versions of the software are available for various purposes. For example, with *MYNTS*-Gas, which features the simulation of gas transport systems, users can set up and control their own subnetworks with master elements to model and control compressor stations (see Figure 1) or mixing chambers. In order to accelerate simulation computations, the software runs on computers with multiple processors.

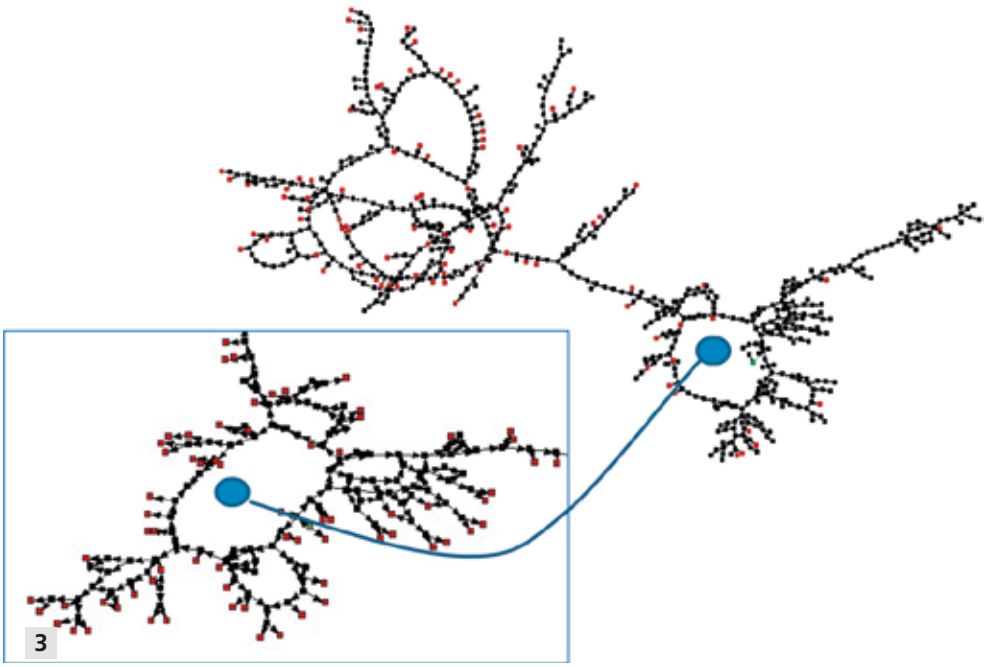
This software is also of interest for smart grids. Intelligent networking and controlling of electricity producers, storage facilities, electricity consumers, and network resources within supply networks are considered to be among the greatest economic and environmental

technology challenges. For example, if bulk consumers could be monitored more efficiently, and power supply adjusted to meet demand at different times – then consumption peaks could be capped, and the use of electric energy could be better matched to supply.

Such bulk consumers include water companies. Studies suggest that three percent of the total electricity production in the USA is used by the water industry where up to 90 percent of this electrical energy is consumed by pumps. Intelligent control of the network would have major economic potential: even minor incremental savings could make a major contribution that benefits the environment.

Extensions of the *MYNTS* technologies are the focus of our ongoing collaboration with the group of Prof. Dr. Caren Tischendorf (Humboldt University of Berlin).

In combination with SCAI's software tools *net'O'graph* and *DesParO*, graph analysis, statistical analysis, and optimization tasks are supported. *net'O'graph* is a novel software library with drivers for analysis and manipulation of networks and graphs. Features include graph reduction, graph matching (see Figure 3), input-output analysis, network decomposition, and layout.



2 *With MYNTS, systems operators can simulate and optimize complex gas, water and power grids even at the planning stage.*
3 *Graphical visualization of two networks, which are matched by net'O'graph ("graph matching").*

COMPUTATIONAL FINANCE

Computational Finance is a new interdisciplinary field of scientific computing. Its aim is to estimate the risks that financial instruments generate as accurately as possible.

Application areas include the pricing and trading of financial securities, the development of hedging strategies, risk assessment and management, asset-liability management, investment decisions, and corporate strategic planning. Current challenges are increasingly complex financial products, market models involving several sources of uncertainty, and the simultaneous management of assets and liabilities as an optimization problem.

The current financial crisis has shown that the interplay between financial products is not yet fully understood and mathematical models for the underlying markets are often inadequate. Numerical simulations can help to better understand these complicated interactions by analyzing the output of simulated scenarios. In comparison runs between different models, or for the same model with different parameters, the model setup with the best predictive behavior can be selected and model risk can be estimated by looking at the variance of the different outputs.

In the Department of Computational Finance, efficient and robust numerical algorithms are developed and realized on parallel supercomputers. Thereby, modern computational methods, such as multilevel Monte Carlo and Quasi-Monte Carlo simulation, dimension-adaptive sparse grid quadrature, and sparse multinomial trees are employed. These new methods allow for the computation of high accuracy solutions and, simultaneously, a substantial reduction of computing times.

Our goal is to develop new approaches for the modeling and simulation of financial products and, furthermore, whole financial companies. In this way, the newest developments in computational finance are integrated into innovative software packages that conform to the latest regulatory standards. Thereby, modern algorithmic design, modular structuring, web-based interfaces and cloud techniques for parallel computing are employed. In this way we hope to aid with the prevention of future financial crises by providing powerful risk management software made by Fraunhofer SCAI.

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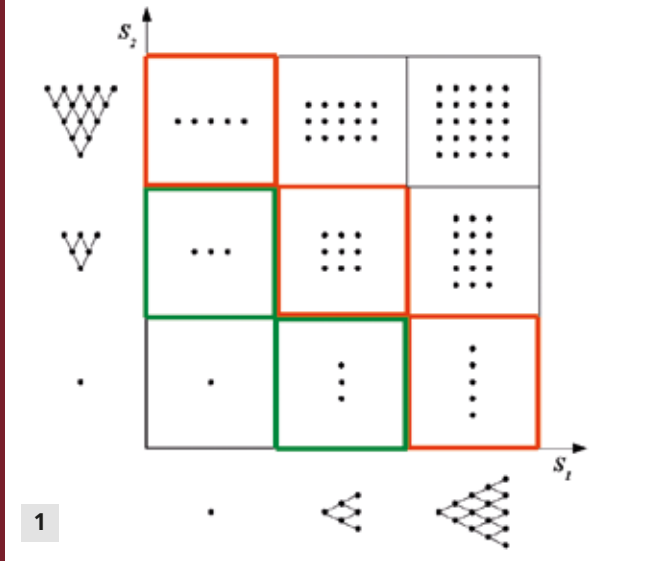
LEFT *Trading room of the Munich Stock Exchange.*



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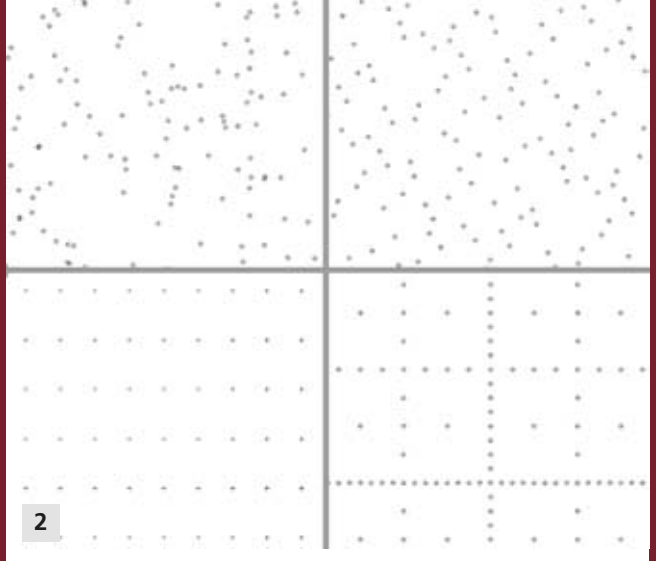

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PRICING OF FINANCIAL DERIVATIVES

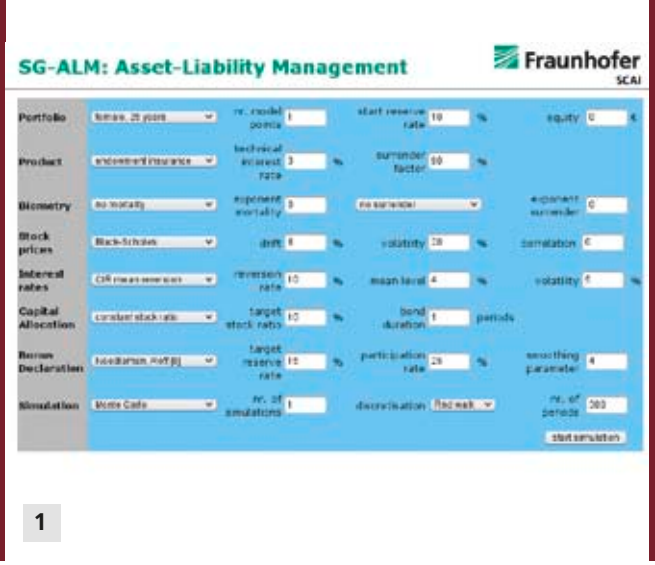
The efficient and accurate valuation of financial derivatives, for example options, is one of the main tasks of computational finance. Thereby, fast and accurate numerical simulation methods are required.

The fair value of a derivative is determined by the payoff structure of the financial product at hand and a suitable stochastic model for the financial market. The resulting problem is then either an expectation (usually a multivariate integral) or a partial (integro-)differential equation. In most cases a closed-form solution for these problems does not exist and numerical methods have to be used for their computation.

In practice, Monte Carlo methods, which are based on the averaging of a large number of simulated scenarios, are usually used. These methods are robust and easy to implement, but suffer from an erratic convergence and relatively low convergence rates. In order to improve an initial approximation by one more digit precision, Monte Carlo methods typically require the simulation of a hundred times as many scenarios as for the initial approximation. Since the simulation of each scenario requires to run over all relevant points in time and all policies in a company's portfolio, often very long computing times are needed to obtain approximations of satisfactory accuracy.

Current challenges include increasingly complex financial products, such as compound or multi-asset options, as well as more and more sophisticated market models, such as jump-diffusion models. In the Department of Computational Finance, we are developing efficient and robust numerical algorithms and implement them on parallel supercomputers. Thereby, modern computational methods, such as multilevel Monte Carlo and Quasi-Monte Carlo simulation, dimension-adaptive sparse grid quadrature, and sparse multinomial trees are employed. These new methods allow the computation of high accuracy solutions and, simultaneously, a substantial reduction of computing times.

1 *Product binomial trees used for the discretization of two stochastic differential equations.*
2 *Pseudo-random numbers, quasi-random numbers, a full grid and a sparse grid.*



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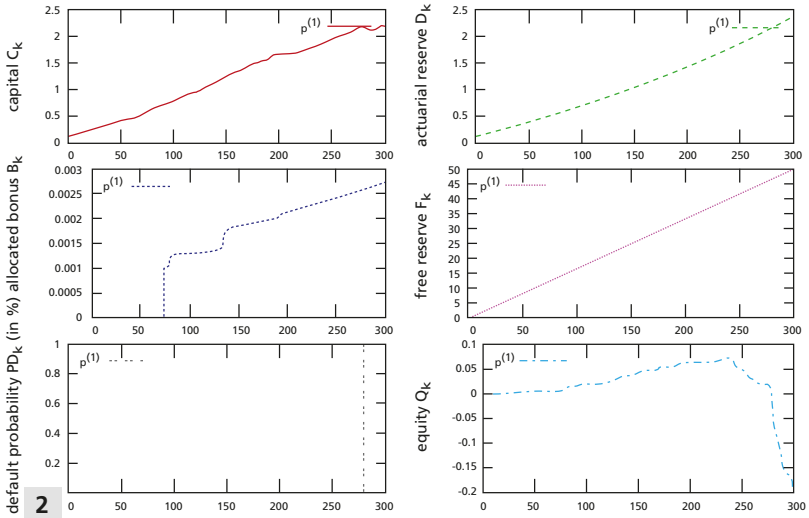

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ASSET LIABILITY MANAGEMENT

Much effort has been spent on the development of stochastic Asset-Liability Management (ALM) models for insurance companies in the last years. Such models are becoming increasingly important due to new accountancy standards, greater globalization, stronger competition, more volatile capital markets and long periods of low interest rates.

ALM models are employed to simulate the medium and long-term development of all assets and liabilities of, e.g. an insurance company. This way, the company's exposure to financial, mortality and surrender risks can be analyzed. The results are used to support management decisions regarding, for example the asset allocation, the bonus declaration, or the development of more profitable and competitive insurance products. The models are also applied to obtain market-based, fair value accountancy standards as required by Solvency II and the International Financial Reporting Standard.

Due to the wide range of path-dependencies, guarantees and option-like features of insurance products, closed-form representations of statistical target figures, such as expected values or variances, which in turn yield embedded values or risk-return profiles of the company, are in general not available. Therefore, insurance companies have to resort to numerical methods for the simulation of ALM models. Due to the long computing times, a frequent and comprehensive risk management, extensive sensitivity investigations, or the optimization of product parameters and management rules are often not possible.

In one of our projects, we focus on approaches to speed up the simulation of ALM models. To this end, we rewrite the ALM simulation problem as a multivariate integration problem and apply quasi-Monte Carlo and sparse grid methods in combination with adaptivity and dimension reduction techniques for its numerical computation. Quasi-Monte Carlo and sparse grid methods are alternatives to Monte Carlo simulation, which are also based on a (weighted) average of different scenarios, but use deterministic sample points instead of random ones. They can attain faster rates of convergence than Monte Carlo, can exploit the smoothness of the integrand, and have deterministic upper bounds on their error. In this way, they significantly reduce the number of required scenarios and computing times.

1 *Web-interface for an asset-liability management simulation.*

2 *Numerical simulation results of an asset-liability management model.*


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NUMERICAL DATA-DRIVEN PREDICTION

Nowadays the automatic collection of data is omnipresent. Efficient analytic tools are necessary to make use of this data deluge. A core aspect is the use of these data collections for predictions, which support decision making.

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The Department of Numerical Data-Driven Prediction develops and investigates numerical algorithms for data-driven prediction. The aim here is to make useful forecasts for the future behavior of systems based on automatically collected current and historical data. Under the assumption that the behavior is similar in similar situations, one uses models built from historical data to forecast upcoming situations.

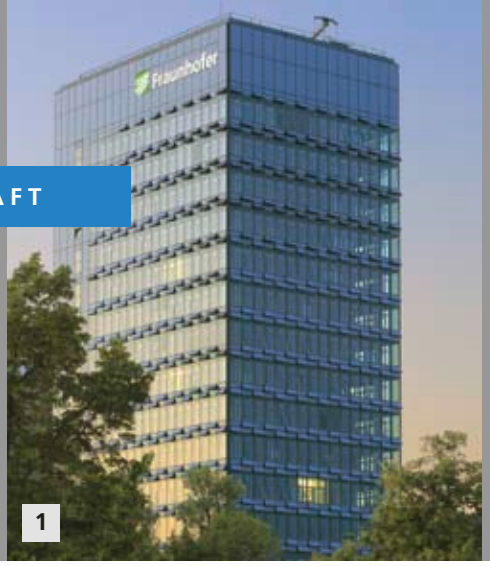
Bringing a mathematical viewpoint to data analysis is the common ground for the different applications and algorithms investigated. Building upon research and development on efficient numerical methods for high-dimensional problems, new approaches are developed within the department. The new approaches are based on the modern numerical methods of "sparse grids" and "low rank tensor decompositions" to represent nonlinear functions. Their computational effort scales only linearly with the number of data instances and they achieve an advantageous prediction quality. Therefore, they can be powerful even in situations where common nonlinear data analysis methods cannot cope with the amount of data due to their need of large computational resources. In particular, the new tools developed in the department have the strong potential to be successfully used for the large amounts of data often found in industrial and commercial applications.

Data-driven predictions appear in many application domains. A special focus of the department's work is on the so-called technical trend prediction for foreign exchange rates and other financial products. We tackle the problem of forecasting time series of traded assets by transforming it into a machine learning regression problem using a delay embedding approach. The machine learning algorithm then learns the typical technical behavior of the time series just from these processed empirical observations of the market.

Further applications are improved recommendation engines for online shops. Here we test the transfer of modern hierarchical solvers from industrial simulation processes to reinforcement learning formulations of recommendation engines.

The services provided to our customers include the development and provision of data analysis software tailored to the specific application needs. Furthermore, SCAI offers consulting and support in the whole data analysis workflow, e.g. in the pre-processing of the raw data, in the algorithmic analysis, or during the deployment of the corresponding results. In joint research projects we develop application specific new approaches or work on the improvement of existing techniques.

THE FRAUNHOFER-GESELLSCHAFT



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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 benefits society in a wider perspective. Its services are solicited by customers and contractual partners in industry, the service sector and public administration.

At present, the Fraunhofer-Gesellschaft maintains more than 80 research units in Germany, including 60 Fraunhofer Institutes. The majority of the more than 20,000 staff are qualified scientists and engineers, who work with an annual research budget of €1.8 billion. Of this sum, more than €1.5 billion is generated through contract research. More than 70 percent of the Fraunhofer-Gesellschaft's contract research revenue is derived from contracts with industry and from publicly financed research projects. Almost 30 percent is contributed by the German federal and Länder 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.

Affiliated international research centers and representative offices provide contact with the regions of 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 relevant 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 allows 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 prospects of starting and developing a career in industry by virtue of the practical training and experience they have acquired.

1 *The "Fraunhofer-Haus" in Munich.*
2 *The organization takes its name from Joseph von Fraunhofer (1787-1826), the illustrious Munich researcher, inventor and entrepreneur.*

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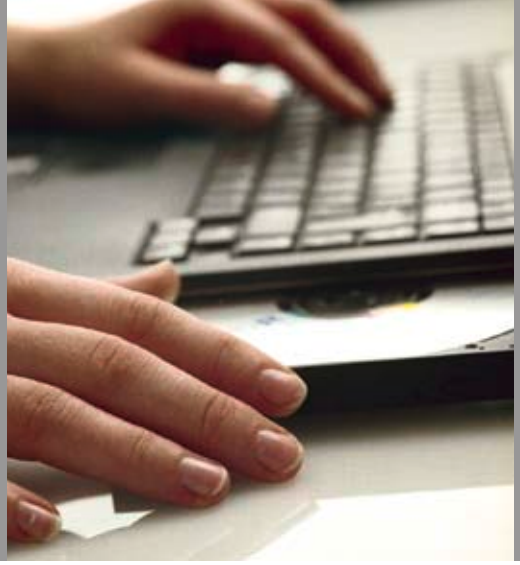

Fraunhofer SCAI works hand in hand with other institutes of the Fraunhofer-Gesellschaft, collaborating in groups and alliances:

Fraunhofer Alliance for Numerical Simulation of Products and Processes

In the Fraunhofer Alliance for Numerical Simulation of Products and Processes, twenty institutes pool their expertise in the development and improvement of simulation techniques.

The simulation of products and processes plays a decisive role in all phases of the product life cycle, from model-based materials development and simulation of manufacturing processes to operating characteristics and product placement on the market. *www.nusim.fraunhofer.de*

Fraunhofer Cloud Computing Alliance

The Fraunhofer Cloud Computing Alliance is a group of six Fraunhofer Institutes that carry out research and industrial projects focusing on different aspects of cloud computing and related topics, such as grid computing, utility computing and service-oriented architectures. By pooling their expertise, the institutes involved are able to offer customers and research partners a central point of contact for questions relating to networking and the optimized utilization of distributed IT resources. *www.cloud.fraunhofer.de*

Fraunhofer Information and Communication Technology Group

As the largest ICT research group in Europe, the Fraunhofer Information and Communication Technology Group serves as a one-stop shop for industrial customers and media enterprises. The strengths of the member institutes are pooled strategically and marketed jointly. This network makes it possible to translate application-oriented research into customized, integrated solutions for a specific sector:

- tailored IT solutions
- competent consulting on technological issues
- pre-competitive research for new products and services *www.iuk.fraunhofer.de*

PUBLICATIONS

The following is a listing of the published work generated by SCAI employees in 2011 and the first half of 2012. This list includes work from peer-reviewed research articles, books and book chapters, conference posters and proceedings.

2011

Armstrong, D.; Djemame, K.; Nair, S.; Tordsson, J.; Ziegler, W.:
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In: Institute of Electrical and Electronics Engineers IEEE: Third IEEE International Conference on Cloud Computing Technology and Science, CloudCom 2011: Athens, Greece, November 29 - December 1, 2011 and New York, NY: IEEE, 2011, pp. 328-331.

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Demonstration of the OPTIMIS toolkit for cloud service provisioning.
In: Abramowicz, W.: Towards a service-based internet. 4th European conference, ServiceWave 2011: Poznan, Poland, October 26-28, 2011; Proceedings. Berlin: Springer, 2011, pp. 331-333 (Lecture Notes in Computer Science 6994).

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In: Cunningham, P.: International Information Management Corp. (IIMC), Dublin: eChallenges e-2011. Proceedings. CD-ROM: Conference & Exhibition, October 2628, 2011: Florence, Italy, Dublin: IIMC, 2011.

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In: Proceedings of The Second International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering: Corsica, France, April 12-15, 2011.

Birkenheuer, G.; Brinkmann, A.; Högqvist, M.; Papaspyrou, A.; Schott, B.; Sommerfeld, D.; Ziegler, W.:
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In: Journal of Grid Computing 9 (2011), No. 3, S. 355-377.

Bürger, M.; Wolf, K.:
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On the construction of sparse tensor product spaces.
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ACADEMIC THESES

Dissertations

2011

Klein, C.:
Information extraction from text for improving research on small molecules and histone modifications.
University of Bonn, 2011.

Klinger, R.:
Conditional random fields for named entity recognition. Feature selection and optimization in biology and chemistry.
TU Dortmund University, 2011.

Menrath, M.:
Stability criteria for nonlinear fully implicit differential-algebraic systems.
University of Cologne, 2011.

Selim, F. F. S.:
The human adenosine A_{2B} receptor: homology modeling, virtual screening, and computer-aided drug design
University of Bonn, 2011.

Wäldrich, O.:
Orchestration of resources in distributed, heterogeneous grid environments using dynamic service level agreements.
TU Dortmund University, 2011.

2012 (up to July)

Hülsmann, M.:
Effiziente und neuartige Verfahren zur Optimierung von Kraftfeld-parametern bei atomistischen molekularen Simulationen kondensierter Materie.
University of Cologne, 2012.

Rettenmeier, M.:
Data compession for computational fluid dynamics on irregular grids.
University of Cologne, 2012.

Wolf, A.:
Revealing the mechanism of thiopeptide antibiotics at atomistic resolution.
University of Bonn, 2012.

Diploma and Master Theses

2011

Bethke, S.:
Zwei Methoden zur gitterunabhängigen Klassifikation von Bauteilen unter Berücksichtigung geometrischer Eigenschaften.
University of Cologne, Diploma Thesis, 2011.

Feld, D.:
Effiziente Vektorisierung durch semi-automatisierte Code-Optimierung im Polyedermodell.
University of Cologne, Diploma Thesis, 2011.

Gries, S.:
Algebraische Mehrgitteransätze für industrierelevante CFD-Probleme – Druckkorrektur im Kontext OpenFOAM.
University of Cologne, Diploma Thesis, 2011.

Hemmersbach, J.:
Regularisierte Approximationsverfahren für eine Dünn-Gitter-basierte, ableitungsfreie Methode zur Optimierung von Kraftfeldparametern im Bereich molekulare Simulation.
University of Cologne, Diploma Thesis, 2011.

Hettkamp, C. J.:
Sensitivitätsanalyse der Prozesskette von Halbleiterbauelement-simulationen.
University of Cologne, Diploma Thesis, 2011.

Ibel, M.:
Consistent initialization of gas pipe networks.
University of Cologne, Diploma Thesis, 2011.

Karla, F. M. P.:
Sensitivitätsanalyse für die Lösungen von DAEs aus der Schaltungssimulation.
University of Cologne, Diploma Thesis, 2011.

Kessler, J.:
Vergleich von Robustheitsmaßen.
University of Cologne, Diploma Thesis, 2011.

Kürz, C.:
Frame-basierte Interpolationsverfahren zur Kompression von transienten Simulationsergebnissen.
University of Cologne, Diploma Thesis, 2011.

Kuppe, C.:
Eine Methode zur Geometrieoptimierung durch lokales Gittermorphing.
University of Cologne, Diploma Thesis, 2011.

Kyrion, T.:
Über dichtkämmende und gleichsinnig drehende Extruderschnecken.
University of Cologne, Diploma Thesis, 2011.

Lammert, D.:
Analyse gegebener Experimentaldaten für und mittels RBF-Metamodellierung.
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Auswirkungen verlustbehafteter Kompression auf das Frequenzspektrum und die Gradienten von CFD-Simulationsergebnissen.
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Adaptiv hierarchische Metamodellierung mittels radialer Basisfunktionen.
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Xuanshi, L.:
Dictionary-based named entity recognition and normalisation in Chinese biomedical publications.
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2012 (up to July)

Bobic, T.:
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Jiali, W.:
A knowledge-based approach to analysing gene expression in specific brain regions and cell types.
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Kalmykov, I.:
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Obermüller, F.:
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Mathematische Modellierung eines Chromatographieprozesses mittels differential-algebraischer Gleichungen.
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Bachelor Theses

Breitenstein, S.:
Entwicklung und Implementierung von Lastausgleichsstrategien zur effektiven Nutzung von Hardware-Beschleunigern in hybriden Computer-Clustern.
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Entwicklung eines verteilten linearen Gleichungssystemlösers.
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Entwurf und Implementierung eines flexiblen C++ Frameworks zum Lösen großer, dünnbesetzter Gleichungssysteme.
University of Cologne, 2012.

TEACHING

Dr. Juliane Fluck

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

Summer semester 2011/2012
- Life Science Knowledge Discovery (lecture and exercise)

Dipl.-Math. Malte Förster

Bonn-Rhein-Sieg University of Applied Sciences

Summer semester 2011
- Mathematik 2 (practical lab)

Winter semester 2011/2012
- Informatik 1 (practical lab)

Summer semester 2012
- Informatik 2 (practical lab)

Prof. Dr. Jochen Garcke

University of Bonn

Winter semester 2011/2012
- Wissenschaftliches Rechnen – Numerische Methoden der Datenanalyse (seminar)

Summer semester 2012
- Selected Topics in Scientific Computing – Numerical Methods for High-Dimensional Problems (lecture)
- Algorithmen im Data Mining (seminar)

Prof. Dr. Thomas Gerstner

Goethe University Frankfurt

Summer semester 2011
- Computational Finance (lecture)
- Mathematik für Informatiker II (lecture)
- Hochdimensionale Quadraturverfahren (seminar)
- Matrix-Algorithmen (proseminar)

Winter semester 2011/2012
- Einführung in die Numerik (lecture)
- Quadraturverfahren (lecture)
- Numerische Methoden für PDEs in Finanzanwendungen (seminar)

Prof. Dr. Michael Griebel

University of Bonn

Summer semester 2011
- Efficient Simulation (seminar)
- Numerical Simulation – Computational Finance (practical lab)

Winter semester 2011/2012
- Particle methods and meshless discretization (practical lab)

Summer semester 2012
- Numerik (seminar)
- Numerical Simulation (post-graduate seminar)
- Numerical Simulation – Computational Fluid Dynamics (practical lab)

Prof. Dr. Martin Hofmann-Apitius

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

Summer semester 2011
- Life Science Knowledge Discovery (lecture and exercise)
- Computational Systems Biology (seminar)
- Current Trends in Applied Life Science Informatics (seminar)
- In Silico Experimentation Using E-Labs (lab course)
- Scientific Programming in JAVA (lab course)
- Jamboree "Knowledge Engineering" (seminar)

Winter semester 2011/2012
- Biological Data Bases (lecture/exercise)
- Current Trends in Applied Life Science Informatics (seminar)
- Grid Computing (seminar)
- LSI Software Practical (lab course)
- Knowledge Discovery Technologies (seminar)

Summer semester 2012
- Life Science Knowledge Discovery (lecture)
- Computational Systems Biology (seminar)
- Current Trends in Applied Life Science Informatics (seminar)
- Jamboree "Knowledge Engineering" (lab course)
- Industrial Systems Biology (tutorial)
- In Silico Experimentation Using E-Labs (lab course)

LEFT *Prof. Dr. Michael Griebel lecturing at the University of Bonn.*

Dr. Roman Klinger

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

Summer semester 2011 and 2012
- Life Science Knowledge Discovery (lecture)

Winter semester 2011/2012
- Knowledge Discovery Technologies (seminar)

Dipl.-Math. Jiri Kraus

Bonn-Rhein-Sieg University of Applied Sciences

Summer semester 2011
- Mathematik für Maschinenbau I u. II (practical lab)

Winter semester 2011/2012
- Ingenieurinformatik (practical lab)

Dr. Dirk Reith

Bonn-Rhein-Sieg University of Applied Sciences

Summer semester 2011
- Modellbildung und Simulation I (lecture)

Winter semester 2011/2012
- Mathematik für Ingenieure I (lecture)

Summer semester 2012
- Mathematik für Ingenieure II (lecture)

Dr. Philipp Senger

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

Summer semester 2011 and 2012
- Analysis of Microarray Data with Methods from Machine Learning and Network Theory (lab course)

Winter semester 2011/2012
- Knowledge Discovery Technologies (seminar)

Prof. Dr. Ulrich Trottenberg

University of Cologne

Summer semester 2011
- Numerical Mathematics I (lecture and practical lab)
- Practical Algorithms for Instruction (seminar for teachers at grammar and comprehensive schools)
- Numerical and Applied Mathematics (graduate class)

Winter semester 2011/2012
- Practical Algorithms for Instruction (seminar for teachers at grammar and comprehensive schools)
- Numerical and Applied Mathematics (graduate class)
- Postgraduate Seminar

Summer semester 2012
- Practical Algorithms for Instruction (seminar for teachers at grammar and comprehensive schools:)

Dr. Marc Zimmermann

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

Winter semester 2011/2012
- Open Pharmacological Space Semantic Technologies for Chemical Information (seminar and lab course)

HOW TO REACH US

By car

Destination entry for car navigation systems:
Destination: Sankt Augustin
Street: Konrad-Adenauer-Strasse

The access road leading to Fraunhofer SCAI is located between Sankt Augustin-Hangelar and Bonn-Hoholz. Travelling on the A 59 motorway, take the exit "Bonn Vilich/Pützchen (41)" or, travelling from the south, the exit "Pützchen (41)".

Follow route B 56 in the direction of Sankt Augustin and Siegburg. In Sankt Augustin-Hangelar at the traffic lights, follow the road signs to Schloss Birlinghoven and Bonn-Hoholz, turning right into Konrad-Adenauer-Straße. Follow Konrad-Adenauer-Straße for approx. 3 km. The entrance to the Institute Center Birlinghoven is on the left hand side of the street.

Traveling on the A 3 motorway, drive up to the interchange "Bonn/Siegburg". Change to the A 560 motorway to "Bonn/Siegburg" and leave at the exit "Sankt Augustin (3)". Follow route B 56 in the direction of Bonn. In Sankt Augustin-Hangelar at the traffic lights, follow the road signs to Schloss Birlinghoven and Bonn-Hoholz, turning left onto Konrad-Adenauer-Straße. Follow Konrad-Adenauer-Straße for approx. 3 km. The entrance to the Institute Center Birlinghoven is on the left hand side of the street.

By plane

From Cologne/Bonn airport take a taxi to "Schloss Birlinghoven". The 25 km ride takes about 20 minutes. Alternatively take bus SB 60 to Bonn central railway station (the bus leaves every 30 minutes during daytime, the bus ride takes about 30 minutes). From Bonn central railway station: see above.

By train, bus or taxi

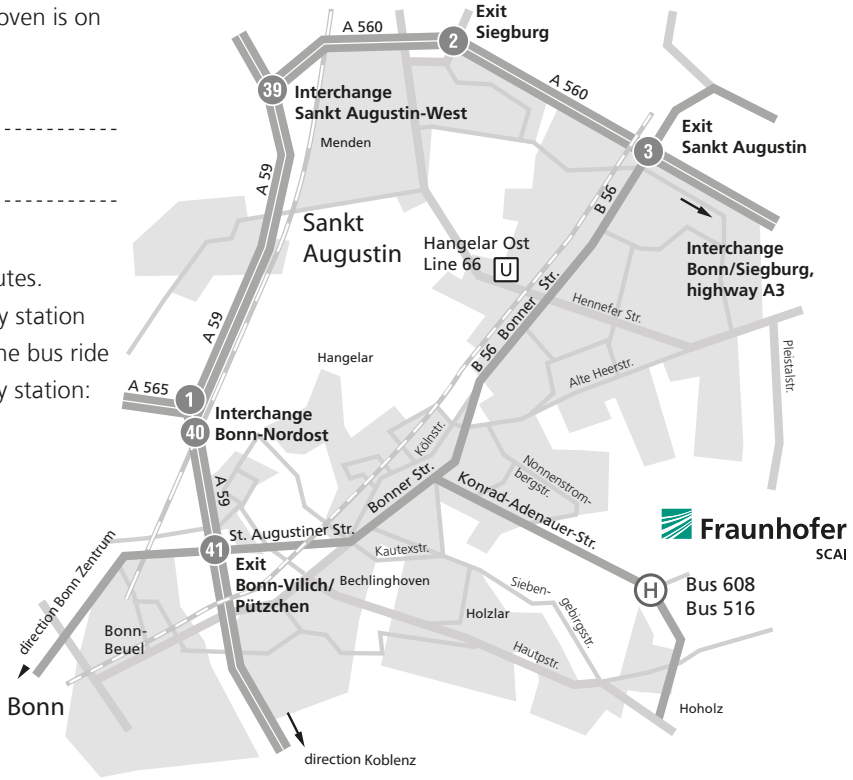
Arriving at Bonn central railway station (Bonn HBF), bus line 608 leaves every 20 minutes at ZOB B3 (departure position B3 of the central bus station) to Fraunhofer Schloss Birlinghoven. The ride by bus takes about 40 minutes.*

By taxi, the ride takes about 20 minutes.

Arriving at Siegburg/Bonn railway station (ICE-Bahnhof Siegburg/Bonn), the tram (line 66, direction Bonn) runs every 10 minutes. Exit at stop Hangelar Ost. From here, a connection bus (line 516) runs to Schloss Birlinghoven approx. every 30 minutes.*

By taxi, the ride takes about 15 minutes from Siegburg/Bonn station to Schloss Birlinghoven.

* Since changes to the bus routes are expected from December 2012 on, please check www.bahn.com (Destination: "Schloss Birlinghoven")



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