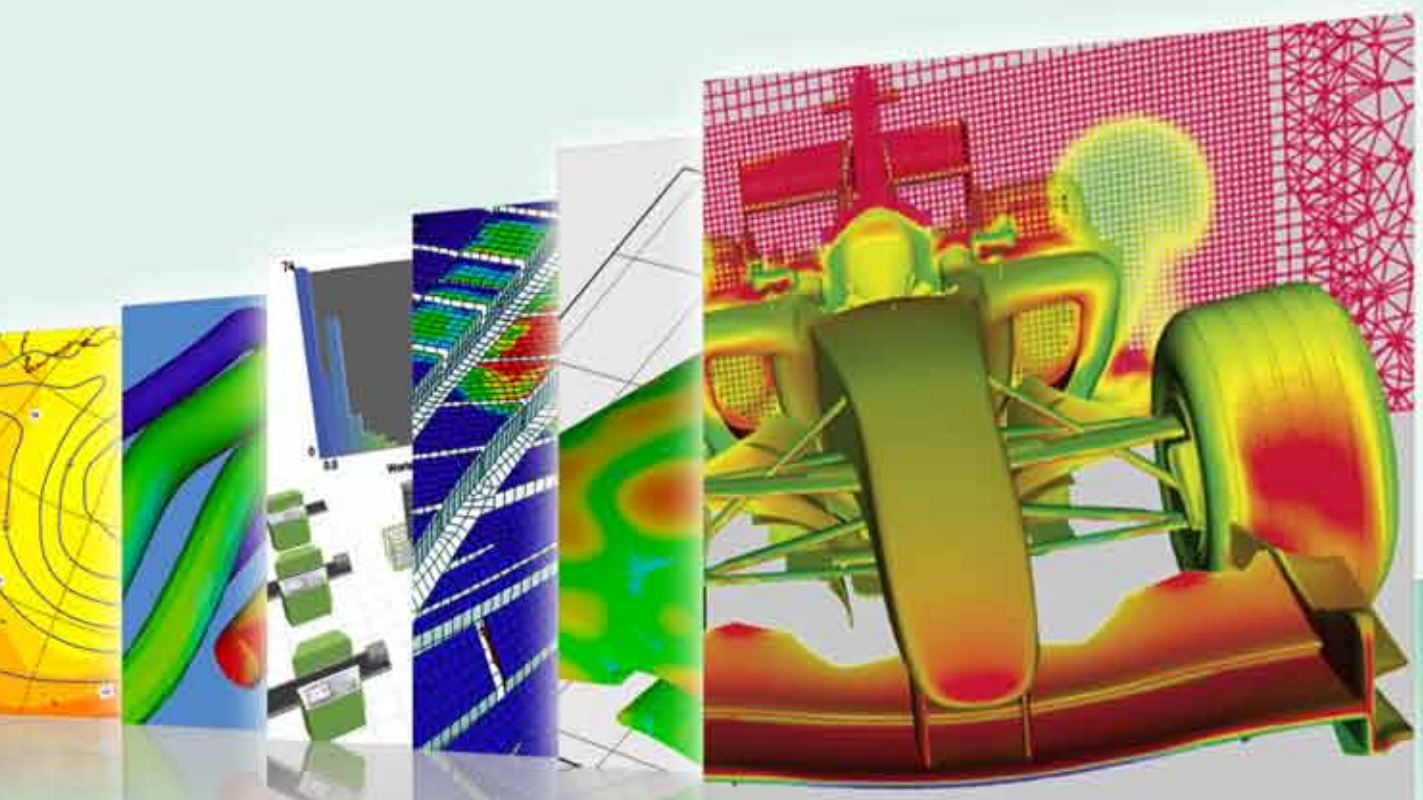
Fraunhofer
SCAI

FRAUNHOFER INSTITUTE FOR ALGORITHMS AND SCIENTIFIC COMPUTING SCAI



ANNUAL REPORT
2008 | 2009

ANNUAL REPORT
2008 | 2009

WELCOME TO FRAUNHOFER SCAI

In 2008, the Fraunhofer Institute for Algorithms and Scientific Computing SCAI had its best economical year since becoming a member of the Fraunhofer-Gesellschaft. This success confirms our long-term strategy to develop innovative mathematical software products for the scientific and technical computing market. Our international customers, mostly industrial companies, continue to rely on SCAI as proven supplier of leading-edge software products for data compression, for optimal cutting and packing, for multidisciplinary coupling ("multiphysics simulations"), for large matrix solutions and for text and image mining. In order to enhance our market outreach, we founded scapos AG, a software house in charge of marketing and sales of the SCAI software products. Located on the Schloss Birlinghoven campus, scapos will further intensify the marketing activities of SCAI, and will extend its scope to other Fraunhofer Institutes in the future.

SCAI has been a partner in a variety of national and international Grid projects, specifically leading the European's flagship SIMDAT project and Germany's SESIS project. Both projects were successfully finished in 2008. SIMDAT gave spectacular results, especially for meteorological applications, while SESIS brought modern Grid-based design technology to Germany's shipbuilding industry.

Whereas Grid technology attracts interest of numerous researchers and today is being replaced by a multiplicity of concepts like service-oriented architectures and cloud computing, a really big challenge is the unsolved problem of bringing real applications to the upcoming many-core computers with millions of processors (cores). Towards this goal, SCAI has formed strategic partnerships with the German Aerospace Center (DLR), Forschungszentrum Jülich (FZJ), Deutscher Wetterdienst (DWD), Microsoft and other industrial partners.

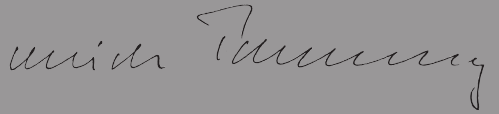
Prof. Dr. Ulrich Trottenberg,
Director of the Fraunhofer
Institute SCAI

The institute's great success was highlighted by the visit of Horst Köhler, Germany's Federal President, and his wife Eva Luise Köhler in August 2008. Apart from the Arithmeum in Bonn, SCAI was the only mathematical institute in Germany honoured by a Presidential visit during the „Year of Mathematics 2008".

The impact of mathematics and its applications is drastically increasing in nearly all areas of society. This is why Germany's Federal Ministry of Education and Research declared 2008 as the "Year of Mathematics" in Germany. Its main goal was to bring a new, fresh, and multi-faceted image of mathematics to the general public, and in particular to the youth. In this context, Fraunhofer SCAI played an active role. Exemplifying this was our science show „Manege der Innovationen," performed at our Sankt Augustin campus, and our exhibition on the science ship „MS Wissenschaft," which captured the fascination of thousands of young people. SCAI also organized, in collaboration with the Fraunhofer Institute ITWM and through Federal Ministry of Education and Research funding, the "Mathematik in der Praxis" congress that took place in Berlin during March 2009. This event attracted approximately 500 experts from science, education, politics and the public, including many students. The congress brought into focus mathematics' key role in innovation, while new ways of mathematical education, based on numerical simulation and algorithms, were highlighted.

SCAI's engagement in education and teaching also becomes visible through its strong links to the universities of Cologne and Bonn: Currently, SCAI supports more than 50 Ph. D. and graduate students in the pursuit of their theses.

You are cordially invited to learn more about our research, our products and services. Please do not hesitate to contact us concerning any questions or comments that you may have.



Prof. Dr. Ulrich Trottenberg

CONTENTS

Welcome to Fraunhofer SCAI

Profile

8 Profile, Advisory Board, facts and figures

12 SCAILights 2008 I 2009

16 Project highlights 2008

17 Selected products

Simulation Engineering

19 Computer simulations for better technologies

20 MpCCI 4.0 – A new level of multiphysics code coupling

22 Meeting the multi-core challenge

23 Cooperative Grid solutions for industry

24 Efficient ways for virtual material and drug design

25 "Grow" creates new molecular models

Numerical Software

27 Fast methods and software for simulations

28 New applications in the airplane industry

29 Simulation results best compressed with FEMZIP

30 Robust Design-parameter studies and optimization

31 Efficient statistical analysis of process chains

CONTENTS

Bioinformatics

33 Information extraction for Life Sciences

34 Chemical information retrieval from literature

35 Organising digital information

36 Knowledge discovery and semantic search

37 Software licenses as Grid services

Optimization

39 Optimizing production, planning and logistics

40 Perfect packing with PackAssistant

41 Simulating material flow for optimal processes

Alliances

43 Regional academic partnership

44 Fraunhofer Information and Communication Technology Group

45 Fraunhofer Transport and Traffic Alliance

45 Fraunhofer Numerical Simulation of Products and Processes Alliance

46 Fraunhofer-Gesellschaft

Annex

47 Selected publications

52 How to reach us

54 Editorial notes and contact

PROFILE

The Fraunhofer Institute for Algorithms and Scientific Computing SCAI focuses on applied research in numerical simulation, optimization and bioinformatics. Due to its innovative computer simulations in product and process development, SCAI is a significant partner of international industry. The institute designs and optimizes industrial applications and conducts calculations on high-performance computers in order to decrease development times, reduce the costs of experiments and improve technical products. The Department of Bioinformatics implements IT solutions for information extraction in life sciences and chemoinformatics.

Scientists from the disciplines of mathematics, informatics, engineering, physics, biology and chemistry work together in interdisciplinary teams to develop software products and services based on modern methods from applied mathematics and information technology.

Organigram

Director	Prof. Dr. Ulrich Trottenberg	+49 2241 14-2760
Deputy director	Dr. Johannes Linden	+49 2241 14-2910
Research departments		
Simulation Engineering	Dr. Johannes Linden	+49 2241 14-2910
Numerical Software	Clemens-August Thole	+49 2241 14-2739
Bioinformatics	Prof. Dr. Martin Hofmann-Apitius	+49 2241 14-2802
Optimization	Dr. Ralf Heckmann	+49 2241 14-2810
Branch Lab Cologne		
Department Numerical Software	Clemens-August Thole	+49 221 470-6082
Central services		
Planning and Controlling	Carl Vogt	+49 2241 14-2692
Marketing and Communications	Michael Krapp	+49 2241 14-2935
IT-Infrastructure	Horst Schwichtenberg	+49 2241 14-2577

1

ADVISORY BOARD

The Advisory Board provides support both to the Fraunhofer-Gesellschaft and to SCAI. The board members share their contacts in the field of industry and science with the institute.

- Professor Dr. Dr. h.c. Norbert Szyperski
  InterScience GmbH, University of Cologne
  Chairman
- Dr. Bernd Thomas
  Continental AG
  Vice Chairman
- Touraj Gholami
  BMW AG
- Dr. Daniel Keesman
  tailormade brand consulting
- Professor Dr. Dr. h.c. Tassilo Küpper
  University of Cologne
- Professor Dr. Thomas Lengauer, Ph.D.
  Max-Planck-Institute for Informatics, Saarbrücken
- Dr. Claus Axel Müller
  T-Systems, Solutions for Research GmbH

SPIN-OFF

In 2009, Fraunhofer has launched the scapos AG at the Schloss Birlinghoven campus. scapos AG is distribution partner for the SCAI products and will offer its services to further Fraunhofer institutes as well.

- Karl Solchenbach
  Chief Executive Officer
- Prof. Dr. Ulrich Trottenberg
  Fraunhofer SCAI
  Chairman of the Supervisory Board
- Professor Dr. Dr. h.c. Norbert Szyperski
  InterScience GmbH, University of Cologne
  Vice Chairman of the Supervisory Board

scapos AG
Schloss Birlinghoven
53754 Sankt Augustin
Germany

Phone +49 2241 14-2820
Fax +49 2241 14-2817

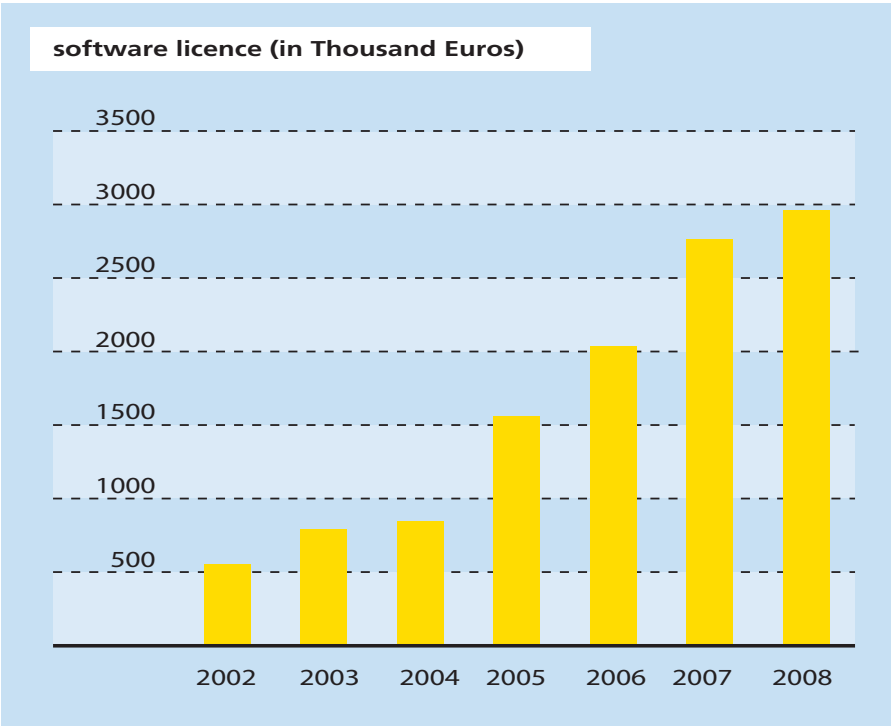
info@scapos.com
www.scapos.com

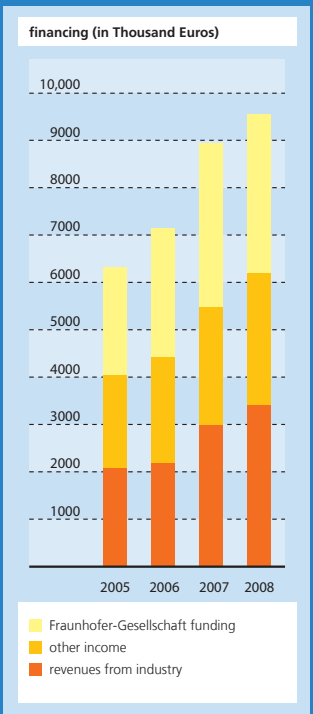
1 *Areal photography of the Schloss Birlinghoven campus.*

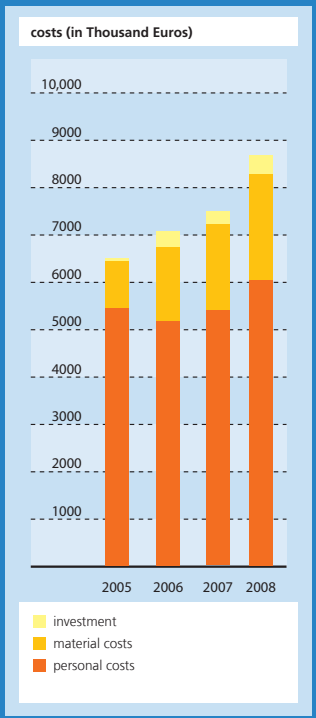
FINANCING, COSTS AND HUMAN RESOURCES

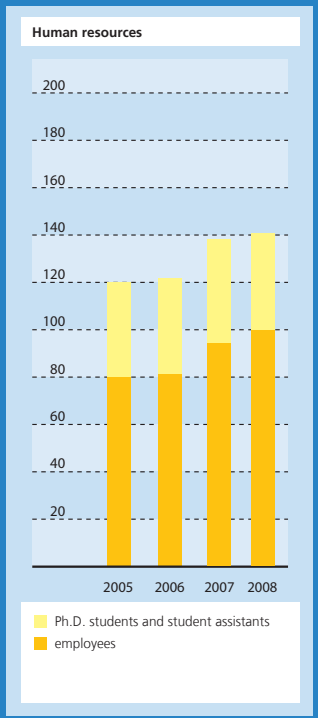
Software Sales

The Fraunhofer Institute SCAI looks back on a successful financial year 2008 with considerable growth rates. From 2005 to 2008 the revenues from software licenses have nearly doubled and now add up to almost €3 million. These substantial revenues represent one third of the overall budget of the institute. With the foundation of the marketing and sales company scapos AG, SCAI expands its leading position in software sales within Fraunhofer. Presumably , the year 2009 will not be as successful as 2008. The half-year results reflect the worldwide financial and economic crisis.









Financing and Costs

In 2008, the revenues from industry increased to €3.4 million – the highest value in the institute's history. The overall capital budget of Fraunhofer SCAI amounted to €9.6 million. The operating expenditure amounted to €8.8 million. This is why the institute was again able to increase its financial reserves in order to invest in innovations and to alleviate a possible drop in industrial revenues due to the worldwide financial and economic crisis in 2009.

At about 70 percent, personnel expenses are the institute's main cost factor. SCAI invested €400,000 in new IT infrastructure dedicated to offering new customer services in the institute's different business areas.

Human resources

At the end of 2008, the institute's staff consisted of 140 employees, including ten Ph.D. students as well as 30 graduate students and student assistants. Noticeably, the number of student assistants has increased due to the institute's close academic relationships with the University of Cologne and the Bonn-Aachen International Center for Information Technology (B-IT) in Bonn. Furthermore, the institute trained four apprentices as IT specialists and one as a media designer.

SCAILIGHTS 2008 | 2009

Closing event of the year of mathematics in Cologne

Horst Köhler and Eva Luise Köhler with Ulrich Trottenberg

2008

Year of Mathematics in Germany

In 2008, mathematics, as academic discipline and educational subject, has been in the public spotlight in Germany. The Year of Mathematics aimed at polishing the image of this discipline in public and particularly in the youth. With various events and science shows, Fraunhofer SCAI helped advance the role of applied mathematics in school education and teacher training.

May 2008

Federal President Horst Köhler fascinated by SCAI's research results

The German Federal President Horst Köhler visited our institute in May 2008. SCAI researchers presented current examples of their work to Köhler, who expressed enthusiasm about the possibilities and perspectives of applied mathematics. The president lauded the institute's innovative operations and pointed out that Fraunhofer SCAI researchers work on future technologies for the collective good.

June 2008

Mathematics and technology on stage!

In the context of the nationwide technology day (Tag der Technik), the Fraunhofer Center Schloss Birlinghoven put on the "Manege der Innovationen" science show. For this day, the terrain around Schloss Birlinghoven was transformed into a colourful circus fairground of science. About 600 students in school and teachers attended the mathematics show. Researchers presented examples of their work and invited children to participate.

July 2008

Discovering science in Bonn

Amazing events in the summer of 2008 made it possible, especially for young people, to experience and explore fascinating mathematical phenomena. Fraunhofer SCAI showed impressive exhibits on the science ship "MS Wissenschaft". In addition, Fraunhofer put on the mathematics show "Manege der Innovationen" at the "Bonner Wissenschaftsnacht". Visitors came to see attractions such as the interactive exhibit "PackAssistant" in a mathematics tent called "Kopf oder Zahl".

Helge Haas, moderator of the show, explains a game

The science-ship "MS Wissenschaft" made a stopover in Bonn

Karl Solchenbach, scapos AG


Congress "mathematics in practice" in Berlin

January 2009

Formation of scapos AG

The software solutions produced by Fraunhofer SCAI are applied by companies all over the world. In order to strengthen sales of its software products, Fraunhofer SCAI founded the company scapos AG. The CEO of scapos is Karl Solchenbach, former Director for Cluster Computing at Intel Corporation. Fraunhofer is a shareholder of scapos AG.

March 2009

Creating the future – applied mathematics

The "mathematics in practice" congress in Berlin delivered insights into the field of applied mathematics and fostered a dialogue about prospects for mathematical knowledge transfer at school and at university. The agenda included lectures and discussions by experts in economics, science and politics, as well as workshops and an exhibition. The event was arranged by the institutes SCAI and ITWM, with funding from the German Federal Ministry of Education and Research.

April 2009

Girls discover research at Fraunhofer

Writing coded electronic messages, dissecting computers, separating genes in food – as part of the nationwide Girls' Day, the Fraunhofer Center invited more than 80 girls to Schloss Birlinghoven to give them an insight into research at Fraunhofer. A multifaceted programme around informatics, digital environments and mathematics fascinated the young ladies and showed the prospects for girls in mathematics and information technology.

May 2009

60 years of Fraunhofer research: Truck on tour

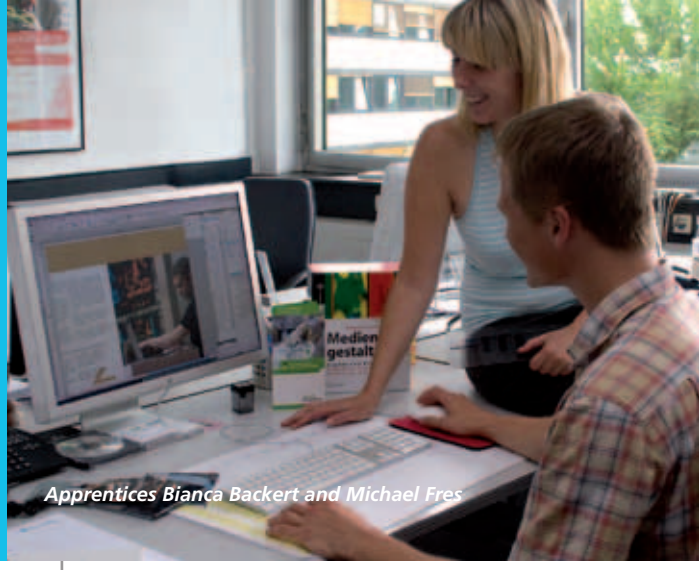
On the occasion of the 60th anniversary of the Fraunhofer-Gesellschaft, an amazing science truck is on tour all around Germany, including a stopover in Bonn. The truck presents selected innovations in the fields of health, environment, energy, security, communication and mobility. In Bonn, the truck also showed the interactive exhibit of SCAI's software "PackAssistant".

Scientist Stefan Rank explains optimization methods


Fraunhofer-Truck shows innovative technologies

Prof. Ulrich Trottenberg


Prof. Carl Adam Petri


Apprentices Bianca Backert and Michael Fres

May 2009

Mathematics open air

Following the motto "mathematics for everybody", Prof. Dr. Ulrich Trottenberg gave a public lecture on applied mathematics in Bonn. Trottenberg showed examples of mathematical algorithms and applications in our everyday life and advocated new teaching methods in mathematics.

2008/2009

SCAI engages in young people's apprenticeship

Fraunhofer SCAI is involved in the professional education of IT specialists and media designers. Furthermore, the institute supports the integrated degree programme in business administration, initiated by the Fraunhofer Center Schloss Birlinghoven and the University of Applied Sciences Bonn-Rhein-Sieg.

2009

Petri honoured with "Computer Pioneer Award"

The world-renowned creator of the Petri net theory and former director of today's Fraunhofer Institute SCAI, Prof. Dr. Carl Adam Petri, was honoured with the 2008 Computer Pioneer Award of the Institute of Electrical and Electronic Engineers (IEEE) in the USA.

2008/2009

SCAI research in dialogue

In order to maintain close relationships with its customers, SCAI regularly arranges symposia and networking meetings. Examples include the yearly MpCCI User Forum and the Fraunhofer Symposium on Text Mining in Life Sciences. Both events are well established in their communities and attract the leading experts in their disciplines.

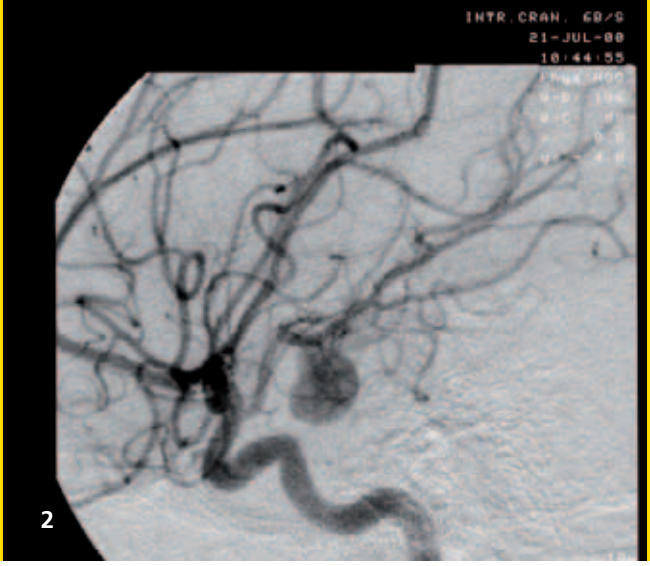
2008/2009

Fraunhofer SCAI presents its solutions at worldwide exhibitions

SCAI continuously presents its innovative products and services at well-established exhibitions and congresses, such as the Hannover Messe, "transport logistic" in Munich and the International Supercomputing Conference in Hamburg.


Outlook on new simulation techniques at the MpCCI User Forum

SCAI fair stand at the "transport logistic" in Munich



PROJECT HIGHLIGHTS 2008

SCAI completes project SIMDAT with great success

Since its launch in 2004, the project Data Grids for Process and Product Development (SIMDAT) has successfully installed Grids in various industrial prototypes in the aerospace, automotive, pharmacology and meteorology sectors. SIMDAT helped to improve collaborative design processes and to increase the competitive advantage in strategic European industrial sectors. The results achieved include the improvement of car safety, low-noise aircraft able to use short runways, faster and targeted drug discovery, and especially the development and enhancement of weather prediction and climate analysis. SIMDAT received 11 million Euro from the European Commission for four years of funding. The project was coordinated by Fraunhofer SCAI.

www.simdat.eu

@neurIST may save patients' lifes

The current process of cerebral aneurysm diagnosis, treatment planning and treatment development is often compromised by the fragmentation of relevant data. The project @neurist, funded by the European Commission, will benefit patients with better diagnostics, prevention and treatment. The SCAI Department of Bioinformatics has developed a disease-specific database harbouring relevant knowledge on genes involved in diseases. Together with partners at the IMIM institute in Barcelona, SCAI has aggregated information on disease-specific genes, their allelic variation and their function as drug targets.

www.aneurist.org

IT Innovation for the ship design process

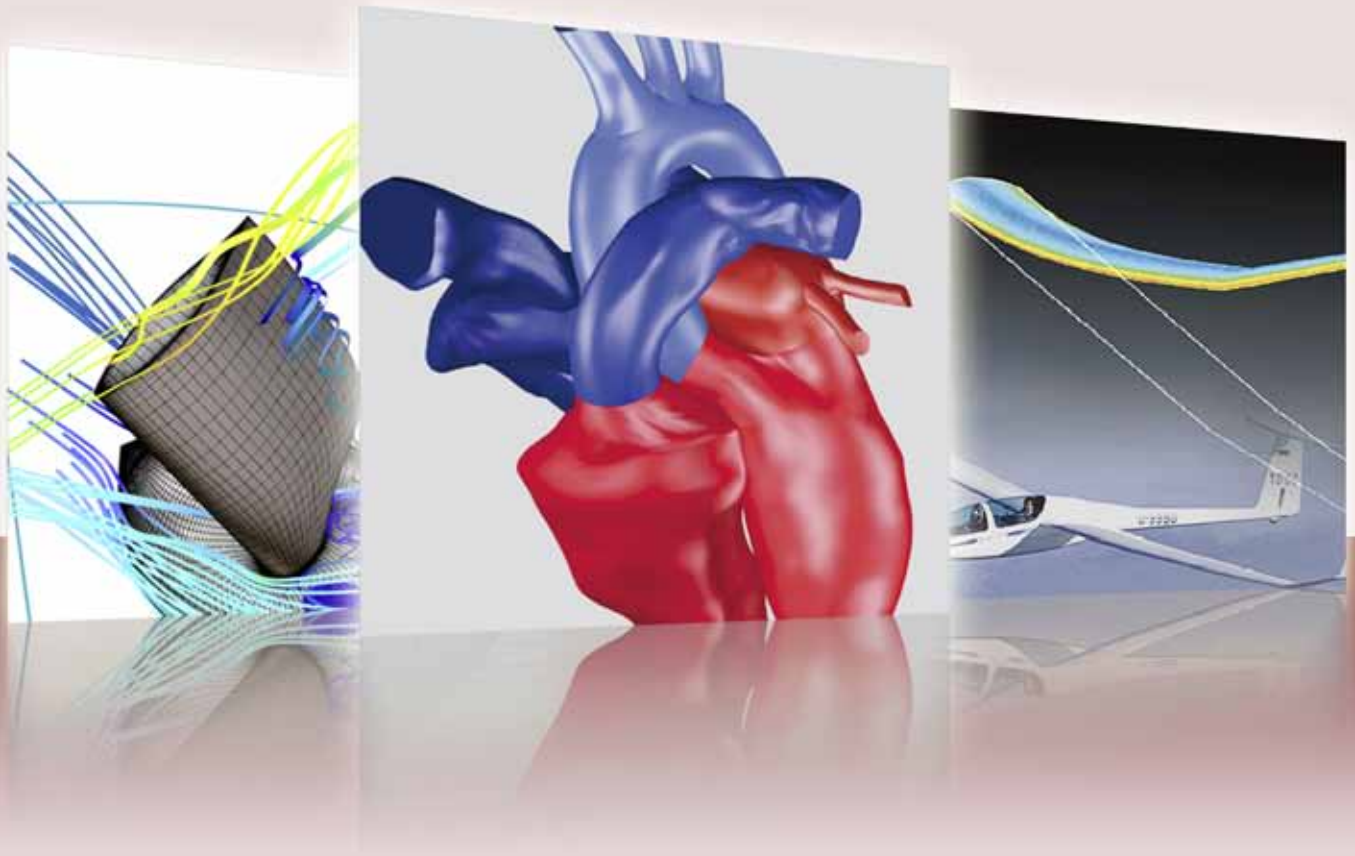
Building a new ship is a highly cooperative process. In the early design phase, where all important parameters of the ship are fixed, a close cooperation between ship yards, their suppliers and consultants is needed. To support them, the innovative Ship Design and Simulation System (SESIS) was jointly developed by a consortium of partners from ship building industries and IT experts. A further result is the development of the software platform Remote Component Environment (RCE). The project, coordinated by Fraunhofer SCAI, started in May 2005 and was funded by the German Federal Ministry of Economics and Technology. SESIS was successfully completed in December 2008.

www.sesis.de

1 *Meteorologists benefit from Grid Computing and achieve more detailed weather forecasts.*
2 *Angiograph of an aneurysm in a cerebral artery.*
3 *SESIS supports the design process for modern ships.*

	Product	Description	Contact
MpCCI	MpCCI	Software for multiphysics simulations. With MpCCI all major CAE codes can be coupled to simulate complex multiphysics phenomena like fluid-structure interaction.	Klaus Wolf +49 2241 14-2557
SAMG	SAMG	Library of subroutines for the highly efficient solution of large linear systems with sparse matrices.	Dr. Klaus Stüben +49 2241 14-2749
FEMZIP	FEMZIP	Tool to compress simulation data for crash and NVH simulations with LS-DYNA, PAM-CRASH and MSC Nastran. Compression rates of up to 10 times can be achieved without significant loss of accuracy.	Clemens-August Thole +49 2241 14-2739
DIFFCrash	DIFF-CRASH	Tool for stability analysis of crash simulations in the automotive industry.	Dr. Tanja Clees +49 2241 14-2983
DesParO	DesParO	System for multiobjective optimization, providing users with control of optimization processes.	Dr. Tanja Clees +49 2241 14-2983
chemoCR	chemoCR	Tool for extracting and reconstructing chemical structural formulas and their chemical structure depictions from scientific literature and patents.	Dr. Marc Zimmermann +49 2241 14-2276
ProMiner	ProMiner	Mining tool for the identification of gene and protein names in huge numbers of scientific publications.	Dr. Juliane Fluck +49 2241 14-2188
AUTO NESTER-T	AutoNester-T and AutoNester-L	Software package for optimized nesting and cutting on fabrics, leather, sheet metal or wood, minimizing material waste.	Dr. Ralf Heckmann +49 2241 14-2810
CUT PLANNER	CUTPLANNER	Software package for use in the textile manufacturing industry for automatic cut order planning.	Dr. Ralf Heckmann +49 2241 14-2810
PACK Assistant	PackAssistant	Software toolbox for optimized packing of complex parts in boxes and containers. The new version includes simulation of bulk goods.	Stefan Rank +49 2241 14-1503
LOGISTIK SIMULATION	Material Flow Simulation	Simulation and analysis of production and material logistics, combined with leading optimization technologies and tools. This service is tailored individually to the customers' needs.	Lydia Franck +49 2241 14-2563
scapos		All SCAI products are distributed by scapos AG.	Karl Solchenbach +49 2241 14-2820

SIMULATION ENGINEERING



COMPUTER SIMULATIONS FOR BETTER TECHNOLOGIES

Due to increasing demands on the quality of innovative products, computer simulation is becoming increasingly important for industry. It accelerates product designs and helps to optimize processes. This reduces development time, replaces "real" experiments, leads to better constructed prototypes and ultimately saves costs.

Physical modelling and numerical simulation have become indispensable in nearly all engineering and scientific disciplines. Understanding the physics of technical processes and devices enables us to design and optimize better technologies. Today in industry and science, modelling and simulations are well accepted and widely used technologies complementing theoretical and experimental work.

The Department of Simulation Engineering covers a broad range of simulation and algorithmic topics with a special focus on multiphysics and multiscale simulations.

The term multiphysics stands for simulations that combine multiple physical models or multiple physical phenomena with software originating from different fields of physical modelling. Examples are the interaction of flow simulation with structural analysis, the thermal coupling of fluid flow, solid conduction and radiation in cooling and heating processes, or the influence of electromagnetic fields on gas flows.

Our central development in this field is the coupling software MpCCI. It enables the user to directly couple different physical models and corresponding simulation codes from different fields. MpCCI delivers a complete multiphysics simulation environment based on code coupling, which includes set-up and control of simulation runs. It includes the exchange of data between simulation codes, the mapping of computational meshes, highly efficient neighbourhood searches, and the interpolation of computational quantities. MpCCI runs with most of the leading simulation codes, e.g. from flow and structural mechanics. Worldwide, it is the leading open platform for code coupling and widely used by a growing multiphysics community in industry and science.

Multiscale computing on the other hand describes the general problem of properly resolving many different length and time scales in order to accurately predict the behaviour of the simulated system. It particularly arises in molecular design problems where effects from the nano- to the micro-scale must be included. This is the focus of our Computational Chemical Engineering group, which develops algorithms and software to improve and accelerate commodity design by way of molecular simulation.

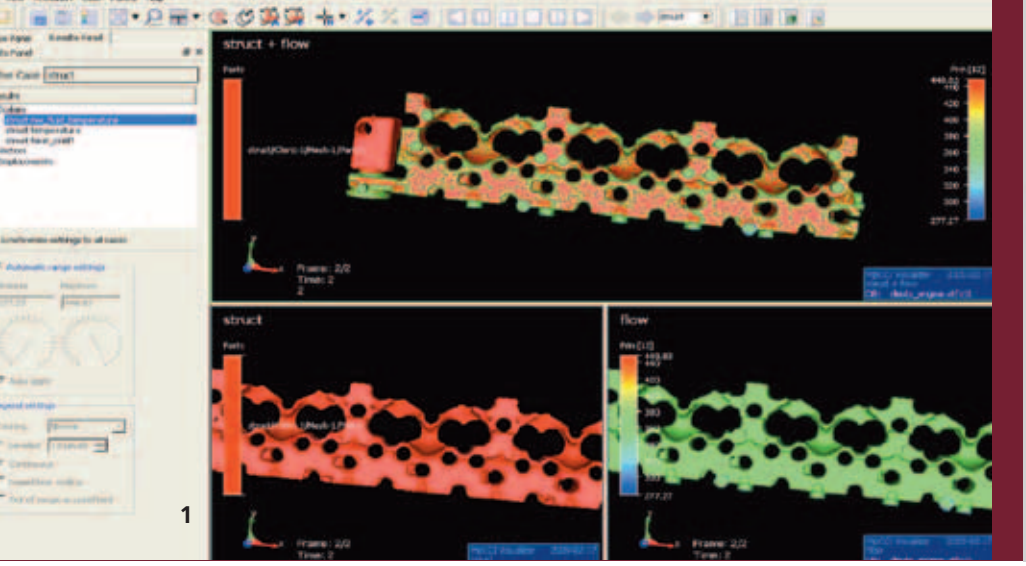
Complementary to our simulation work, we address various aspects of High Performance and Distributed Computing. Here, the emphasis is currently placed on the efficient use of "many-core" systems and heterogeneous architectures including GPUs for numerical calculations, and on Grid and Cloud techniques for integrated computing and data environments.

In all 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 modelling, computational studies and ready-to-use applications.

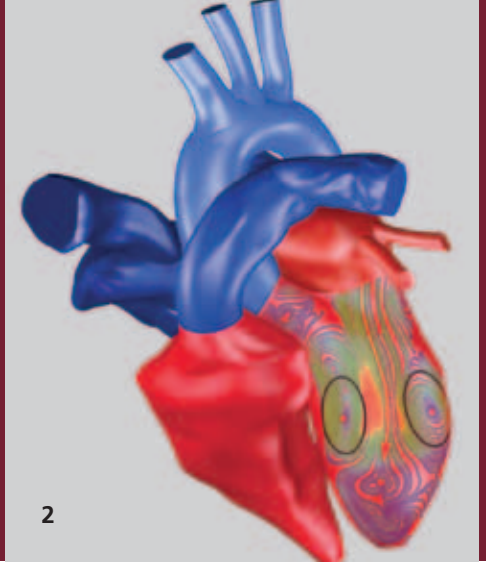
HEAD OF DEPARTMENT
Dr. Johannes Linden
Phone +49 2241 14-2910
Fax +49 2241 14-2167
johannes.linden@
scai.fraunhofer.de

DEPUTY HEADS
Dr. Anton Schüller
Phone +49 2241 14-2572
Fax +49 2241 14-2181
anton.schueller@
scai.fraunhofer.de

Dipl.-Inform. Klaus Wolf
Phone +49 2241 14-2557
Fax +49 2241 14-2181
klaus.wolf@
scai.fraunhofer.de



1



2

MPCCI 4.0 – A NEW LEVEL OF MULTIPHYSICS CODE COUPLING

MpCCI has been developed at Fraunhofer SCAI in order to provide an application independent interface for the coupling of different simulation codes. Currently, Fraunhofer SCAI´s developers release version 4.0 of the coupling software with many important new features.

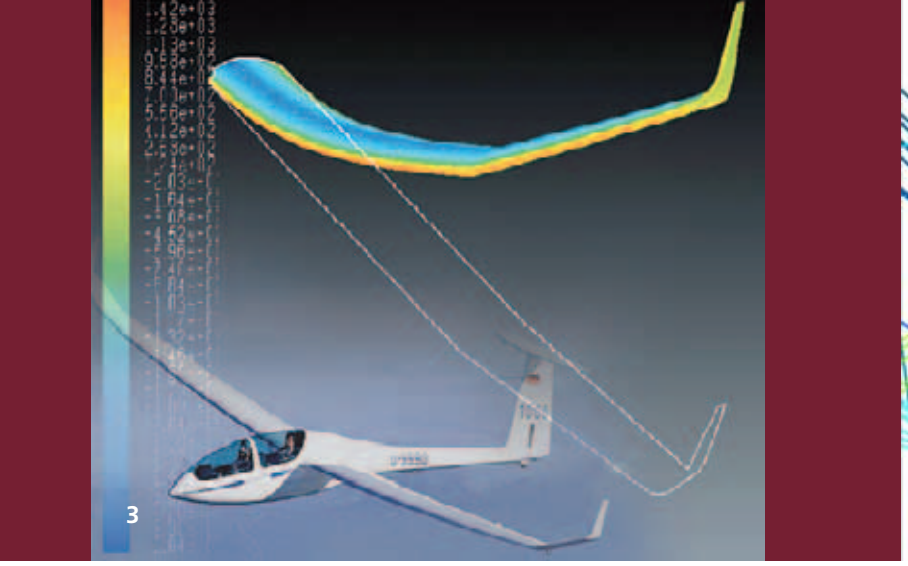
MpCCI (Mesh-based Code Coupling Interface) is a software environment that enables the direct exchange of physical quantity data between the computational models of two or more simulation codes. It performs the neighbourhood calculation of the coupled models and uses advanced interpolation methods when transferring physical data from one code to the other.

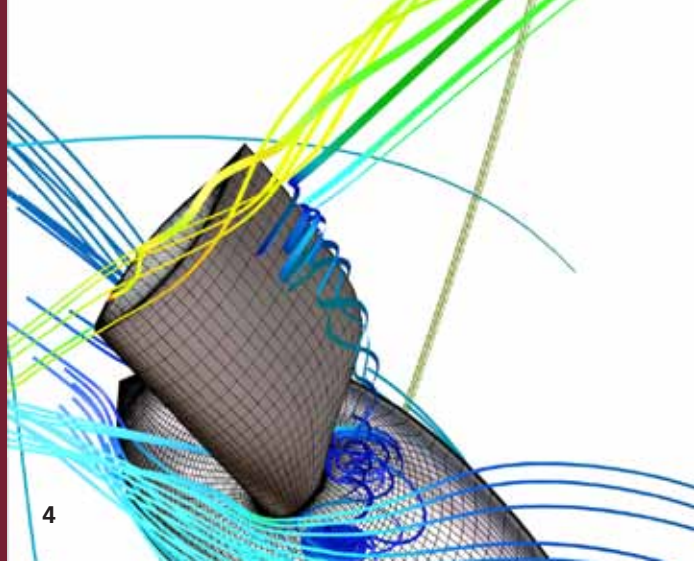
The new MpCCI version 4.0 provides a completely redesigned coupling server, which is faster and more efficient with respect to CPU and memory usage. The internal operator management allows specifying mapping workflows per coupling quantity. Predefined operators for prefiltering, neighbourhood search, post-filter actions, integration, and hole filling methods offer a flexible solution for the exchange of physical quantities in coupled applications.

The core algorithms of MpCCI for neighbourhood search and interpolation were re-implemented during 2008. The outcome was a dramatic improvement in CPU performance and memory usage. These new algorithms now support:

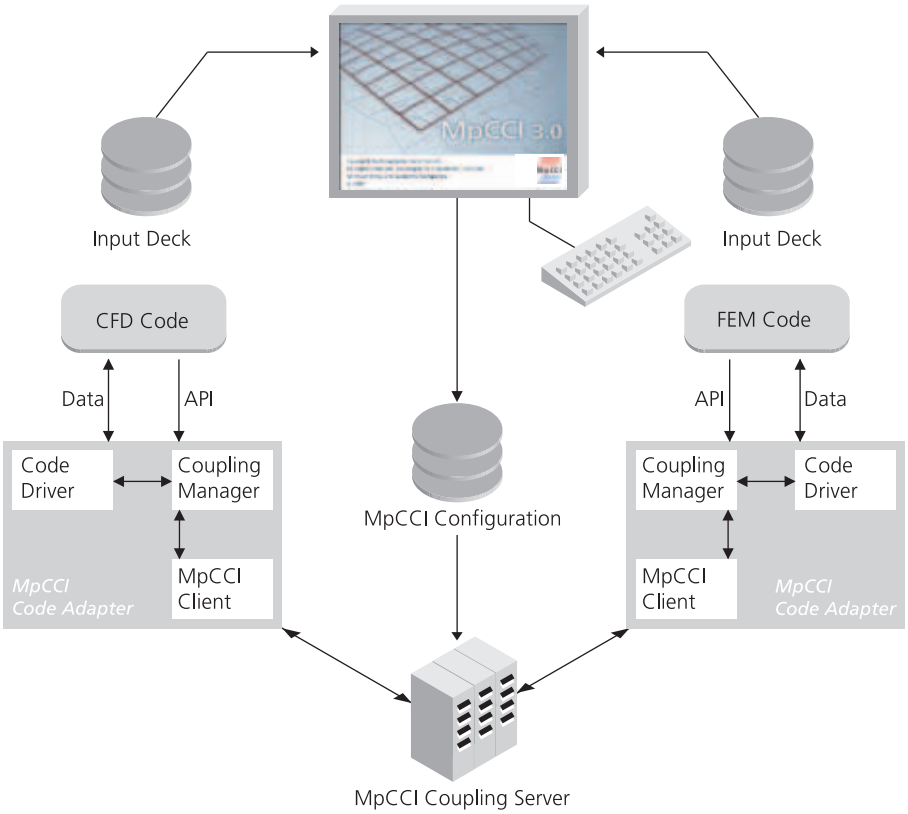
- adaptive remeshing of coupling areas
- combinations of static and moving reference-frames
- extrapolation for orphaned regions
- polygon/polyhedra meshes

The MpCCI server system offers an asynchronous communication model. The coupled codes may run asynchronously – even coupling on demand can now be realized. MpCCI provides a new visualizer, based on a third-party solution from Ceetron. It offers synchronized single and superimposed views. Online communication between simulation and visualizer through socket communication can be used to monitor even batch jobs.





During 2009, MpCCI 4.0 will support Abaqus, ANSYS, Flowmaster, FLUENT, Flux, ICEPAK, MSC.Marc, MD Nastran, Numeca FineHexa & FineTurbo, Permas, Samcef, StarCD 3 & 4, and RadTherm. Adapters for further codes like STAR-CCM are under development. There is also a strong request for combinations of commercial codes with dedicated in-house codes. This is especially true in the aerospace industry, where engineers trust their own high-end in-house tools for aerodynamics; on the other side, they use commercial FEM codes to analyse, for example, deformations and stresses in structure. Likewise, universities and research institutes have also realized their own codes either for educational purposes or for evaluating specific details in CFD or FEM.



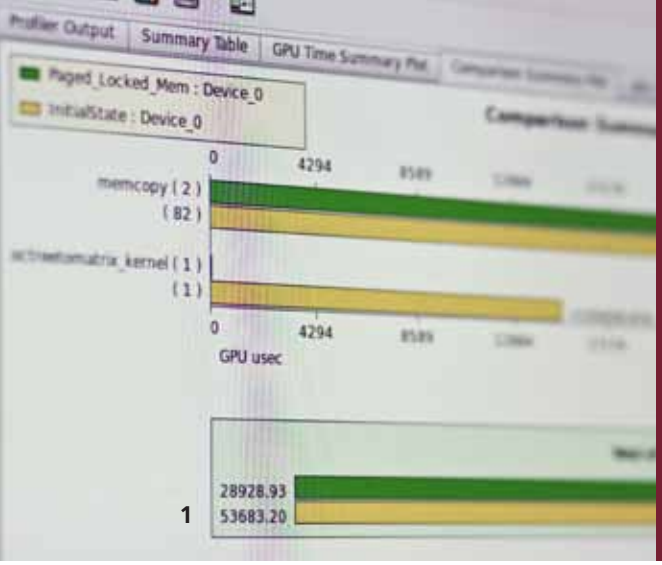
1 *The user interface of the MpCCI visualizer displays coupling processes.*

2 *By simulating cardiac bloodstream, coupled simulations with MpCCI achieve high accuracy.*

3 *MpCCI couples fluid and structure simulation programs for the design optimization of airfoils.*

4 *In this figure, streamlines around a deformed airfoil of a wind turbine are shown.*

Dipl.-Inform. Klaus Wolf
Phone +49 2241 14-2557
Fax +49 2241 14-2181
klaus.wolf@
scai.fraunhofer.de



1

2

MEETING THE MULTI-CORE CHALLENGE

Today, multi-core processors seem to be the only answer to the quest for more compute performance. Nevertheless, their architecture causes some serious problems, among them the memory bandwidth gap. SCAI researches are taking up the challenge to meet these problems and looking for solutions on the algorithmic side.

Originally, Moore's law heuristically predicts the evolution of the number of transistors on a single silicon die. Implicitly, it is being applied to describe the increase of the peak performance of processors and, since, became a self-fulfilling prophecy. Facing physical limits hardware developers struggle to double the compute power of CPUs every 18 to 24 months, as predicted by the law. Currently, multi-core CPUs seem to be the only viable solution. They comprise a set of classical CPU cores all embedded in a common infrastructure on the same piece of silicon. Furthermore, multi-core CPUs have a significant advantage over classical mono-core CPUs: They are more energy efficient. And when it comes to energy efficiency, other classes of processing units are currently being pursued: Graphics Processing Units (GPUs) and the Cell Broadband Engine Architecture.

It is conceivable that the trend towards CPUs offering even more compute cores than today will continue. But unfortunately, the bandwidth between cores and the main memory is not increasing in the same manner. This already now leads to significant problems with the bandwidth performance ratio. In order to overcome those kinds of problems, new algorithms are needed. Heterogeneous hardware architectures including Cell and GPUs offer interesting opportunities. Nevertheless, for achieving a benefit from these architectures, task/thread scheduling and memory access patterns have to be trimmed for extreme efficiency.

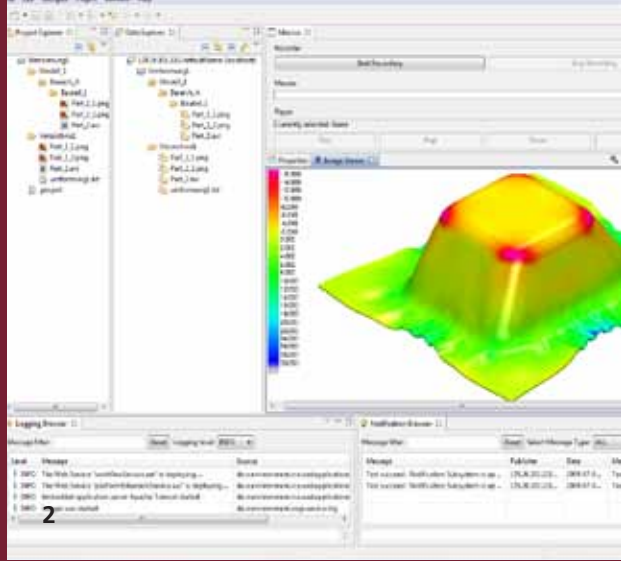
Fraunhofer SCAI focuses on the integration of heterogeneous architectures into high performance computing, ranging from the desk-side supercomputer towards Peta-scale facilities. Towards the Peta-FLOPS end, SCAI works, for example, with the leading stakeholders in the field of weather and climate research. Companies benefit from SCAI's expertise at cluster and desk-side level.

Moreover, SCAI researchers collaborate with partner institutes, funded by the Fraunhofer MAVO programme (Marktorientierte Strategische Vorlaufforschung), on developing tools and finding solutions to given problems.

1 *SCAI researchers always seek for the best solution when optimizing algorithms and applications on various hardware architectures.*
2 *With Deskside Supercomputers and compact clusters, the SCAI HPC group solves individual problems. Even small companies can directly benefit from high performance computing.*

Dr. Thomas Soddemann
Phone +49 2241 14-3414
Fax +49 2241 14-4-3414
thomas.soddemann@scai.fraunhofer.de

1



2

COOPERATIVE GRID SOLUTIONS FOR INDUSTRY

Industrial design and production processes are increasingly based on division of labour. Instead of completely covering the value chain, enterprises concentrate on their core competences and purchase goods and services from specialized third-party companies.

In the case of PartnerGrid, a distributed IT platform has been developed to support these collaboration processes in a very efficient way. Its core technology is based on the Remote Component Environment (RCE), developed by Fraunhofer SCAI in cooperation with the German Aerospace Center (DLR). RCE is a service-based software infrastructure to manage collaborative processes. It hides the complexity of heterogeneous and distributed IT systems behind common user interfaces and thereby enforces security in the access of data and services.

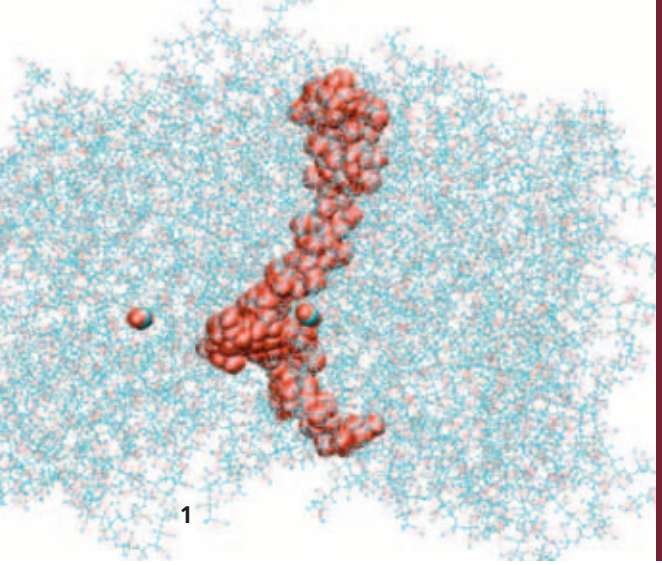
RCE serves as an integration platform to connect the software components of the distributed application scenario. A web-based portal developed by Fraunhofer IAO serves as a user interface. Pre-processing tools, simulation programs and visual postprocessors share data on the base of the RCE data management. Workflows are defined by the RCE workflow tool and are submitted for execution in a Grid environment.

The application scenario is the collaboration of metalworking suppliers in the automotive industry. Virtual design techniques and computer simulations are indispensable tools in today's product design. GNS in Braunschweig offers construction and simulation services for metal forming, mainly for car manufacturers and their suppliers. The exchange of product design and simulation results between the partners is managed by the PartnerGrid platform in an efficient and secure way. This facilitates an immediate online collaboration between customer and supplier providing an important advantage in the development of new and better customer relationships.

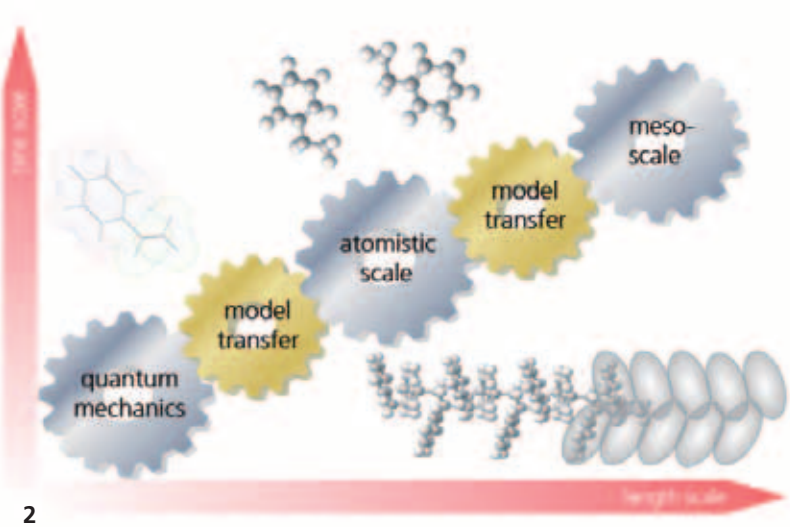
RCE is a flexible environment for managing distributed resources, which can easily be applied to various applications. SCAI offers the adaptation of RCE for specific needs in new application areas. The project is funded by the Federal Ministry of Education and Research.
More information is available at the project website www.partnergrid.de

1 *RCE has been developed in cooperation with ship building industries in the SESIS project.*
2 *The RCE user interface is integrated in a web-based portal.*

Ottmar Krämer-Fuhrmann
Phone +49 2241 14-2202
Fax +49 2241 14-2181
ottmar.kraemer-fuhrmann@scai.fraunhofer.de



1



2

EFFICIENT WAYS FOR VIRTUAL MATERIAL AND DRUG DESIGN

The development of new high-tech materials and modern medicine requires understanding the microscopic behaviour and mechanisms of chemical systems. Multiscale simulations provide important information needed for successful commodity design, linked together at different chemical resolutions and time scales.

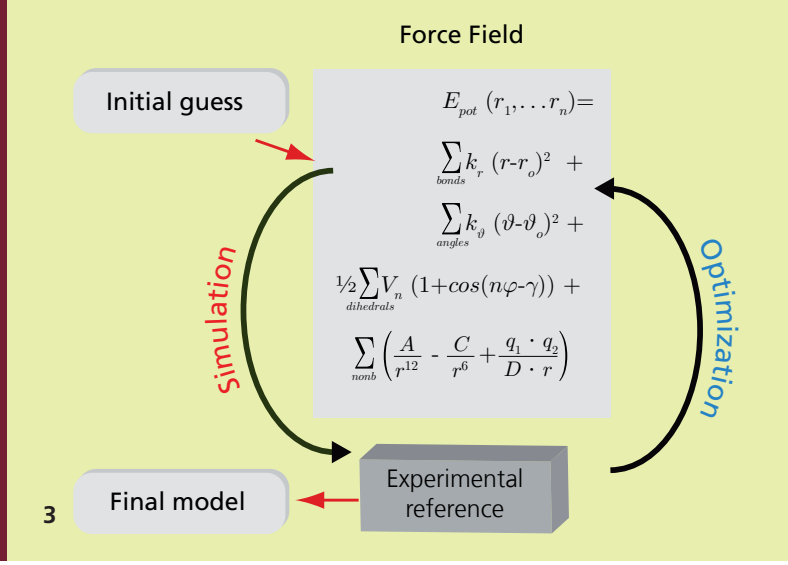
Many properties of chemical systems can be understood and rationalized by a thorough investigation of their microscopic details (e.g. molecular forces, dynamics, and structure). Molecular models, ranging from atomistic to coarse graining, are appropriate and efficient ways to investigate and obtain these microscopic details.

Atomistic simulations explicitly account for each atoms in a given system and allow the exploration of specific interactions in high resolution, such as the process of how drugs bind to receptors. This detailed treatment of a system's degrees of freedom prohibits the consideration of macroscopic properties that are dependent upon longer molecular time frames. Coarse graining approaches to the mesoscale enable researchers to access these longer time frames by creating system-specific "super atoms," each composed of several individual atoms. Approximating the chemical system via super atoms allows for more of the macrosystem to be represented; subsequently, this facilitates the investigation of large-scale motions, such as polymer entanglement.

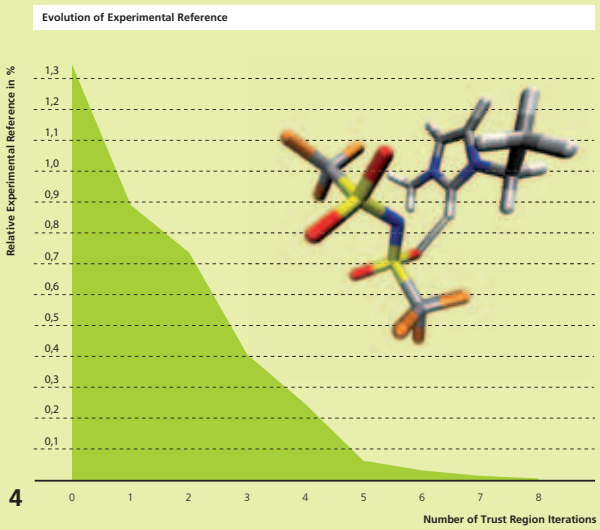
The CoChE group is developing efficient procedures for both atomistic and coarse-graining simulations, as well as creating methodologies for moving between these simulation techniques. This ultimately allows for a wide range of chemical behaviour to be well understood, which promotes designing and optimization of new commodities.

In recent years, the above methods have proven to be robust and reliable. That means, for example, experimental data can be qualitatively reproduced and new insight gained. We are currently able to derive properties for a large variety of chemical systems by means of multiscale simulations. Typical systems include organic polymers in melts or solution (e.g. polystyrene and polyacrylic acid), biochemical polymers (e.g. carbohydrates, protein, and nucleic acids), and low-molecular liquids (e.g. organic solvents and ionic liquids). We are capable of studying, to name a few, potential energy surfaces, molecular conformations, interaction energies, surface adsorption effects, system annealing and quenching, gas permeation, and the calculation of transport coefficients like thermal conductivity or shear viscosity.

This computationally gained knowledge and our long experience directly benefits industry in its desire to optimize production, steer key developments in a better direction, and design new products more cost effectively.



3



4

"GROW" CREATES NEW MOLECULAR MODELS

The Computational Chemical Engineering Group (CoChE) has developed the software GROW, which enables users to robustly generate new molecular models for all kinds of chemical substances. Organized as a modular tool kit, it is extendable for further optimization and integration into third-party simulation programs.

Molecular simulation methods, most prominently molecular dynamics (MD) and Monte-Carlo, are powerful tools to gain insight into the microscopic processes that govern the macroscopic behaviour of matter. Driven by the progressive growth of computational resources, it is forecasted that these molecular methods will increasingly become more important in the coming decades.

Key to the success of molecular simulations is the accuracy of its foundation, the force field. A force field describes the intra- and intermolecular interactions by a semi-empirical equation and its associated parameters. While the equation's functional form is usually clear, the force field parameterization is often tedious. Therefore, manual adjustment and optimization is, at best, extremely time-consuming. Hence, an automated parameterization scheme is essential in our pursuit to create tailor-made models for our customers in a timely fashion. This has been realized and implemented into a Gradient-based Optimization Workflow (GROW) for the automated development of molecular models.

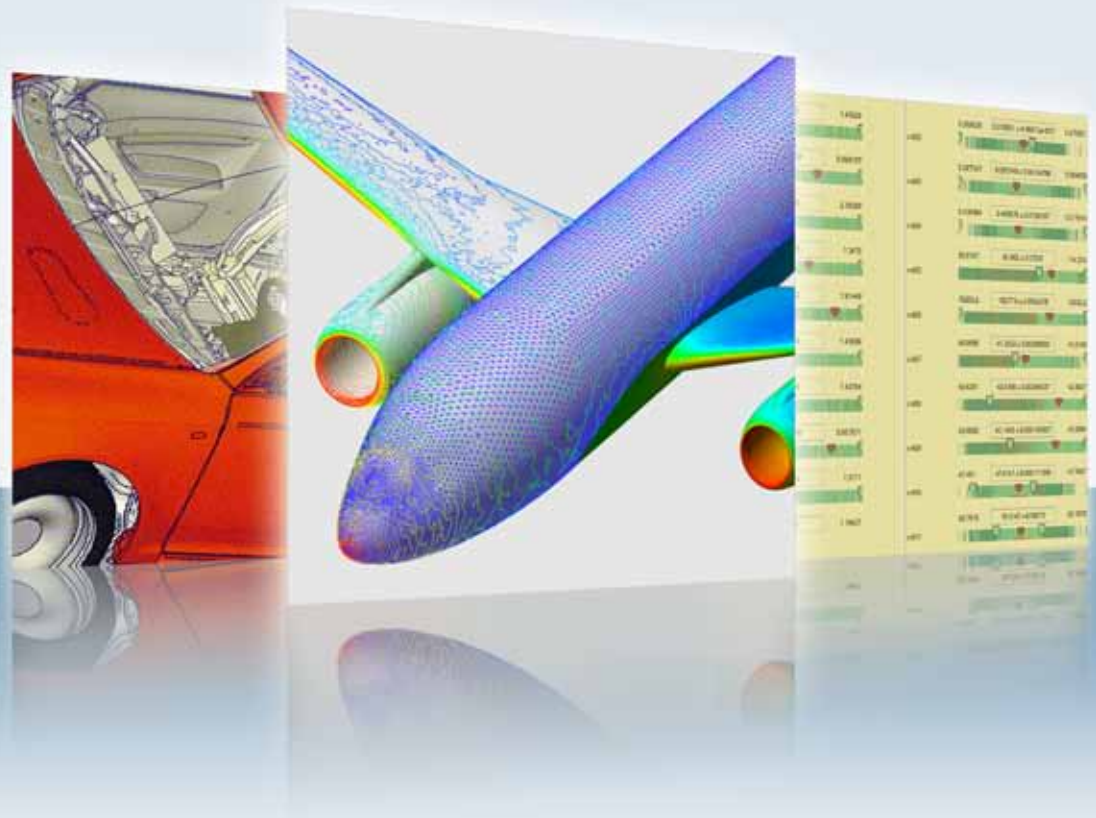
GROW is a program tool kit to facilitate the use of gradient-based numerical optimization of force field parameters. Its components include various optimization algorithms (including quasi-Newton algorithms or trust region methods), analysis scripts and I/O-handling. GROW can be "attached" to various standard MD simulation engines like GROMACS, AMBER, and ESPResSo(++), making it a powerful companion for many application fields (e.g. bio-molecules, ionic liquids, and polymers).

GROW's application in creating and optimizing reliable molecular models has proven extremely valuable in several demonstrated cases. Experimental target values, used for verification purposes only, can be typically matched within a few percent for common properties (e.g. density, thermal and electrical conductivity, diffusion and vapour pressure).

1 *Snapshot of a gas permeation simulation. Some representative molecules for each species are highlighted.*
2 *Scale-Bridging involves molecular models at three different levels: quantum (including electrons), atomistic (atoms only) and mesoscale models ("super atoms").*
3 *Schematic representation of GROW: Force field parameters are iteratively optimized until some control observables have reached an acceptable accuracy.*
4 *Iteration results for an exemplary molecule.*

Dr. Dirk Reith
Phone +49 2241 14-2746
Fax +49 2241 14-1328
dirk.reith@
scai.fraunhofer.de

NUMERICAL SOFTWARE



FAST METHODS AND SOFTWARE FOR SIMULATIONS

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

Reducing product cycle time, for example in the automotive industry, is not possible without more use of numerical simulation. For oil field exploitation, it is only through numerical simulation that knowledge about processes inside an oil reservoir can be obtained. Numerical simulation facilitates an analysis of the various recovery strategies in order to guarantee optimal exploitation.

The creativity and experience of the engineer determines the quality of a product. Enhancing the engineer's abilities can be achieved by:

- integrating simulation software more strongly into optimization processes
- increasing the precision of the models involved
- carrying out simulation interactively

Here, current numerical simulation often reaches its limits. Particularly, the typical long run-times of simulations must be substantially reduced. In addition, various tools for detailed analysis and reuse of simulation results are simply not available.

Our first goal is to develop new methods and tools that enable more efficient use of industrial software. This is achieved through the development of highly efficient numerical methods for the optimal and scalable solution of large systems of linear equations, as they occur at the heart of industrial simulation packages, specifically via modern hierarchical approaches (products SAMG and HLIBpro).

Our second goal is the analysis of data and design optimization, especially with regard to robust design. Our toolbox, DesParO, supports the user in computer-aided optimization of highly complex processes, even when combined with calculation-intensive simulation programs.

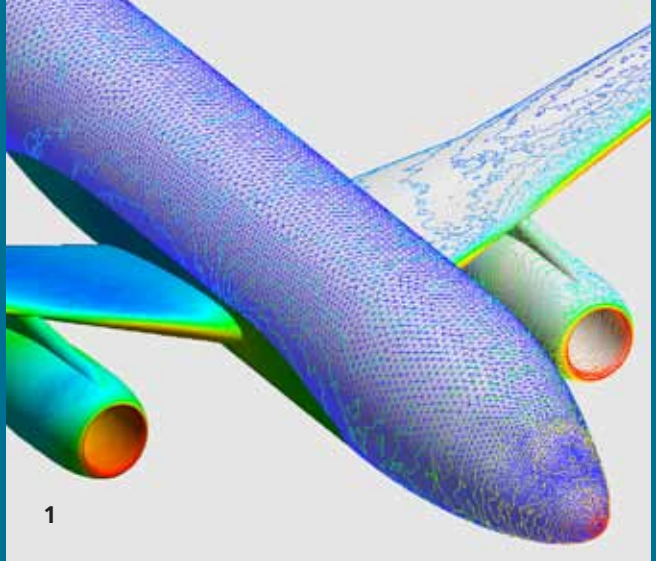
The use of data-mining techniques for software-oriented reuse (analysis and evaluation) of large data repositories, in the sense of automatic knowledge recovery, plays an ever more important role. SCAI is investigating suitable methods and is developing relevant software tools to this end. Moreover, SCAI has specialized and optimized compression tools for the efficient storage of large data archives.

Most of the technologies and methods mentioned above are already available as individual products suitable for industrial use. The strong interest expressed by many companies, especially in the oil and automotive industries, supports the relevance of these developments for numerical simulation.

A great challenge of the future is the combination of interactive simulation with robust design, which has been made possible by extremely efficient and scalable solver technology. Interactive simulation – i.e. push a button for alternative models, in real time, analysed and evaluated – is the strategic work that NUSO is oriented towards.

HEAD OF DEPARTMENT
Dipl.-Math.
Clemens-August Thole
Phone +49 2241 14-2739
Fax +49 2241 14-2102
clemens-august.thole@
scai.fraunhofer.de

DEPUTY HEAD
Dr. Klaus Stüben
Phone +49 2241 14-2749
Fax +49 2241 14-2102
klaus.stueben@
scai.fraunhofer.de



1

NEW APPLICATIONS IN THE AIRPLANE INDUSTRY

Increasing demands in computational flight testing call for hierarchical solvers like algebraic multigrid (AMG) for resulting sparse linear systems. With respect to this, Fraunhofer SCAI is taking part in the joint research project ComFliTe in order to investigate possible extensions of its AMG-based solver package SAMG.

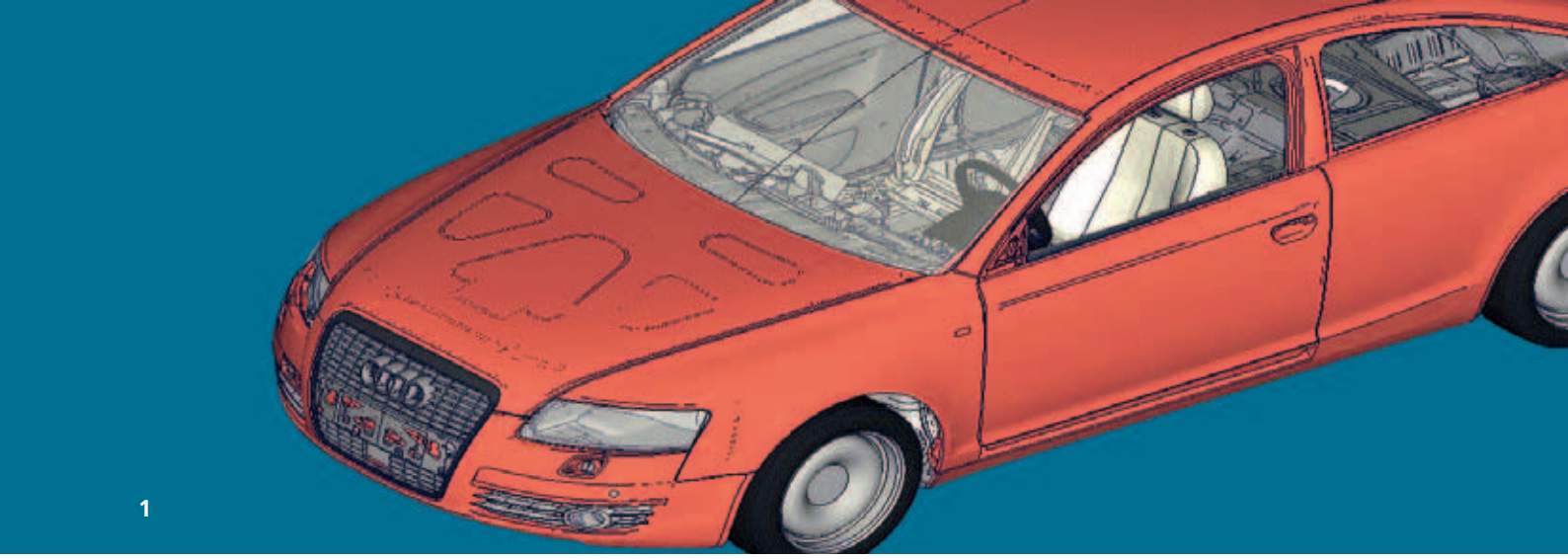
Over the past years, numerical simulations have become an increasingly important technology in the design process of aircraft components. Nevertheless, significant time is still invested in constructing expensive prototypes and testing them in wind tunnels. Consequently, efforts are currently going into the development of a "numerical wind tunnel" for virtual flight-testing. The aim is to reduce the costs in each stage of the design process. In cooperation with the German Aerospace Center, Airbus and other research and industry partners, Fraunhofer SCAI is working to achieve this aim. SCAI is adept in the development of fast linear solvers towards this aim.

The underlying models to be solved numerically are based on the compressible Navier-Stokes equations (for flow simulations) and the elasticity equations (for mesh deformation). A detailed aircraft Grid in three dimensions, for example, leads to problems with millions of variables. Standard "h-dependent" solvers are not scalable and thus not practicable to solve such large equation sets in an acceptable time.

As a hierarchical solver, SAMG is well suited to solving large sets of equations very efficiently. In contrast to geometric multigrid, which explicitly exploits information on the Grid structure, algebraic multigrid merely operates on the matrix equations. Therefore, SAMG is easy to integrate as a plug-in solver into existing simulation codes. Being a toolbox instead of a plain solver, certain algorithmic components of SAMG can be adjusted or exchanged to meet the new requirements, that are specific for aviation industry simulations. This flexible framework has already been successfully proven in the past. In fact, the SAMG package has become a well-established tool in various industrial simulation processes, such as the simulation of oil and water reservoirs, casting and moulding processes, semiconductor processes and devices, and in electrochemical processes.

1 *Pressure distribution on an aircraft, using a very fine mesh with more than 16 million elements.*

Dr. Klaus Stüben
Phone +49 2241 14-2749
Fax +49 2241 14-2102
klaus.stueben@
scai.fraunhofer.de



1

SIMULATION RESULTS BEST COMPRESSED WITH FEMZIP

Simulation programs open new prospects for product development. Yet this creates problems for archiving the resulting terabytes and petabytes of data, and communicating it internally and externally. SCAI has developed compression tools to alleviate this problem.

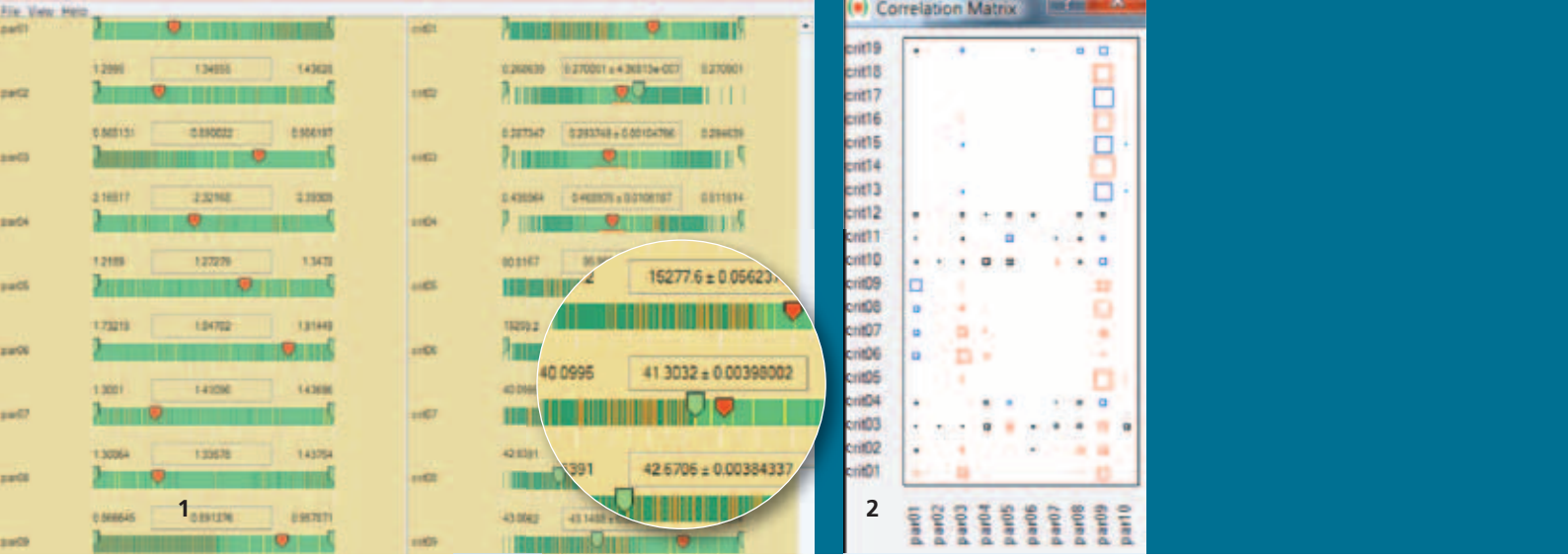
A product design is performed by a network of developers and their external consultants, usually spread around the globe. Simulation results need to be regularly exchanged among these partners, and archived for future reference and re-analysis. We have developed specialized tools to compress data from engineering applications. Particularly, in the field of crash simulation, FEMZIP has evolved into a standard tool that is extensively used in automotive industry in Europe, Japan, the US and other countries. It not only drastically reduces archive sizes, but in the newest versions also accelerates access to the data for visualization purposes, one of the main uses of the data in this field. The FEMZIP developments were awarded the Fraunhofer Prize in 2007. The latest SCAI compression tool adds support for simulation results in OP2 format as, for example, generated by MSC Nastran.

Simulation results are usually stored in a 32-bit floating point representation. Due to numerical approximation errors and inaccuracy in the model description itself, this representation is usually far too accurate. FEMZIP allows the user to specify his accuracy preferences in a parameter file. Expressed mathematically, the information in the parameter file quantizes the data. Approximation and interpolation is used to predict the remainder as accurately as possible (patented). For the difference between approximation and quantized data, lossless compression techniques are applied. Typically, the size of the resulting files is reduced by a factor of ten for crash and NVH (noise, vibration & harshness) simulation results.

FEMZIP's compression and decompression modules are available as executable files for almost all platforms. To support the user's workflow, compressed files can be directly read in by a growing number of pre- and post-processing tools. As a huge benefit, the read-in times for a compressed PAM-CRASH file, for example in GNS Animator3, is up to three times shorter than opening an uncompressed crash result file.

1 *The new software tool FEMZIP-N was partially funded by the European Commission in the SIMDAT project.*

Josua Lidzba, Matthias Rettenmeier, Rodrigo Iza-Teran
Phone +49 221 470-6081
Fax +49 221 470-6076
femzip@scai.fraunhofer.de



ROBUST DESIGN-PARAMETER STUDIES AND OPTIMIZATION

Production processes and the properties of resulting products usually depend on many different kinds of parameters. Software tools supporting an analysis of the parameter dependences are as necessary as a robust optimization that takes parameter variations efficiently into account.

Often, several conflicting criteria have to be fulfilled for optimization. Consequently, compromises must be determined, such as pareto-optimal solutions. The thickness of a certain part, for example, should be minimized while its stability should be maximized.

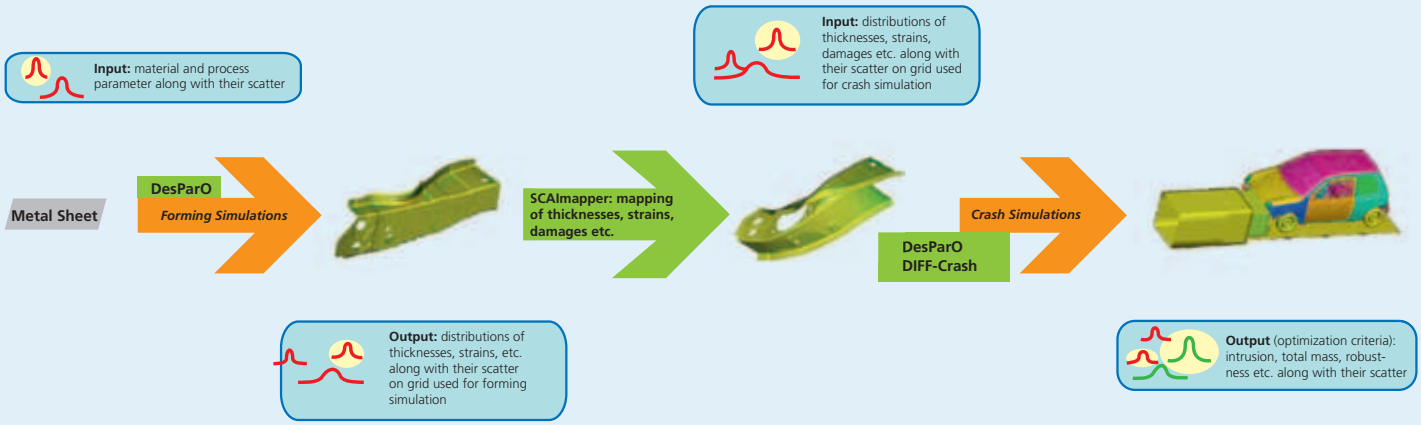
Our software package DesParO accomplishes these tasks by means of innovative, interactive and intuitive methods. As a basis, DesParO builds up a high-quality meta-model (response surface model) for the parameter-criteria relationships. Examples for parameters (possibly several hundred) include temperatures, pressures or parameterized material properties. Often, criteria (responses, outputs) are just simple functions of the parameters, such as total mass or quality measures, obtained by physical experiments or simulations. In advanced situations, outputs are given on highly resolved Grids, for example local thicknesses, strains and concentrations. Very efficient numerical techniques support handling of large data.

Typical tasks supported by DesParO:

- Interactive exploration (see figure 1) and/or an automated analysis of the model
- Sensitivity and robustness analysis; multi-objective robust optimization
- Determination of influencing/critical parameters (figure 2 shows one method)
- Adaptive refinement of the model; storage and re-use for further analysis steps

DesParO efficiently avoids common drawbacks, such as a solution trapped at a local optimum or exhaustive experimentation required by Monte-Carlo-like strategies. Current application areas include crash, metal forming, semiconductor process/device/circuit simulation, fluid mechanics, analysis of experimental data (automotive, chemical, electronic industry) and more.

1 *The DesParO graphical user interface shows a realistic case: 10 parameters, 19 criteria.*
2 *The correlation matrix of DesParO shows the influence of critical parameters.*



1

EFFICIENT STATISTICAL ANALYSIS OF PROCESS CHAINS

Products are often fabricated in a series of different process steps. At minimum, the most important process steps and their interplay should be analysed in order to obtain realistic information on output variations and their dependence on input variations (scalar parameters or data on fine Grids).

Our tools DesParO and DIFF-CRASH support an analysis of entire process chains. Examples include:

- metal forming/casting → crash simulation
- semiconductor process → device → circuit simulation

Recently, efficient methods have been developed for a new, reduced representation of the design space and simulation results. In a process chain that runs from a forming simulation to a crash simulation, for instance, the strategy consists of the following steps (see figure 1):

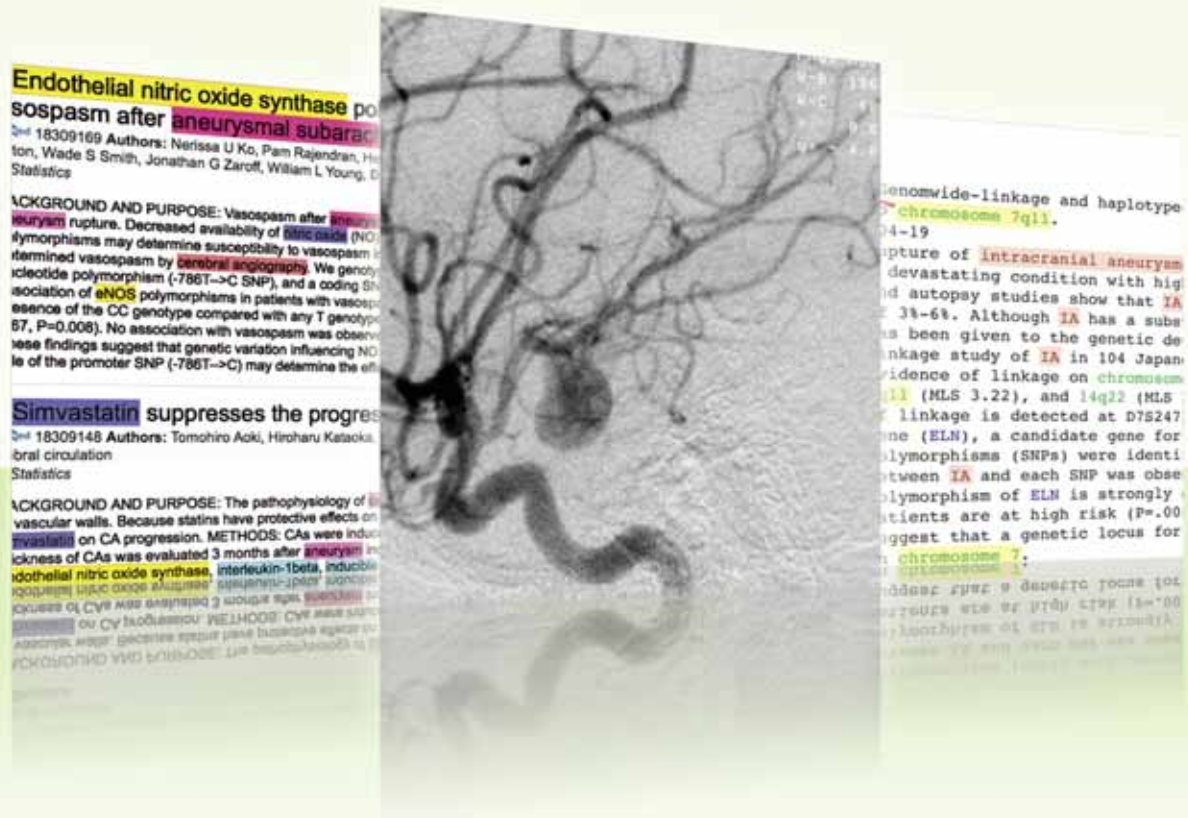
- forming simulation
  - → setup of appropriate input
  - → parameter sensitivity analysis
  - → reduction of parameters
  - → construction of a reduced database
- mapping of database
- crash simulation
  - → reduction of necessary simulation runs
  - → stability, sensitivity, robustness analysis
- multi-objective robust design-parameter optimization

Our methods and software tools are successfully used for industrial applications. The analysis of a metal blank of a B-pillar in a car, for example, has shown that not only the usual thickness and strains have to be taken into account: It is crucial to include damage information as well. Comparisons to physical experiments have demonstrated the abilities of the proposed strategy.

1 *This exemplary scenario illustrates a process chain from forming simulation to crash simulation.*

Dr. Tanja Clees
Phone +49 2241 14-2983
Fax +49 2241 14-4-2983
tanja.clees@
scai.fraunhofer.de

BIOINFORMATICS



INFORMATION EXTRACTION FOR LIFE SCIENCES

The collaborative research and development projects of the Department of Bioinformatics deliver data management solutions to the pharmaceutical and biotech industry, as well as the publishing industry. Positioned at the boundary between pure commercial and pure academic research, we maintain strong links and provide a bridge between both communities.

The Department of Bioinformatics conducts applied research and development in the fields of:

- information extraction and semantic text analysis
- applied chemoinformatics
- distributed and Grid computing

The Bioinformatics team works closely with industrial partners – including SMEs – to enhance their competitiveness through mediating knowledge and technology transfer from academic research to industrial application.

Our products solve information management problems prevalent in the pharmaceutical and publishing industries:

ProMiner is a system for the detection and disambiguation of biomedical named entities in texts, such as gene names, protein names, disease names and drug names. During 2008 and 2009 we completed our approach to the recognition of named entities in texts through methods based on machine learning. For example, Linda.IUPAC, a recognizer for IUPAC-like expressions used to encode chemistry, has been included in our text-mining solution. Moreover, with SCAIView we have developed a mining environment that allows biologists, chemists and medical researchers to use text-mining technology without needing to understand the computer science behind it.

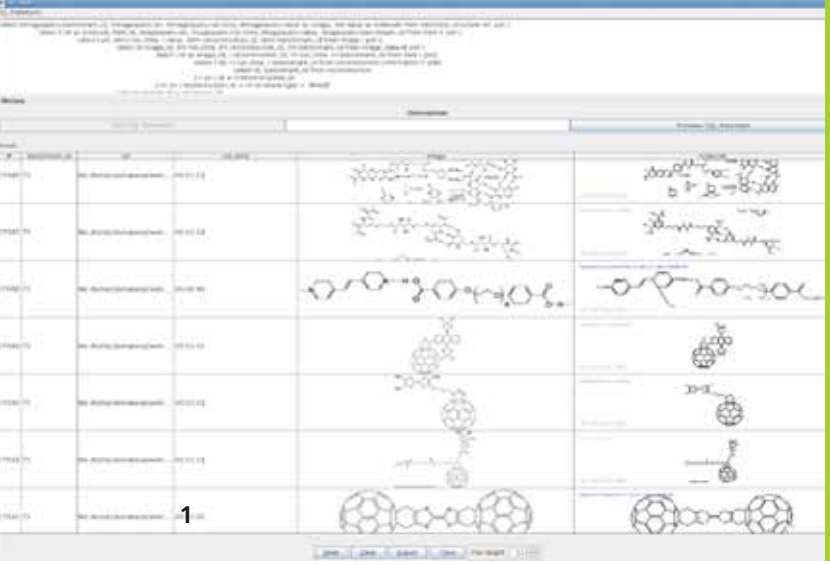
chemoCR is a system for reconstructing chemical information from chemical structure depictions. This tool has been developed to gain access to one of the largest sources of chemical information: images containing chemical structure depictions. Although communicating chemical information via images is quite common amongst chemists, the information contained in images could not be used by machines. chemoCR solves this problem by reconstructing chemical information from images.

Both ProMiner and chemoCR reveal hidden information in scientific texts and image sources, making it available for improved retrieval, information extraction and knowledge discovery. Our industrial partners use our tools for indexing large document collections, normalizing named entities in scientific literature, and interpreting high-content data.

A brand new approach to distributed licence management began in 2008: elasticLM. It addresses specific challenges that arise with distributed use of commercial software. At the end of 2009, elasticLM will be available for beta testing. We have already received significant interest in the elasticLM approach from various industrial partners.

HEAD OF DEPARTMENT
Prof. Dr. Martin Hofmann-Apitius
Phone +49 2241 14-2802
Fax +49 224114-2656
martin.hofmann-apitius@scai.fraunhofer.de

DEPUTY HEAD
Dr. Marc Zimmermann
Phone +49 2241 14-2276
Fax +49 2241 14-2656
marc.zimmermann@scai.fraunhofer.de



1

CHEMICAL INFORMATION RETRIEVAL FROM LITERATURE

chemocr is a tool for chemical structure reconstruction. It extracts chemical structural formulas and their depictions from scientific literature and patents. The software package converts the structure depictions into a format the computer can use to process the information contained in the depictions.

In scientific texts, chemical entities can appear as trivial and brand names, assigned catalogue names or IUPAC names. The preferred representations of entities are often two-dimensional depictions of the chemical structure, which can be found as images in nearly all electronic sources of chemical information (e.g. journals, reports, patents, and database web interfaces).

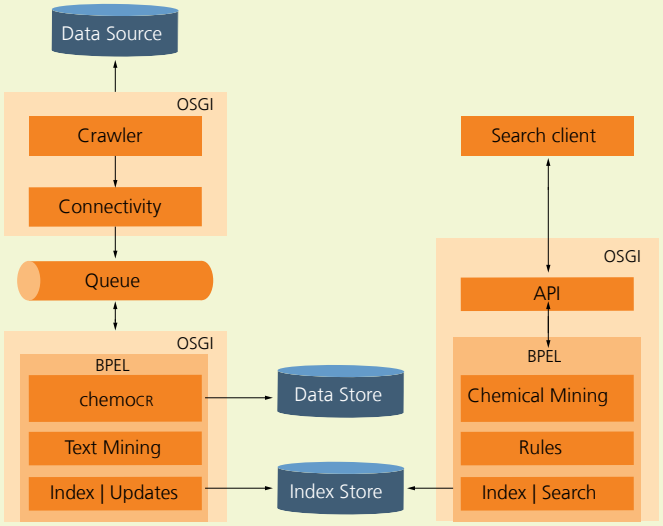
Chemical structure extraction is a key feature and a technological challenge. In contrast to multipurpose search engines, such as Google, the extraction of the so-called connection table from images allows chemical-relevant queries. By using Google image search, a user could ask: "Find all documents that show aspirin in an image." By searching for the term aspirin in the caption or surrounding text, the resulting images can be identified. A chemical structure extraction enables semantically-rich queries like "Find chemical similar structures of aspirin." This search doesn't rely on the text and accordingly even works for Asian patents without translating them.

To solve the problem of recognizing and retrieving chemical structures in image documents, chemocr combines pattern recognition techniques with a chemical rule-based expert system. The workflow consists of three phases:

1. page segmentation: analysing a full page scan, separating text from images, and extracting single images containing a structure diagram using image classification techniques
2. connection table reconstruction: performing image vectorization, optical character recognition, and molecule assembly using a chemical rule system
3. retrieval task: feeding the resulting molecules in a structure-searchable database

Main software features:

- conversion of PDF documents into full page scans
- segmentation of full page scans into chemical schemes
- classification and selection of chemical depictions
- conversion of chemical depictions into computer-readable chemical file formats
- chemical intelligence for post-processing
- fully automatic batch processing mode
- scoring scheme for the reconstruction process based on known chemical scaffolds
- training ability to improve the automatic system by expert-teaching
- graphical user interface (GUI) for manual curation
- connection to database management systems



2

ORGANISING DIGITAL INFORMATION

Fraunhofer SCAI is involved in an extensive research programme initiated by the Federal Ministry of Economy and Technology. THESEUS aims at developing a new Internet-based infrastructure in order to better use and utilize the knowledge available on the Internet. SCAI's contribution to the project is its expertise in extracting information from chemical depictions.

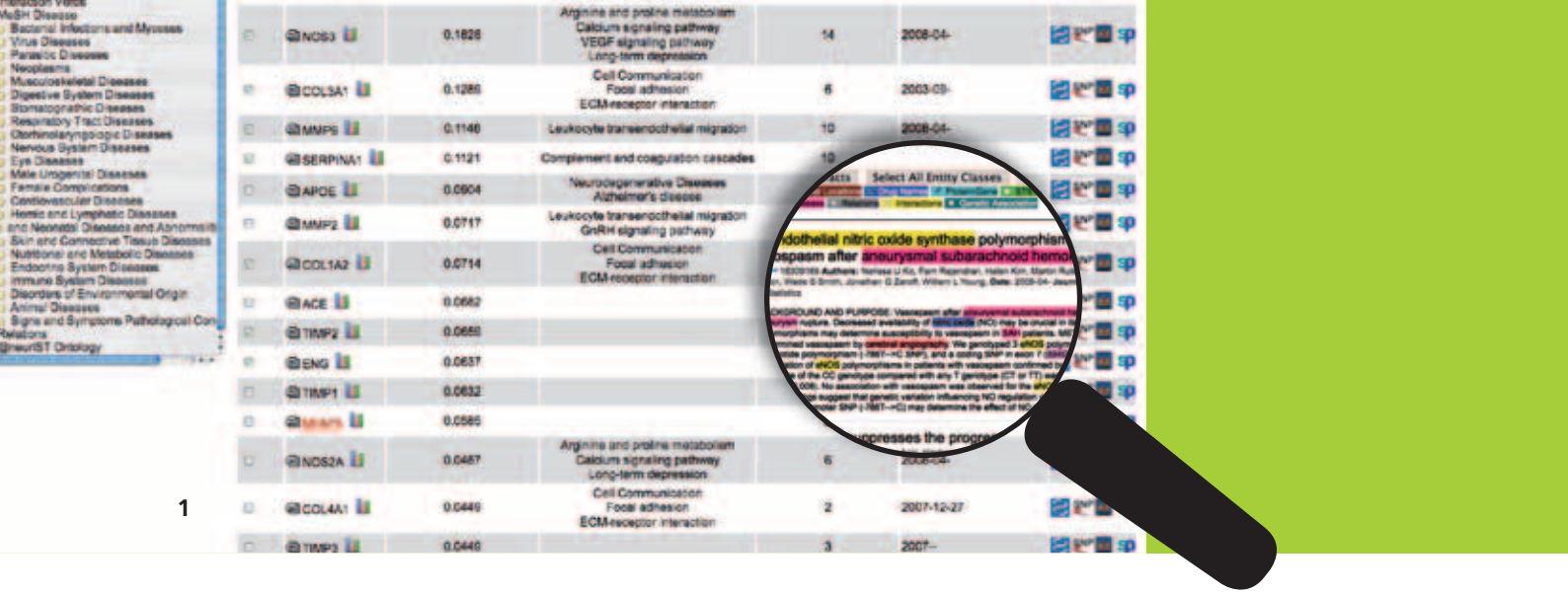
The research programme focuses on semantic technologies. These determine contents (words, images and sounds) not by conventional methods (e.g. combinations of letters), but by recognizing the meaning of content and placing it in its proper context. By using these technologies, computer programs can intelligently comprehend the context in which data is stored. Furthermore, by applying rules and order principles, computers can draw logical inferences from content and autonomously recognize and produce connections between pieces of information from different sources.

The application scenario ORDO is intended to research and develop semantic technology, thereby creating new services and software tools that will enable users to organize their entire store of digital information. In contrast to the solutions used up till now, this personalized linking allows structured and unstructured data to be organized in a uniform manner, enabling efficient, individual knowledge management. Part of the ORDO application scenario is the development of innovative procedures for automatically recognizing and comprehending content.

The Department of Bioinformatics is contributing its expertise in information extraction from chemical depictions: the computer becomes a "chemistry expert". chemocr (a tool for chemical compound reconstruction) extracts chemical structural formulae and depictions from scientific literature. The software package converts the structure depictions into a format that the computer can then use to search for and process information contained in the depictions. chemocr has been successfully integrated in the SMILA (Semantic Information Logistics Architecture) – the open source (Eclipse project) semantic search engine framework developed in ORDO. This allows SMILA to automatically crawl all kinds of documents, search them for chemical depictions, and reconstruct the molecules. Later the user can pose queries like: "Show all patented core structures in last year's Asian patents."

1 *Snapshot of the retrieval system. An SQL interface allows querying and displaying the images and the reconstructed molecules.*
2 *chemocr is integrated into SMILA as pipelet in the extraction pipeline performing PDF conversion, page segmentation, image classification and chemical structure reconstruction.*

Dr. Marc Zimmermann
Phone +49 2241 14-2276
Fax +49 2241 14-2656
marc.zimmermann@scai.fraunhofer.de



1

KNOWLEDGE DISCOVERY AND SEMANTIC SEARCH

ProMiner, a tool for biological name recognition, and SCAIView, an advanced search engine, address questions of interest to biomedical researchers. Most of the biological and medical knowledge is given as unstructured text (publications and text fields in databases).

ProMiner is able to work with voluminous dictionaries, complex thesauri and large controlled vocabularies derived from ontologies. The system addresses several fundamental issues in named entity recognition in the field of life sciences:

- recognition of biomedical entities and their spelling variants in text
- mapping of synonyms to reference names and data sources
- context-dependent disambiguation of biomedical termini and resolution of acronyms

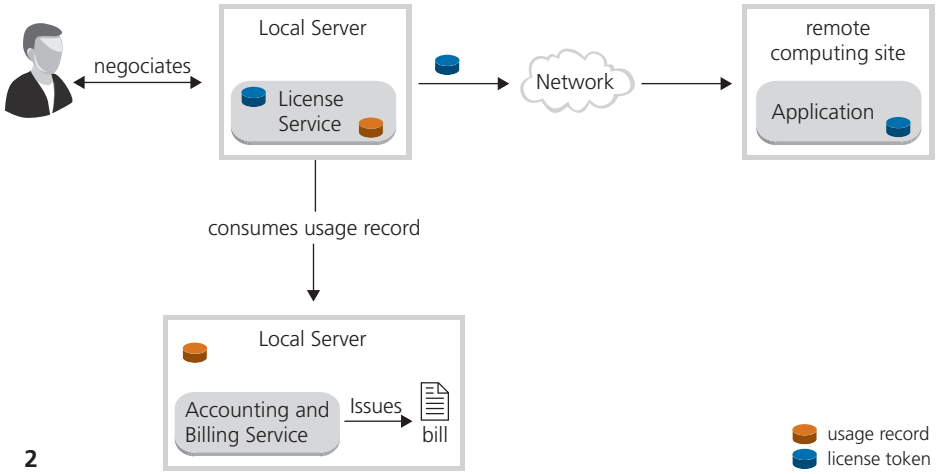
SCAIView allows searches for full text and biomedical concept, based on the ProMiner biomedical terminologies and text mining technologies. Advanced retrieval technology facilitates answering complex questions such as:

- Which genes/proteins are related to a certain context (e.g. disease/pathway/epigenetics)?
- Which relevant biomedical concepts are in my subcorpus?
- Which drugs are relevant for this context?
- To which diseases is my gene associated?
- Which chromosomes show linkage to the disease?
- Which variations are mentioned in the context of the disease and could they be found in dbSNP?
- What other diseases are possibly co-occurring with my relevant disease?

The documents are retrieved via free text queries in combination with semantic or ontological search of biomedical entities of interest. The entities are embedded in searchable hierarchies and span from genes, proteins and accompanied SNPs to chemical compounds and medical terminology. SCAIView supports fast retrieval from large corpora and provides rankings based on relative entropy for the retrieved results. Even if some proteins like insulin are mentioned quite often in the context of a search, it will be ranked low if it is not mentioned over-proportional in the specific query result set. Links to relevant biomedical databases (e.g. EntrezGene, dbSNP, KEGG, GO, DrugBank), as well as document visualisation with user-defined highlighting are supported.

1 *ProMiner retrieves up to date information about biomedical entities in scientific texts.*
2 *Basic scenario of elasticLM: There is no bidirectional network link required at run-time.*

Dr. Juliane Fluck
Phone +49 2241 14-2188
Fax +49 2241 14-2656
juliane.fluck@scai.fraunhofer.de



SOFTWARE LICENSES AS GRID SERVICES

Funded by the European Commission, the SmartLM project aims at producing mechanisms for managing and using software licenses in a more flexible way. Based on the SmartLM software prototype developed within the project, a product called elasticLM has been implemented.

The general approach is to treat and implement software licenses as Grid services, thus providing platform independent access just like to any other virtualized resources.

- Licenses will become Grid services; a promising approach to overcome the limitations of monolithic licensing models.
- Licenses will be managed as agreements, extending the conventional Service Level Agreements (SLAs) which are made today between sellers and buyers in the market.
- Licenses will be dynamic in order to support agreements that may change over time and where dynamic negotiation between service provider and consumer is needed.

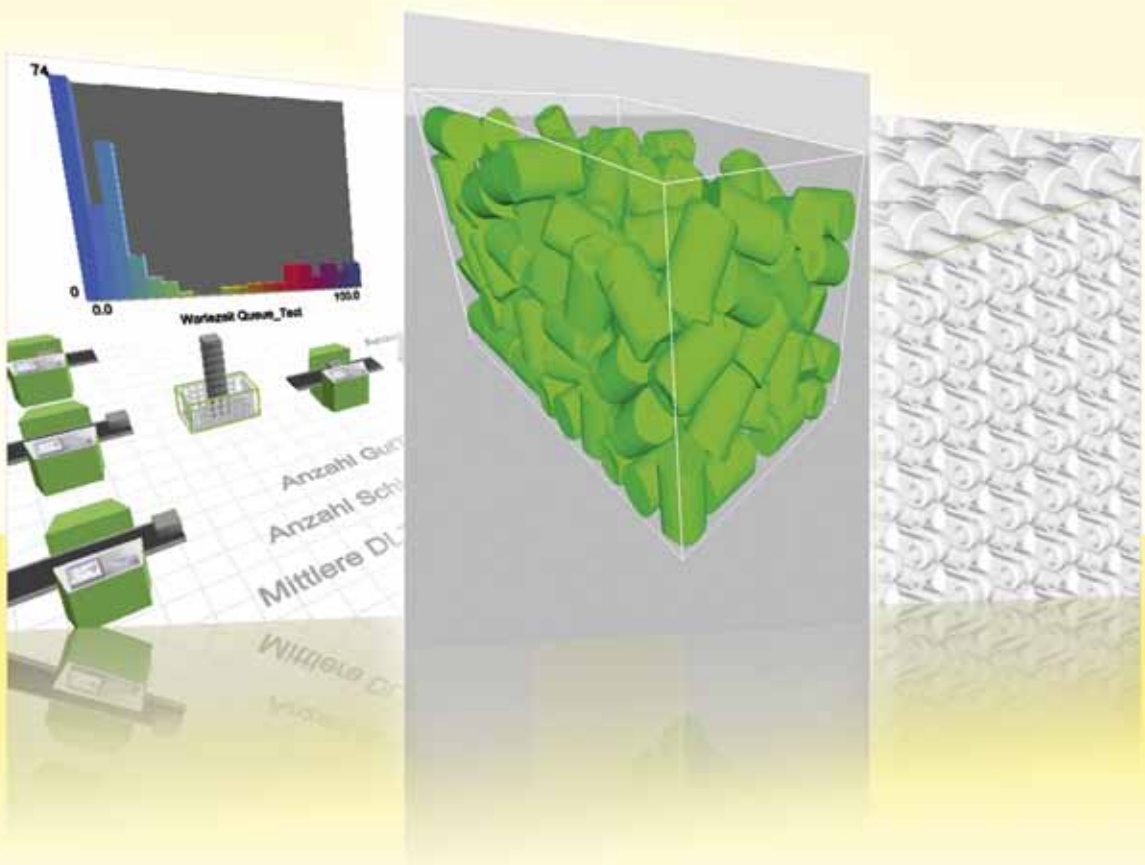
elasticLM is implemented as a framework of Web Services. Together with the built-in mechanisms to evaluate different policies prior to taking a decision on the user's license request, elasticLM achieves maximum flexibility. Thus, adapting the functionality and behaviour of elasticLM to the needs of the respective environments is easy. elasticLM is based on open standards to ease the integration into existing environments and leveraging interoperability. Moreover, this approach renders the elasticLM system extensible with components adding site-specific functionality, e.g. billing.
In contrast to most of the other existing license management systems, elasticLM comes with an integrated, modular solution for accounting and billing, supporting comprehensive analysis of license usage. Moreover, the integrated approach allows determining the costs for license usage based on user requests and other parameters, like previous usage or department-specific pricing.
Finally, this integration allows checking users' license requests against predefined budgets per user, department etc. License usage is granted only if the request does not lead to a violation of the budget constraints.

Aspects of security have been examined with special care:

- authentication and authorization of users, services, servers
- security and confidentiality of the communication between different actors or components
- disclosure of sensitive information, e.g. compromise of licenses
- integrity of the process to inhibit non-repudiation
- security of the licensing mechanism itself, e.g. the license generators, manipulation of the executables, or clock tweaking

Wolfgang Ziegler
Phone +49 2241 14-2258
Fax +49 2241 14-42258
wolfgang.ziegler@
scai.fraunhofer.de

OPTIMIZATION



OPTIMIZING PRODUCTION, PLANNING AND LOGISTICS

How can a production line be run to its best capacity without resulting in delivery delays caused by long set-ups? How can storage be optimized so that all components are made available for the production process with small stock in short time? These are questions asked daily in the manufacturing industry. The answers can be found with the specialists at the Optimization Department of Fraunhofer SCAI.

HEAD OF DEPARTMENT
Dr. Ralf Heckmann
Phone +49 2241 14-2810
Fax +49 2241 14-2656
ralf.heckmann@
scai.fraunhofer.de

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

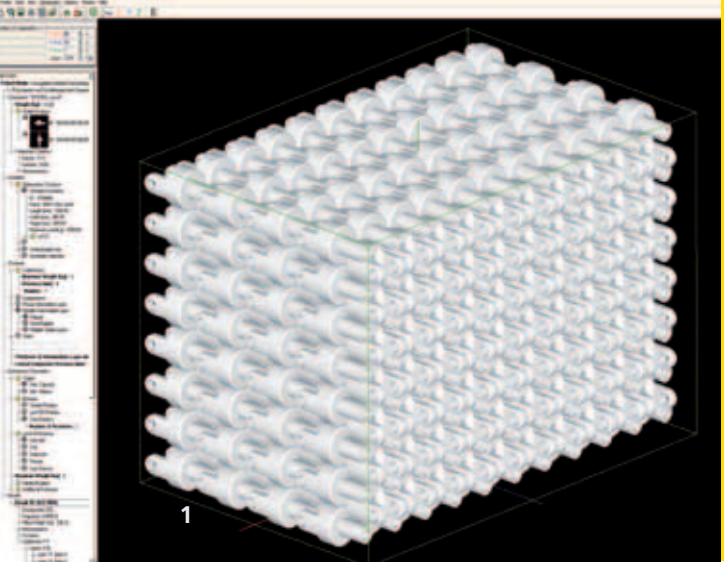
- Production: machine scheduling, work schedules, material consumption, cutting and packing
- Logistics: transport optimization, route planning, location choice
- Material flow: utilizing means of transportation, machines and workers, work piece cycle-times, stock of buffers and intermediate storage, resource dimensions
- Planning: Optimal utilization of area and space, location of safety equipment, communication networks

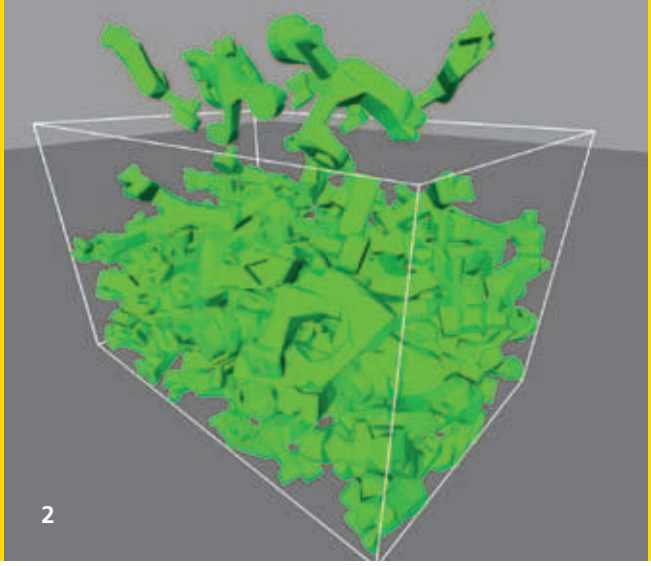
The Optimization Department at Fraunhofer SCAI provides research and optimization services for trade, commercial or industrial companies. We are receptive to all kinds of problems that could be solvable by optimization methods. Amongst others, we offer the following services:

- Problem analysis and consulting
- Specifying mathematical and methodological descriptions of the problem
- Custom-made optimization software
- Standard products developed by us or with partners
- Software maintenance, training and ongoing support
- Further development and customization of our tailor-made and standard solutions

SCAI has about 20 years of experience in optimization and a large library of optimization methods for creating solutions for new problems. We identify and employ the most suitable state-of-the art optimization technique enriched with our special knowledge and improvements, and aided by problem specific constraints. Typical optimization techniques include branch and bound, simulated annealing, Great Deluge, record-to-record travel, genetic or evolutionary algorithms, simulated trading, greedy algorithms, tabu search, linear and integer programming, multi-objective optimization, and ant colony optimization.

The institute has a strong background and a team of experts specialized in solving cutting and packing problems. We have developed several solutions for industrial partners in the field of one-, two-, and three-dimensional cutting, packing and arrangement problems. Furthermore, we offer a suite of standard products for these kinds of applications. Our product AutoNester can be used to solve nearly any two-dimensional nesting task, and our PackAssistant product can calculate the optimal packing arrangement of identical parts in standard containers.





PERFECT PACKING WITH PACKASSISTANT

In industry, engineers and warehouse managers are often confronted with the challenge of efficient packing and logistics planning. Simulation can find precise solutions for the best possible arrangement of components in containers or for loading production systems. The simulation results optimize production and logistics processes for companies.

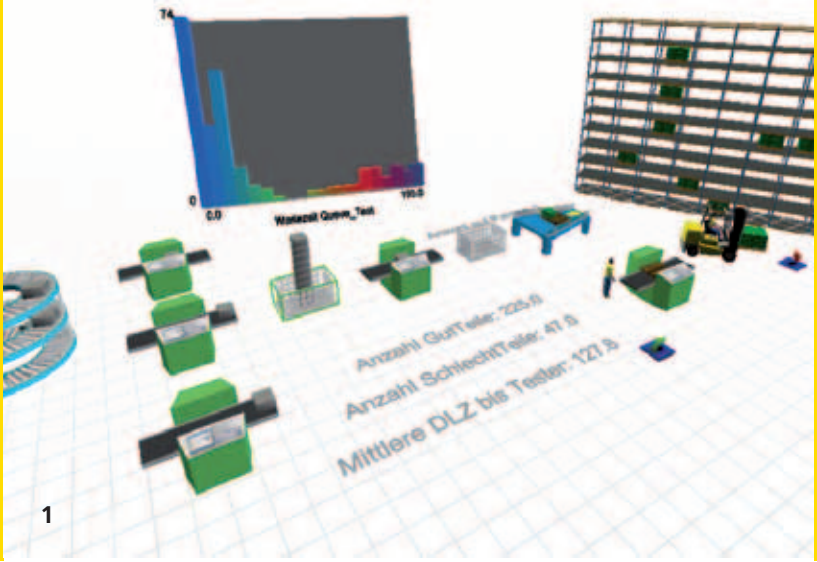
Experienced packing planners usually spend a lot of time meticulously arranging and packing components with complex shapes. In the majority of cases, this manual approach cannot achieve a packing density comparable to PackAssistant. The industry-leading simulation software is used in production and logistics planning for optimizing the packing of identical components in containers. This provides enormous benefits for packing planners and warehouse managers, including fast, space-saving, economical planning, as well as the timely planning of transport, container and storage capacities.

1 *PackAssistant calculates an optimized packing of components in a container.*
2 *The new version of the software is able to estimate the loading of containers with bulk goods.*

The software allows the calculation of models with arbitrary complex shapes and a vast data volume in an efficient, memory saving and accurate way. Within minutes, packing planners can compute how many components optimally fit into a container for different types of packing structures. These include compartments, planar intermediate layers, flexible intermediate layers like plastic foil or corrugated cardboard, and stacks. Now, PackAssistant can even estimate the loading of containers with bulk goods. The software is also able to compute the smallest container for a specified number of components. PackAssistant creates a Microsoft Word document with images to illustrate the packing arrangement and key data, such as container dimensions and the number of components.

PackAssistant is used worldwide by many customers from the automotive and other industries. Fraunhofer SCAI's software engineers constantly maintain and enhance the software and provide customer support.

Stefan Rank
Phone +49 2241 14-1503
Fax +49 2241 14-2656
stefan.rank@
scai.fraunhofer.de



1

2

SIMULATING MATERIAL FLOW FOR OPTIMAL PROCESSES

Modelling and simulating processes in production and logistics help to increase efficiency and to create new production systems. Through sensitivity analysis, the SCAI team examines the behaviour of such production systems under exceptional conditions and develops contingency plans jointly with the customer. Our activities in simulation and optimization focus on intralogistics, so far.

An example of a successful material flow simulation project is a process enhancement for BPW Bergische Achsen in Wiehl, Germany. We conducted a simulation study in order to optimize the manufacturing processes in the axle plant.

The main problem was a large stock, which led to undesirable capital commitment and required a high effort for order picking. On the other hand it assured on-time delivery even during bottlenecks and breakdowns. Within this project, we aimed at reducing stock and simultaneously maintaining a high-level adherence to delivery dates. Furthermore, we were asked to conduct sensitivity analyses for exceptional conditions, such as extreme order mix or low material availability, and to develop compensatory measures.

First of all, we modelled the current status in the simulation software Plant Simulation. Based on this simulation, we developed measures for optimizing processes and maintaining performance in collaboration with BPW, such as:

- capacity expansion in certain divisions
- acceleration of clocked machines
- shortening planning intervals
- changing the decoupling point
- common usage of resources
- stronger concatenation of working stations
- globally optimal job scheduling
- variation of the stock's removal strategy
- elimination of the stock and compensation by innovative concepts

The most promising ideas were implemented in the model, simulated, and evaluated. BPW began implementing selected optimization activities before the project was even finished.

What did we achieve? We managed to reduce stock considerably without compromising on-time delivery. Furthermore, the project improved inter-divisional communication. After updating the model, it can be reused for future simulations.

1 *Within the services in material flow simulation, SCAI researchers generate models of a production line in Flexsim.*
2 *SCAI supported BPW in achieving a process enhancement in the production of axles. Here, a BPW axle is shown.*

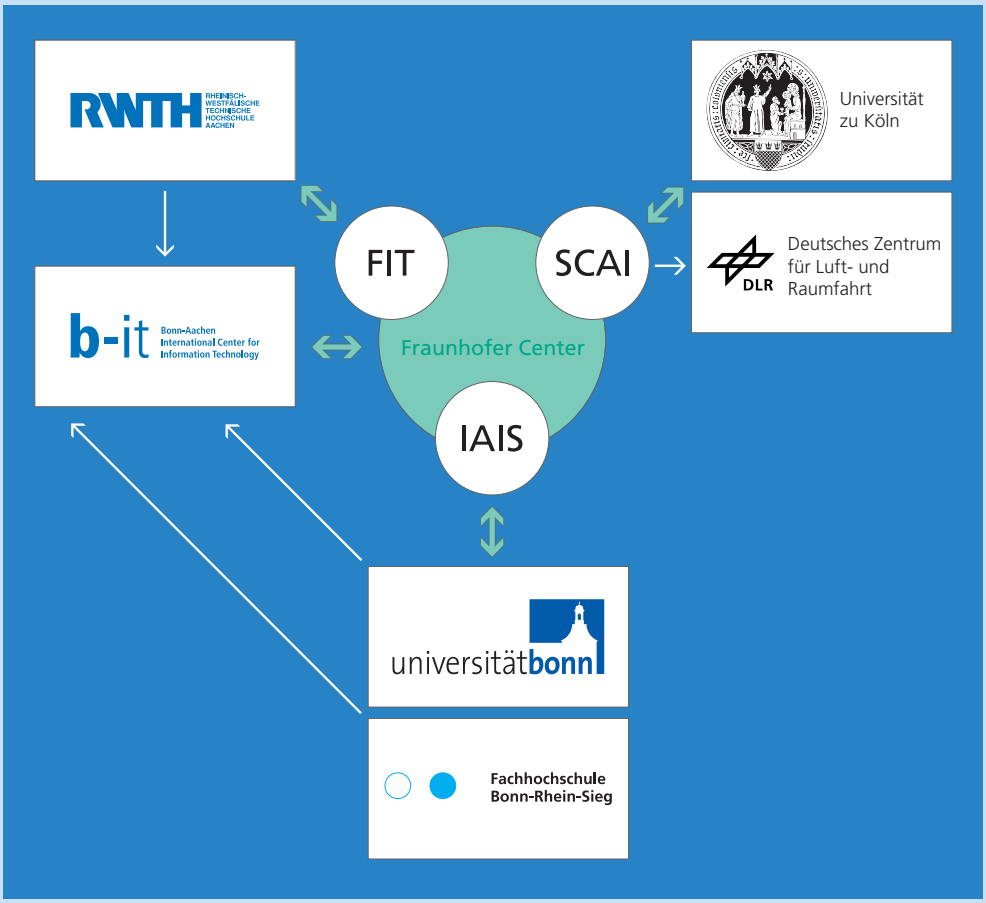
Lydia Franck
Phone +49 2241 14-2563
Fax +49 2241 14-2656
lydia.franck@scai.fraunhofer.de

ALLIANCES


Contours of Static Temperature (k)
Mar 25, 2004
FLUENT 6.1 (3d, dp, segregated, ke

REGIONAL ACADEMIC PARTNERSHIP

Via the chairs of the institute directors the Fraunhofer Center Schloss Birlinghoven is strongly linked with regional universities and other research institutes. SCAI has especially close relationships to the University of Cologne, the German Aerospace Center (DLR) and the Bonn-Aachen International Center for Information Technology (B-IT).



FRAUNHOFER ALLIANCES

Cooperation and competency bundling are very important strategies in Fraunhofer Research and Development. The Fraunhofer Institute SCAI is an active member of three Fraunhofer Alliances.

Fraunhofer Information and Communication Technology Group

Chairman of the alliance:
Prof. Dr. Dieter Rombach
Fraunhofer Institute IESE

Deputy chairman:
Prof. Dr. Matthias Jarke
Fraunhofer Institute FIT

Shorter innovation cycles have turned IT knowledge into a perishable commodity. The Fraunhofer Information and Communication Technology Group (ICT) provides support in the form of customized studies, technology consulting, and contract research for new products and services. In addition to feasibility studies, it also investigates end-user acceptance and produces market analyses and cost-benefit assessments. The Fraunhofer ICT Group comprises thirteen institutes as full members and two associate members, representing a workforce of roughly 2,800 employees. It manages an annual budget of about €168 million. Its central office in Berlin serves as a one-stop shop, referring customers to the appropriate contacts.

The complementary focal fields of the participating institutes cover the entire value chain of the ICT industry. The ICT Group conducts activities within a wide range of business fields, including information and communication technologies for:

- medicine and life sciences
- culture and entertainment
- e-government
- digital media
- security
- traffic and mobility
- e-business
- production
- software
- communication systems & interdisciplinary applications

The member institutes possess considerable experience in the innovative development of new technologies, particularly mobile networks and data transmission, information security, software engineering, knowledge management and information logistics, e-learning, embedded systems, electronic commerce, and virtual and simulated reality.

www.iuk.fraunhofer.de

Fraunhofer Transport and Traffic Alliance

Chairman of the alliance:
Prof. Dr.-Ing. Uwe Clausen
Fraunhofer Institute IML

The Fraunhofer Transport and Traffic Alliance currently represents the combined traffic-engineering expertise of twenty Fraunhofer Institutes. They cooperate to develop adequate technical and conceptual solutions for public and industry partners and put these solutions into practice by means of transport-related research.
The Alliance creates a new choice in transport R&D by bundling existing potential and broad system competency. The alliance's missions and R&D clusters are:

- Convenience and design concepts
- Intelligent lightweight construction systems
- Sustainable propulsion concepts
- Transport management systems
- Safety and security systems
- Logistics structures and processes
- Mobility and transport strategies
- Innovative transportation systems

Due to their participation in international research programmes, the member institutes have worldwide contacts with companies and research organizations involved in the fields of transportation engineering and management.

www.verkehr.fraunhofer.de

Fraunhofer Numerical Simulation of Products and Processes Alliance

Spokesman of the alliance:
Andreas Burblies
Fraunhofer Institute IFAM

In the Fraunhofer Alliance for Numerical Simulation of Products and Processes, 20 institutes pool their expertise in the development and improvement of simulation techniques.
The simulation of products and processes today 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.
The object of the alliance is to address institute-wide issues and represent the interests of the member institutes as a central point of contact for public-sector and industrial customers.
In particular, the pooling of expertise from the I&C sector with materials and components know-how, as well as with surface technology and production engineering, promises to yield innovative results. The alliance's business areas are:

- Numerical methods & software engineering
- Materials modelling and component simulation
- Simulation of manufacturing methods and production processes
- Simulation in surface engineering, photonics and microelectronics

www.nusim.fraunhofer.de

FRAUNHOFER-GESELLSCHAFT

Research of practical utility lies at the heart of all activities pursued by the Fraunhofer-Gesellschaft. Founded in 1949, the research organization undertakes applied research that drives economic development and serves the wider benefit of society. Its services are solicited by customers and contractual partners in industry, the service sector and public administration. The organization also accepts commissions from German federal and Länder ministries and government departments to participate in future-oriented research projects with the aim of finding innovative solutions to issues concerning the industrial economy and society in general.

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, accelerating technological progress, improving the acceptance of new technologies, and not least by disseminating their knowledge and helping to train the urgently needed future generation of scientists and engineers.

As an employer, the Fraunhofer-Gesellschaft offers its staff the opportunity to develop the professional and personal skills that will allow them to take up positions of responsibility within their institute, in other scientific domains, in industry and in society. Students working 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.

At present, the Fraunhofer-Gesellschaft maintains more than 80 research units, including 56 Fraunhofer Institutes, at 40 different locations in Germany. The majority of the 12,500 staff are qualified scientists and engineers, who work with an annual research budget of €1.2 billion. Of this sum, more than €1 billion is generated through contract research. Two thirds of the Fraunhofer-Gesellschaft's contract research revenue is derived from contracts with industry and from publicly financed research projects. Only one third is contributed by the German federal and Länder governments in the form of institutional 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 research centers and representative offices in Europe, the USA and Asia provide contact with the regions of greatest importance to present and future scientific progress and economic development.

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

ANNEX

Selected Publications

Allodi, M. A.; Kirschner, K. N.; Shields, G. C.: Thermodynamics of the hydroxyl radical with isoprene. In: The Journal of Physical Chemistry/A, Molecules, spectroscopy, kinetics, environment & general theory 112 (2008), 30, S. 7064-7071.

Bayrasy, P.; Kelsall, D.: Coupling of 1D and 3D simulation. In: Wolf, K. (Hrsg.): 9th MpCCI User Forum, 2008, S. 106-117.

Bougé, L.; Forsell, M.; [...] Ziegler, W. (Hrsg.): Euro-Par 2007 Workshops: Parallel Processing: HPPC 2007, UNICORE Summit 2007, VHPC 2007, Rennes, France, Aug. 28-31, 2007; revised selected papers. Berlin: Springer, 2008.

Breton, V.; Jacq, N.; Kasam, V.; Hofmann-Apitius, M.: Grid-added value to address malaria. In: IEEE Transactions on Information Technology in Biomedicine 12 (2008), 2, S. 173-181.

Brodbeck, C.: MpCCI FS morphing capabilities. In: Wolf, K. (Hrsg.): 9th MpCCI User Forum, 2008, S. 36-43.

Clees, T.: Computer aided robust design for multi-disciplinary processes. In: Wolf (Hrsg.): 10th MpCCI User Forum, 2009, S. 20-29.

Clees, T.; Burblies, A.: Computer Aided Robust Design – auf dem Weg zur simulierten Realität. wt Werkstattstechnik online, Jahrgang 98, Heft 1/2, 2008.

Dunlop, R.; Arbona, T.; [...] Friedrich, C. M.: @neurIST – chronic disease management through integration of heterogeneous data and computer-interpretable guideline services. In: Solomonides, T.: Global healthgrid: e-science meets biomedical informatics; HealthGrid 2008, proceedings. Amsterdam: IOS Press, 2008, S. 173-177.

Faroughi, A.; Faroughi, R.; [...] Ziegler, W.: Attributes and VOs: Extending the UNICORE authorisation capabilities. In: Bougé, L. u.a.: Euro-Par 2007 Workshops, 2008.

Friedrich, C. M.; [...] Hofmann-Apitius, M.: @neuLink: a service-oriented application for biomedical knowledge discovery. In: Solomonides, T.: Global HealthGrid, 2008, S. 161-164.

Furlong, L. I.; Dach, H.; Hofmann-Apitius, M.; Sanz, F.: OSIRISv1.2: a named entity recognition system for sequence variants of genes in biomedical literature. In: BMC Bioinformatics 9, Art. 84, 2008.

Gosch, Th.; Abels, W.; [...] Krämer-Fuhrmann, O.; [...]: SESIS – Entwicklung eines integrierten schiffbaulichen Entwurfs- und Simulationssystems. In: Bundesministerium für Wirtschaft und Technologie: BMWi-Statustagung Schifffahrt und Meerestechnik: Tagungsband, Rostock-Warnemünde, 11.12.2008.

Grimme, Ch.; Lepping, J.; [...] Ziegler, W.: Towards a standards-based Grid scheduling architecture. In: Gorlatch, S. u.a. (Hrsg.): CoreGRID Integration Workshop 2008, April 2-4, 2008, Hersonissos, Greece. New York: Springer, 2008, S. 147-158.

Groeper, R.; Grimm, C.; [...] Ziegler, W.; [...] A concept for attribute-based authorization on D-Grid resources. In: Future Generation Computer Systems. 25 (2009), 3, S. 275-280.

Gruber, R.; Ziegler, W.: ÏANOS: intelligent application-oriented scheduling for HPC Grids with ÏANOS. 2008.

Hartt, G. M.; Shields, G. C.; Kirschner, K. N.: Atmospheric OCS with one to four water molecules. In: The Journal of Physical Chemistry/A, (2008), 19, S. 4490-4495.

Hofmann-Apitius, M.; Fluck, J.; [...] Kolárik, C.; Klinger, R.; [...] Mevissen, T.; [...] Friedrich, C.M.: Knowledge environments representing molecular entities for the virtual physiological human. In: Philosophical Transactions of the Royal Society: Series A, Mathematical, Physical and Engineering Sciences 366 (2008), 1878, S. 3091-3110.

Iavindrasana, J.; Lo Iacono, L.; [...] Friedrich, C. M.; [...] Hofmann-Apitius, M.: The @ neurIST project. In: Solomonides: Global HealthGrid, 2008, S. 161-164.

Jambor, R.; Kasná, B.; Kirschner, K. N.; [...]: [{2,6-(Me 2 NCH 2) 2 C 6 H 3 }Sn] 2: An intramolecularly coordinated diorganodistannyne. In: Angewandte Chemie 47 (2008), 8, S. 1650-1653.

Joppich, W.; Pott, S.: Results

ANNEX

obtained with a semi-lagrangian mass-integrating transport algorithm by using the GME grid. In: Lirkov, I. u.a.: Large-Scale Scientific Computing: 6th International Conference, Sozopol, Bulgaria, June 5-9, 2007; revised papers. Berlin: Springer, 2008, S. 417-424.

Joseph, L. C.; Bennett, J. A.; Kirschner, K. N. [...]: Antiestrogenic and anticancer activities of peptides derived from the active site of alpha-fetoprotein. In: Journal of Peptide Science. 15 (2009), 4, S. 319-325.

Keller, V.; Rasheed, H.; Wäldrich, O.; Ziegler, W.; [...]: Models and internals of the ÏANOS resource broker. In: Computer Science - Research and Development. 23 (2009), 3-4, S. 259-266.

Kirschner, K. N.; [...]: GLYCAM06: a generalizable biomolecular force field. Carbohydrates. In: Journal of Computational Chemistry 29 (2008), 4, S. 622-655.

Klinger, R.; Kolárik, C.; Fluck, J.; Hofmann-Apitius, M.; Friedrich, C. M.: Detection of IUPAC and IUPAC-like Chemical Names. In: Bioinformatics 24 (2008), 13, S. 268-276.

Klinger, R.; Pesch, R.; Mevissen, T.; Fluck, J.: International Society for Biocuration: Methodical and Representation issues: 3rd International Biocuration Conference, Nature Proceedings, Berlin, 16.-19.4.09. Berlin, 2009.

Köddermann, T.; Paschek, D. Ludwig, R.: On the Validity of Stokes-Einstein and Stokes-Einstein-Debye Relations in Ionic Liquids and Ionic Liquids Mixtures. ChemPhysChem, 9: 1851-1858, 2008.

Köddermann, T.; [...]: What far-infrared spectra can contribute to the development of force fields used in molecular dynamics simulations. In: ChemPhysChem. 10 (2009), 8, S. 1181-1186.

Kolárik, C.; Hofmann-Apitius, M.: Linking chemical and biological information with natural language processing. In: Banville, D. L. (Hrsg.): Chemical information mining: facilitating literature-based discovery. Boca Raton: CRC Press, 2009, S. 123-150.

Kolárik, C.; Klinger, R.; Hofmann-Apitius, M.: Identification of histone modifications in biomedical text for supporting epigenomic research. In: BMC bioinformatics 10: Supplement 1 (2009): Selected papers from the 7th Asia-Pacific Bioinformatics Conference: Beijing, China, 13-16 Jan. 2009.

Krämer-Fuhrmann, O.: RCE - Reconfigurable Computing Environment: an open integration platform for distributed design. In: International Association for the Engineering Analysis Community: Simulation Data Management - Integration into the Product Development Process: NAFEMS Seminar, 18.-19.03.2009. Wiesbaden, 2009.

Larson, G.; Deryl, S.; Vanden Abeele, D.; Clees, T.: Application of single-level, pointwise algebraic, and smoothed aggregation multigrid methods to direct numerical simulations of incompressible turbulent flows. In: Computing and Visualization in Science 11, 2008, 1, S. 27-40.

Li, J.; Wäldrich, O.; Ziegler, W.: Towards SLA-based software licenses. In: Priol, T. u.a. (Hrsg.): From Grids to service and pervasive computing: 2008 CoreGRID Symposium, Feb. 25-26, Canary Islands, Spain. New York: Springer, 2008, S. 139-152.

Lob, M.; Peetz, J.-V.: Gekoppelte Simulationen in verteilten Rechnerumgebungen. In: Weisbecker, A. u.a. (Hrsg.): Software. Fraunhofer Enterprise Grids, 2008, S. 40-42.

Mei, L.; Thole, C.-A.: Data analysis for parallel car-crash simulation results and model optimization. In: Simulation Modelling Practice and Theory 16, 2008, 3, S. 329-337.

Müller, Th. J.; [...] Maaß, A.; Reith, D.: Economic simplex optimization for broad range property prediction: strengths and weaknesses of an automated approach for tailoring of parameters. In: Fluid Phase Equilibria 274, 2008, S. 27-35.

Peetz, J.-V.; Steckel, B.; Ettrich N.: Maths in flood protection. In: ERCIM News, 2008, 73, S. 23-24.

Peetz, J. V.: 3ZM-GRIMEX - coupled simulation environment for flood. In: Wolf (Hrsg.): 10th MpCCI User Forum, 2009, S. 122-125.

Pichot, A.; Wieder, Ph.; Wäldrich, O.; Ziegler, W.: Dynamic SLA Negotiation based on WS-Agreement. In: Cordeiro, J. u.a.: WEBIST 2008:

ANNEX

4th International Conference on Web Information Systems and Technologies, proceedings. Setúbal: Insticc Press, 2008.

Prätzel-Wolters, D.; Trottenberg, U.: Mathematik – Schlüssel zu Innovationen. In: Fraunhofer-Magazin, 2008, 4, Mathematik erleben, S. 2-3.

Qu, C.; Zimmermann, F.; Kumpf, K.; [...]: Semantics-enabled service discovery framework in the SIMDAT pharma grid. In: IEEE Transactions on Information Technology in Biomedicine 12, 2008, 2, S. 182-190.

Raekow, Y.; Simmendinger, C.; Krämer-Fuhrmann, O.: License management in Grid and high performance computing. In: Computer Science, Research + Development 23 (2009), 3-4: ISC '09 Scientific Day proceedings: International Supercomputing Conference, 23.-26.06.2009, Hamburg, S. 275-281.

Rajasekaran, H.; Lo Iacono, L.; [...] Friedrich, C. M.; Hofmann-Apitius, M.; [...]: @neurIST – Towards a system architecture for advanced disease management through integration of heterogeneous data, computing, and complex processing services. In: Computer Society/Technical Committee on Computational Medicine: 21st IEEE International Symposium on Computer-Based Medical Systems; June 17-19, 2008, Jyväskylä, Finland; proceedings. Los Alamitos: IEEE Computer Society Press, 2008, S. 361-366.

Rasheed, H.; Gruber, R.; Keller, V.; [...] Ziegler, W.: ÏANOS: an intelligent application oriented scheduling framework for an HPCN Grid. In: Gorlatch: CoreGRID, 2008, S. 237-248.

Ruau, D.; Kolárik, C.; Mevissen, H.-T.; [...] Hofmann-Apitius, M.; [...]: Public microarray repository semantic annotation with ontologies employing text mining and expression profile correlation. In: BMC Bioinformatics 9 (2008), Supplement 10, Art. 05.

Salisburg, A. M.; Deline, A. L.; [...] Kirschner, K. N.: Ramachandran-type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. In: Journal of computational chemistry. 30 (2009), 6, S. 910-921.

Scholz, J.; Toska, K.; Luborzewski, A.; Maaß, A.; [...]: Endogenous tetrahydroisoquinolines associated with Parkinson's disease mimic the feedback inhibition of tyrosine hydroxylase by catecholamines. In: The FEBS Journal 275 (2008), 9, S. 2109-2121.

Schwarz, F.: ALLTYPES in the Web. In: ACM Communications in Computer Algebra 42 (2008), 165/166, S. 185-187.

Schwarz, F.: Loewy Decomposition of Third-Order Linear PDE's. In: Gonzales-Vega, L.: ISSAC 2008: ACM-SIGSAM International Symposium on Symbolic and Algebraic Computation, July 20-23, 2008, Hagenberg, Austria, proceedings. New York: ACM, 2008, S. 277-286.

Seidel, J.; Wäldrich, O.; [...] Ziegler, W.: Using SLA for Resource Management and Scheduling – A Survey. In: Talia, D. u.a.: Grid Middleware and Services: Challenges and Solutions. New York: Springer, 2008.

Shahid, M.; Ziegler, W.; Kasam, V.; Zimmermann, M.; Hofmann-Apitius, M.: Virtual High Throughput Screening (vHTS) on an optical high speed testbed. In: Solomonides, T.: Global HealthGrid, 2008, S. 125-134.

Sherer, E.C.; Kirschner, K. N.; [...]: Efficient and accurate characterization of the Bergman cyclization for several enediynes including an expanded substructure of esperamicin A(1). In: The Journal of Physical Chemistry/B, Condensed matter, materials, surfaces, interfaces & biophysical chemistry 112 (2008), 51, S. 16917-16934.

Smith, L.; Tanabe, L. K.; [...] Klinger, R.; Friedrich, C. M.; [...]: Overview of BioCreative II gene mention recognition. In: Genome Biology 9, 2008.

Solomonides, T.; Hofmann-Apitius, M.; [...] (Hrsg.): Healthgrid research, innovation and business case: proceedings of HealthGrid 2009, 29 June - 1 July, Berlin. Amsterdam: IOS Press, 2009.

Steffes-Lai, D.; Thole, C.-A.; Nikitin, I.; Nikitina, L.: Interactive Optimization with DesParO. In: ERCIM News (2008), 73, S. 29-30.

Stork, A.; Thole, C.-A.; [...] Nikitin, I.; Nikitina, L.; [...]: Towards interactive simulation

ANNEX

in automotive design. In: The Visual Computer 24, 2008, 11, S. 947-953.

Talia, D.; Yahyapour, R.; Ziegler, W. (Hrsg.): Grid Middleware and Services: Challenges and Solutions. New York: Springer, 2008.

Thole, C.-A.: PICKEffizienter Austausch von Simulationsergebnissen mit FEMZIP. In: Weisbecker u.a. (Hrsg.): Software. Fraunhofer Enterprise Grids. 2008, S. 43-45.

Trottenberg, U.: Begeisterung durch Anwendungen und Algorithmen. In: Der mathematische und naturwissenschaftliche Unterricht 61 (2008).

Trottenberg, U.: Mathematik ist Technologie: Essay. In: Fraunhofer-Magazin (2008), 1, S. 30-31.

Trottenberg, U.; Clees, T.: Multigrid Software for Industrial Applications – From MG00 to SAMG. In: Hirschel, Ernst Heinrich; Krause, Egon (Hrsg.): 100 Volumes of 'Notes on Numerical Fluid Mechanics', 40 Years of Numerical Fluid Mechanics and Aerodynamics in Retrospect. Notes on Numerical Fluid Mechanics and Multidisciplinary Design, Vol. 100, Berlin: Springer, 2009.

Trottenberg, U.; Prätzel-Wolters, D.: Rechnen für Fortschritt und Zukunft. Innovationen brauchen Mathematik. In: Jahresbericht 2007, Fraunhofer-Gesellschaft. München: Fraunhofer-Gesellschaft 2008, S. 47-55.

Trottenberg, U.: Das Superrechnerprojekt SUPRENUM (1984-1989). In: Reuse, B. u.a.: Informatikforschung in Deutschland. Berlin: Springer, 2008, S. 176-187.

Tyagi, S.; Arnold, A.; Holm, Ch.: Electrostatic layer correction with image charges: A linear scaling method to treat slab 2D+h systems with dielectric interfaces. In: The Journal of Chemical Physics 129 (2008), 20, Art. 204102, 9 S.

Väänänen, J.; Trottenberg, U.: Maths for everyday life. In: ERCIM News (2008), 73, S. 10-11.

Weisbecker, A.; Pfreundt, F.-J.; Linden, J.; Unger, St. (Hrsg.): Grid check. Fraunhofer Enterprise Grids. Stuttgart: Fraunhofer IRB-Verlag, 2008.

Weisbecker, A.; Pfreundt, F.-J.; Linden, J.; Unger, St. (Hrsg.): Software. Fraunhofer Enterprise Grids. Stuttgart: Fraunhofer IRB-Verlag, 2008.

Wieder, Ph.; Ziegler, W.; Keller, V.: ÏANOS – efficient use of HPC Grid resources. In: ERCIM News, 2008, 74: Special issue, S. 27-29.

Wolf, A.; Hofmann-Apitius, M.; [...]: DockFlow - a prototypic PharmaGrid for virtual screening integrating four different docking tools. In: Solomonides, T. u.a.: HealthGrid 2009, S. 3-12.

Wolf, K.(Hrsg.): 9th MpCCI User Forum. Proceedings. 19.-20.02.08, Sankt Augustin: Fraunhofer SCAI, 2008.

Wolf, K. (Hrsg.): 10th MpCCI User Forum. Proceedings. 17-18.02.09, Sankt Augustin: Fraunhofer SCAI, 2009.

Ziegler, W.: Phosphorus: A European optical Grid test-bed. 2008.

ANNEX

Academic theses

Brühl, B.: Absatzprognosen für die Automobilindustrie in der Bundesrepublik Deutschland. Univ. Köln, Thesis, 2008.

Crngarov, A.: Analyse und OpenMP-Parallelisierung der Setup-Phase des algebraischen Mehrgitter-Codes SAMG. FH Bonn-Rhein-Sieg, Master Thesis, 2008.

Engbroks, B.: Lösung linearer Gleichungssysteme durch approximative Schur-Komplemente. Ein Vergleich verschiedener Verfahrensklassen. Univ. Köln, Thesis, 2008.

Frings, N.: Vergleich von Bildklassifikationsalgorithmen für chemische Strukturformeln. FH Koblenz, Bachelor Thesis, 2008.

Hahn, D.: Kompression von Simulationsergebnissen aus der numerischen Strömungsmechanik. FH Aachen, Thesis, 2008.

Heikamp, K.: Atomistic Simulations for the Polymer Precursor Methyl Methacrylate (MMA). FH Koblenz, Bachelor Thesis, 2008.

Kaiser, O.: AMG in der Erdölreservoirsimulation – Vergleich und Bewertung von Lösungsansätzen. Univ. Köln, Thesis, 2008.

Kavaliauskas, S.: PaperMaker: Consistency Analysis of Scientific Biomedical Literature. Univ. Bonn, Master Thesis, 2008.

Klimm, B.: A minimization based mapping algorithm for data transfer between simulation meshes. Univ. Köln, Thesis, 2009.

Kuznecov, E.: Entwicklung einer Retrieval- und Analyseapplikation für Chemiedaten basierend auf InfoZoom SDK. Univ. Bonn, Thesis, 2008.

Lainé, P.: Enhancing Methods for the Biomedical Knowledge Discovery Process. Univ. Bonn, Master Thesis, 2008.

Monroy Kuhn, J. A.: Beschleunigung der Echtzeit-Interpolation von FE-Daten mittels SVD. Univ. Köln, Thesis, 2009.

Oeckerath, A.: RBF-basierte Interpolation zwischen Finite-Element-Gittern in der Crash-Umform-Simulation. Univ. Köln, Thesis, 2008.

Oster, M.: Using Latent Semantic Indexing for the Disambiguation of Global Abbreviations in Biomedical Literature. FH Bonn-Rhein-Sieg, Thesis, 2008.

Qiong, L.: Network-based Approach for Analyzing Pathway Interactions. Univ. Bonn, Master Thesis, 2008.

Schneiders, F.: Numerische Konvergenzuntersuchungen am Lokal-Modell des Deutschen Wetterdienstes. Univ. Köln, Thesis, 2008.

Strötgen, J.: UTEMPL – Aufbau und Evaluierung einer UIMA basierten Textmining Pipeline für biomedizinische Literatur. Univ. Heidelberg, Thesis, 2009.

Thomas, Ph.: Automated extraction of variation mentions from literature sources and mapping to a unique database identifier. Univ. Tübingen, Master Thesis, 2008.

Younesi, E.: Analysis of molecular interaction networks associated with breast cancer tomour susceptibility. Univ. Bonn, Master Thesis, 2008.

HOW TO REACH US

We are looking forward to your visit to the Fraunhofer Institute SCAI. The institute is located next to Schloss Birlinghoven in Sankt Augustin, Germany (close to Bonn).

By car

From north and northeast: Follow the Autobahn A 59 to exit 41, Bonn-Beuel Ost. There turn right onto route B 56 to Sankt Augustin-Hangelar.*

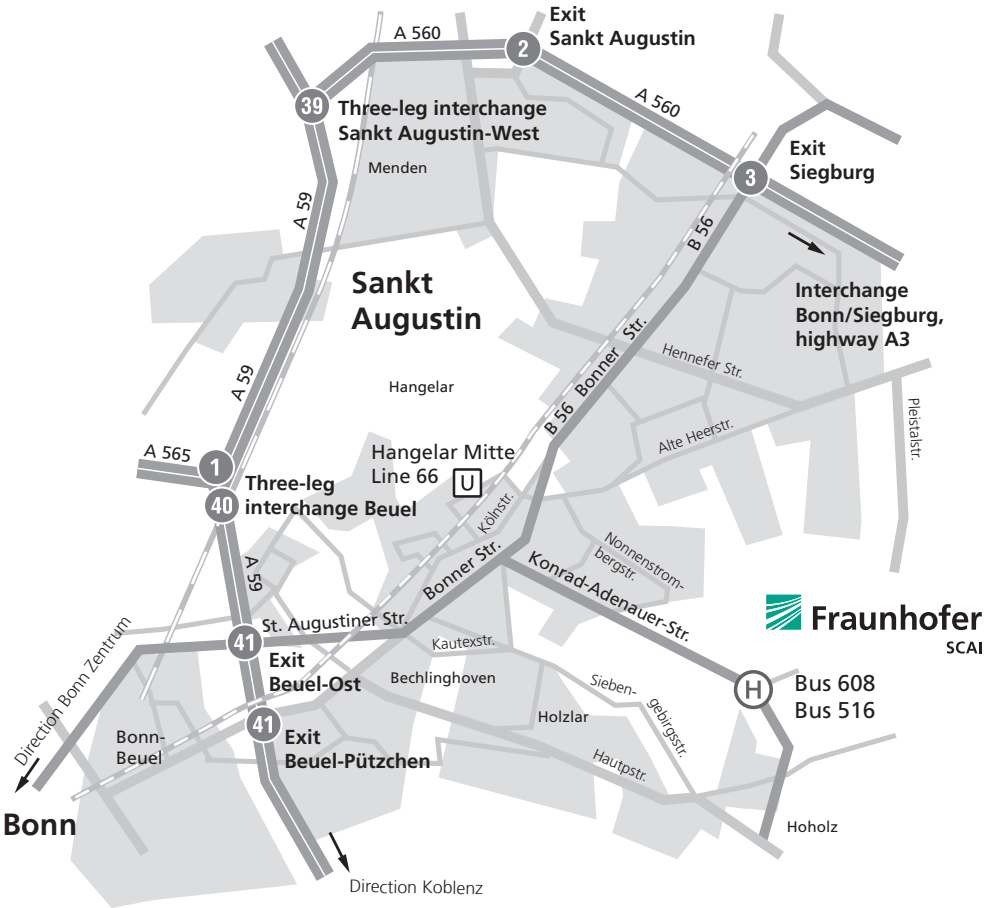
From south: Follow the Autobahn A 3 to exit 5, Bonn/ Siegburg. Turn onto the Autobahn A 560 to exit 3, Siegburg. Follow route B 56 to Sankt Augustin-Hangelar.*

From west: Follow the Autobahn A 59 to exit 41, Beuel-Ost and take route B 56 to Sankt Augustin-Hangelar.*

*At the crossing Bonner Straße/Konrad-Adenauer-Straße (sign to Schloss Birlinghoven and Bonn-Hoholz) turn into Konrad-Adenauer-Straße. About 3 kilometres farther, the entrance to Schloss Birlinghoven is on the left side.

By train

To reach Schloss Birlinghoven, take the train to Bonn Central Station or Siegburg/Bonn Station.
From Bonn Central Station, it takes about 20 minutes to get to Schloss Birlinghoven by taxi and from Siegburg/Bonn Station about 15 minutes.



To arrive by public transport, a tram (line 66) runs every 10 minutes during the day from direction Bonn or Siegburg/Bonn to stop Hangelar Mitte. From here, a connection bus (line 516) runs to Schloss Birlinghoven (only!) in the morning and evening.

From Bonn Central Station, you can also go by bus line 608 (destination Hoholz) leaving from bus platform B3. During weekday peak hours, the bus leaves every 20 minutes, the ride takes about 35 minutes.

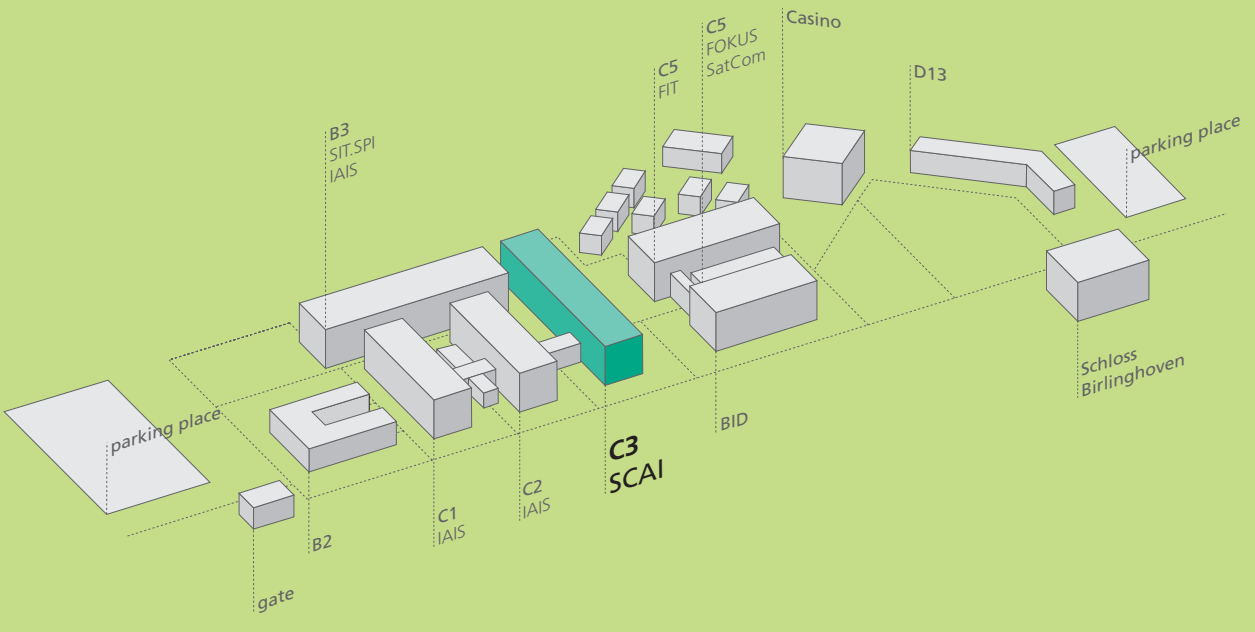
By plane

From Cologne Bonn Airport you can take a taxi to Schloss Birlinghoven, about 25 minutes away.

Alternatively you can take the Airport-Express-Bus 670 (destination Bonn Hbf). It leaves every 20 minutes and takes 35 minutes to Bonn Central Station. Then follow "By train".

From Düsseldorf Airport and Frankfurt Airport take the InterCity or the ICE to Bonn or Siegburg/Bonn. Then follow "By train".

Campus Map



EDITORIAL NOTES

A publication of the Fraunhofer Institute for Algorithms and Scientific Computing SCAI

Editorial team
Dipl.-Journ. Michael Krapp
Katrin Berkler, M.A.

Layout
Bianca Backert
Dipl.-Des. Till Martensmeier

Photos
page 13, MS Wissenschaft: Ilja C. Hendel
page 16, picture 2: Lucien Monfils, Creative Commons
page 16, picture 3: LINDENAU
page 20, picture 2: Inst. f. Strömungslehre, Univ. Karlsruhe
page 21, picture 3: ETH Zürich
page 21, picture 4: NUMECA International
page 23, picture 1: Flensburger Schiffbau-Gesellschaft
page 28, airplane: fotolia.de/sharply_done#7856923
page 40, picture 1: NVIDIA Corporation
page 41, picture 2: BPW Bergische Achsen

The editors express their gratitude to cooperation partners, who released their pictures for publication.

CONTACT

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

Phone +49 2241 14-2500
Fax +49 2241 14-2460
info@scai.fraunhofer.de

www.scai.fraunhofer.de