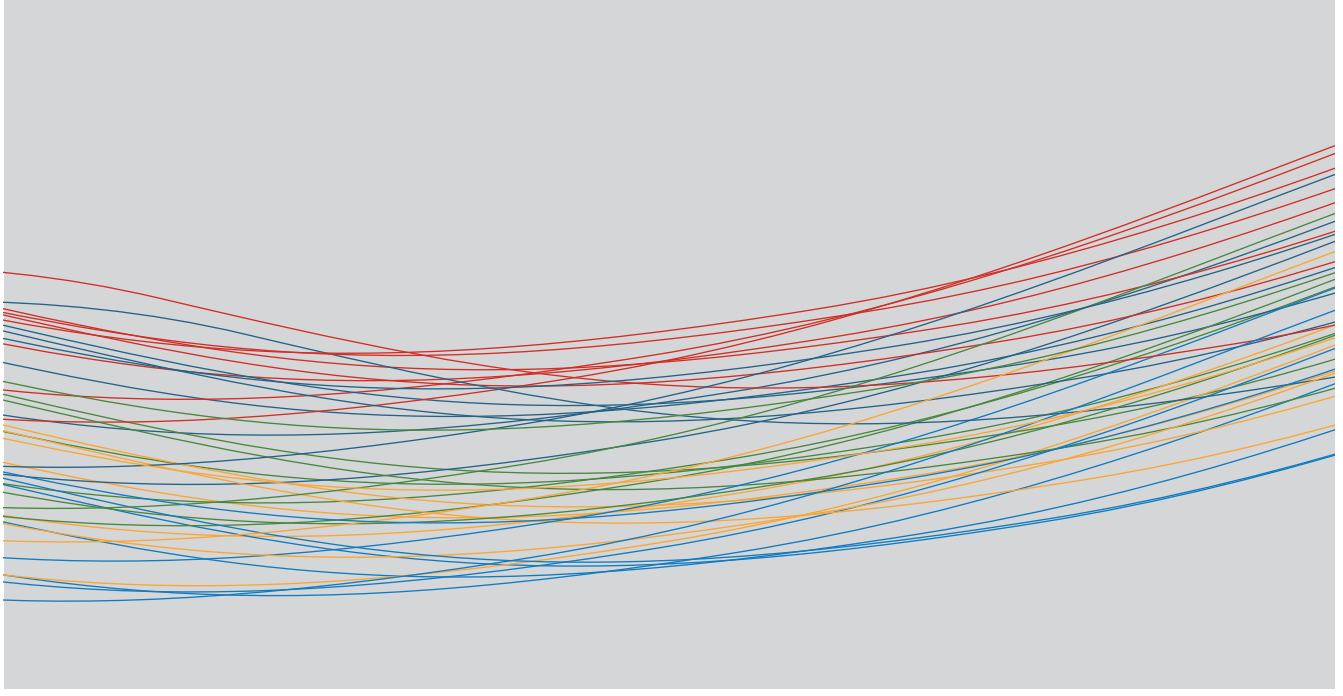
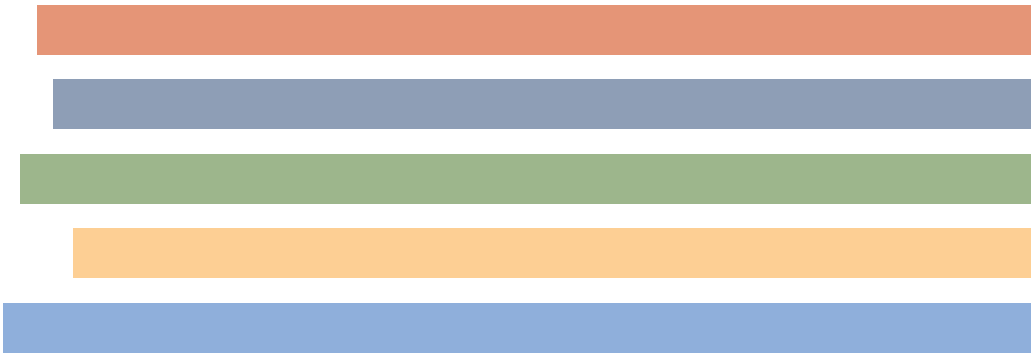
SCAI

Fraunhofer Institut
Algorithmen und Wissen-
schaftliches Rechnen

ANNUAL REPORT 2006





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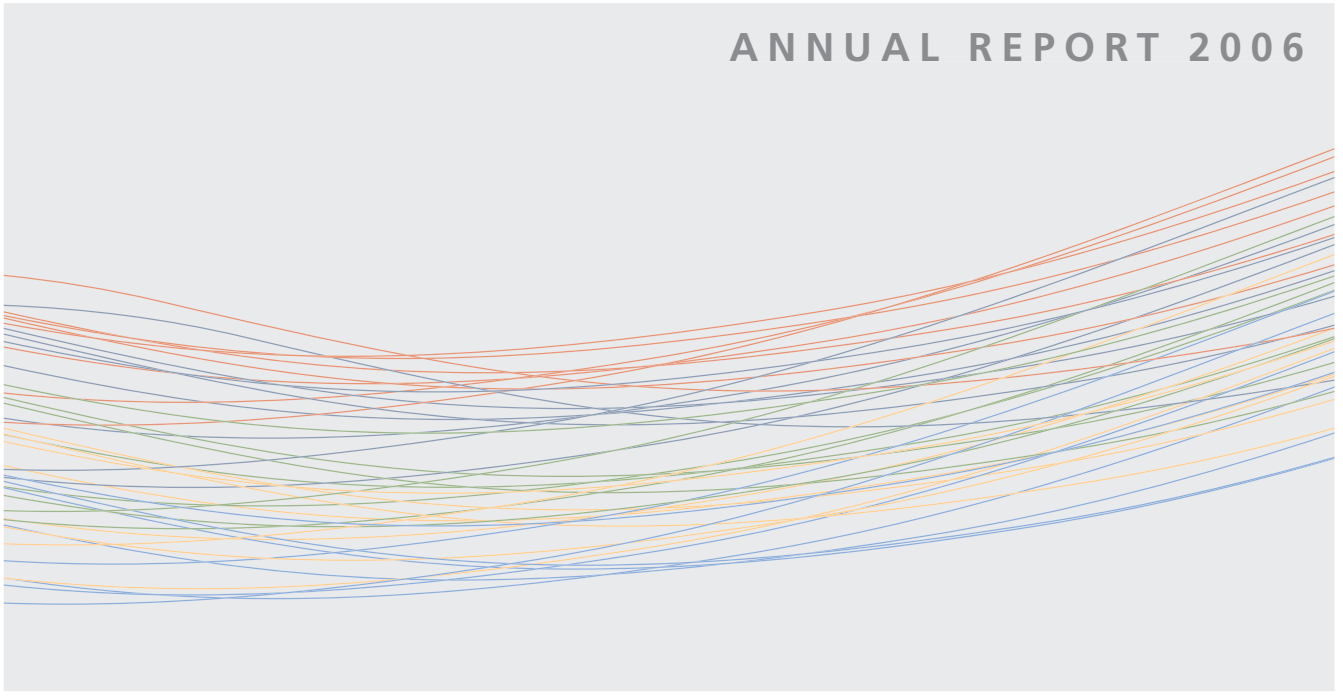


»Our products and services are based on highly innovative technologies in the fields of applied mathematics, computer science and engineering. Our fast algorithms and intelligent tools for data handling represent selling points in each of our departments.«

FRAUNHOFER SCAI

Prof. Dr. Ulrich Trottenberg

Director of the Fraunhofer Institute SCAI

Computer Simulation is the key technology in industrial product and process development. This technology is one of the main areas in which the Fraunhofer Institute for Algorithms and Scientific Computing SCAI is engaged in. Several of the software products and services provided by SCAI have worldwide visibility and reputation.

The SCAI researchers develop and combine methods from applied mathematics and information technology with know-how in engineering, applied and life sciences, as well as with business and production-oriented applications. The key competencies lie in scientific computing, the development of algorithms for complex industrial problems, software design, bioinformatics, information extraction, data and text mining and optimization. Our customers profit from integrated software solutions for distributed cooperative applications.

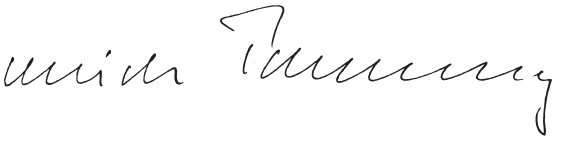
SCAI is not only a synonym for innovative competence, it also stands for unconventional and flexible approaches. SCAI develops industrial applications, provides customer-tailored solutions and advises business partners in the fast-increasing field of Grid Computing. We provide products and services to companies of all sizes. Not only large international industrial corporations work with our products and trust in our top-class services, but also small and medium-sized companies from various sectors.

Our institute consists of 4 research departments with a total number of 125 employees (including 10 Ph.D. and 30 graduate students), computer scientists, physicists, engineers, chemists, and biologists. They work in the fields of computer simulation, optimization and bioinformatics.

Fraunhofer SCAI is nationally and internationally linked to leading research institutions. Regionally, strong links exist first of all to the University of Cologne (through my chair of Applied Mathematics and Scientific Computing), then to the German Aerospace Center (DLR) (through the Simulation and Software Technology Group SISTEC headed by me), and last – but not least to the Bonn-Aachen International Center for Information Technology (B-IT) in Bonn where Fraunhofer SCAI members hold teaching positions.

2008 is the Year of Mathematics in Germany. This is a great opportunity for us to present our ideas for enhancing the competitive strength of the German economy and for organizing our living and working conditions in a networked world.

May I invite you to have a look at our research work and the services we offer. Your questions and ideas will be most welcome.



CONTENTS

SELECTED PRODUCTS

	PRODUCT	DESCRIPTION	CONTACT
MpCCI	MpCCI	MpCCI links simulation programs, thereby solving multidisciplinary problems. The software supports the leading industrial simulation tools.	Klaus Wolf +49 (0) 2241 / 14 - 2557
SAMG Algebraic Multigrid Methods for Systems	SAMG	Library of subroutines for the highly efficient solution of large linear systems of equations with sparse matrices.	Dr. Klaus Stüben +49 (0) 2241 / 14 - 2749
FEMZIP	FEMZIP	Tool for compressing LS-DYNA™ (FEMZIP-L) and PAM-CRASH™ (FEMZIP-P) results. It reads and reconstructs the native data formats.	Clemens-August Thole +49 (0) 2241 / 14 - 2739
DIFFCrash	DIFF-Crash	Stability of crash simulations in the automotive industry.	Helmut Schwamborn +49 (0) 2241 / 14 - 2312
DesParO	DesParO	System for multiobjective optimization, providing the user with complete control of optimization processes.	Clemens-August Thole +49 (0) 2241 / 14 - 2739
chemocr chemical compound reconstruction	ChemoCR	The tool extracts and reconstructs chemical structural formulas and their chemical structure depictions from scientific literature.	Dr. Marc Zimmermann +49 (0) 2241 / 14 - 2276
ProMiner	ProMiner	Tool for the identification of gene and protein names in scientific text.	Dr. Juliane Fluck +49 (0) 2241 / 14 - 2188
AUTO NESTER-L automatic nesting	AutoNester-L	Software package for automatic marker making on leather hides.	Dr. Ralf Heckmann +49 (0) 2241 / 14 - 2810
AUTO NESTER-T automatic marker making	AutoNester-T	Software package for automatic marker making on fabrics, sheet metal or wood.	Dr. Ralf Heckmann +49 (0) 2241 / 14 - 2810
CUT PLANNER automatic cut planning	CUTPLANNER	Software package for use in the textile manufacturing industry for automatic cut order planning.	Dr. Ralf Heckmann +49 (0) 2241 / 14 - 2810
PACK Assistant	PackAssistant	Software in the field of optimizing packing configurations of identical parts into containers.	Thorsten Bathelt +49 (0) 2241 / 14 - 2932

THE INSTITUTE IN PROFILE

The Fraunhofer-Institute for Algorithms and Scientific Computing SCAI engages in computer simulations in product and process development and is a strong partner in industry. SCAI designs and optimizes industrial applications and does calculations on high-performance computers. The aim is to reduce development times, make experiments less expensive and optimize technical products. The department of Bioinformatics focuses on solutions for information extraction in life sciences and chemoinformatics.
Scientists from the disciplines of mathematics, information technology, engineering, physics, biology and chemistry work together in interdisciplinary teams.

HUMAN RESOURCES, COSTS AND FINANCING

Human resources

In 2006 the staff numbers of the Fraunhofer SCAI remained constant. At the end of the year 2006 the staff consisted of 125 employees on 87 full-time positions, including eight Ph.D. and 30 graduate students. Due to the institute´s close relation with the universities of Cologne and with the Bonn-Aachen International Center for Information Technology (B-IT), the number of graduate assistants has been rising significantly. As in 2005 three apprentices began their training at the institute.

Costs and Financing

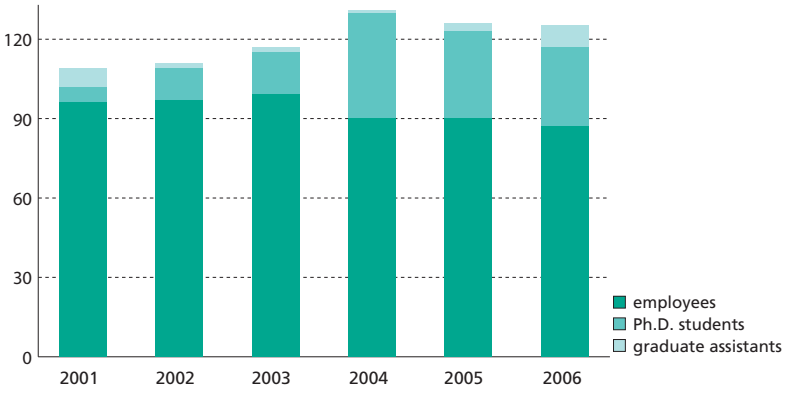
With 77 percent the biggest cost factor at Fraunhofer SCAI is determined by personnel costs, which is why the operating budget is growing with the number of staff. The operating expenditure of the institute amounted to 6.8 Million Euro, remaining on the previous years level.

In the period reported 0.5 Million Euro were invested in a cluster computer needed for a scientific project with the german D-Grid initiative as well as for additional hardware, software and network components.
The overall capital budget of the Fraunhofer SCAI amounted to 7.3 Million Euro.

Fraunhofer SCAI´s resources are generated 30 percent from revenues with industry, 30 percent from public-sector research and other earnings and 40 percent from Fraunhofer-Gesellschaft funding.

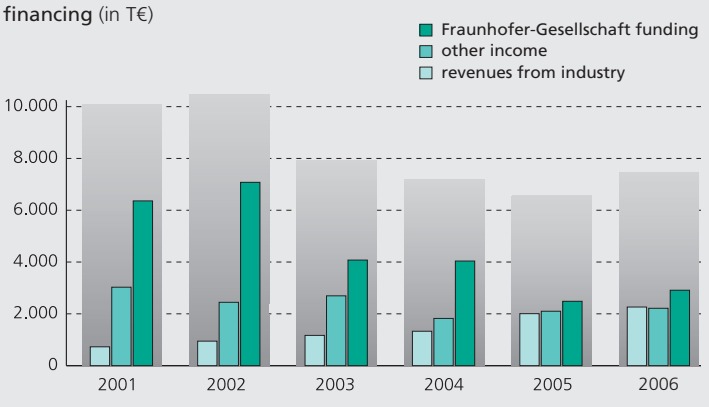
Director		Prof. Dr. Ulrich Trottenberg	+49 (0) 2241 / 14 - 2760
Deputy director		Dr. Johannes Linden	- 2910
Research departments			
	Simulation Engineering	Dr. Johannes Linden	- 2910
	Numerical Software	Clemens-August Thole	- 2739
	Bioinformatics	Prof. Dr. Martin Hofmann-Apitius	- 2802
	Optimization	Dr. Ralf Heckmann	- 2810
Central services			
	Administration, Planning and Controlling	Carl Vogt	- 2692
	Marketing and Communications	Michael Krapp	- 2935
	IT-Infrastructure	Horst Schwichtenberg	- 2577

Human resources



costs (in T€)

financing (in T€)



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Karl Solchenbach
Intel GmbH

The advisory board provides support both to the Fraunhofer-Gesellschaft and to SCAI. The board members share their contacts to industry, science and local organizations with the institute.
The constitutive meeting of the advisory board took place at Schloss Birlinghoven on 13th November 2005. From the left: Prof. Dr. Dennis Tsichritzis (former member of the executive board of the Fraunhofer-Gesellschaft), Prof. Dr. Ulrich Trottenberg (Director of Fraunhofer SCAI), Dr. Daniel Keesman (tailormade brand consulting), Prof. Dr. Martin Hofmann-Apitius, Carl Vogt, Klaus Wolf, Prof. Dr. Norbert Szyperski (Chairman of the institute´s advisory board, InterScience GmbH, Universität zu Köln), Karl Solchenbach (Intel GmbH), Dr. Johannes Linden, Prof. Dr. Tassilo Küpper (Universität zu Köln), Dr. Bernhard Thomas (Deputy chairman of the institute´s advisory board, Continental AG), Gerd Fiala (Fraunhofer-Gesellschaft), Dr. Ralf Heckmann, Clemens-August Thole, Prof. Dr. Thomas Lengauer (Director of the Max-Planck-Institut für Informatik, Saarbrücken), Dr. Eva Eggeling, and Stephan Springstubbe.

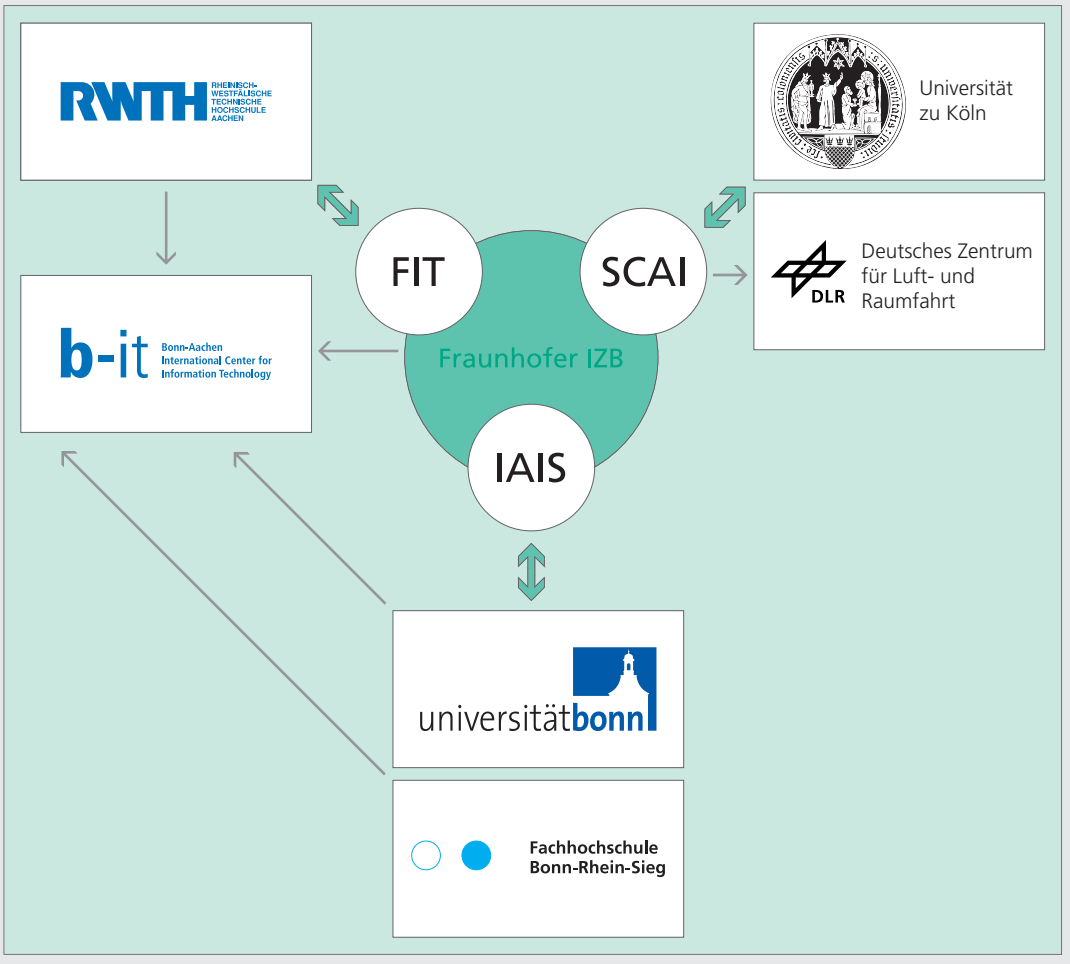
STRATEGIC RESEARCH PARTNERS IN THE AACHEN, BONN AND COLOGNE AREA

The Fraunhofer center Schloss Birlinghoven is associated via the chairs of the institute directors to the following universities:

- RWTH Aachen University (Prof. Jarke)
- University of Bonn (Prof. Wrobel)
- University of Cologne (Prof. Trottenberg)

Furthermore there is close cooperation with:

- Bonn-Aachen International Center for Information Technology (B-IT)
- Bonn-Rhein-Sieg University of Applied Sciences
- The German Aerospace Center (DLR)



THE FRAUNHOFER ICT ALLIANCE

Shorter innovation cycles have turned IT knowledge into a perishable commodity. The Fraunhofer Information and Communication Technology Alliance (ICT-Alliance) 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 Alliance comprises thirteen institutes as full members and two associated members, representing a workforce of roughly 2800 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 member institutes cover the entire value chain of the ICT industry. The ICT Alliance conducts activities within a wide range of business fields, including information and communication technologies for:

- Medicine and life sciences
- Traffic and mobility
- Culture and entertainment
- E-business
- E-government
- Production
- Digital media
- Software
- Security
- Communication systems and 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, virtual and simulated reality.

The alliance comprises the Fraunhofer Institutes for

- Algorithms and Scientific Computing SCAI
- Applied Information Technology FIT
- Computer Architecture and Software Technology FIRST
- Computer Graphics Research IGD
- Digital Media Technology IDMT
- Experimental Software Engineering IESE
- Industrial Engineering IAO
- Industrial Mathematics ITWM
- Information and Data Processing IITB
- Integrated Circuits IIS (associated member)
- Intelligent Analysis and Information Systems IAIS
- Open Communication Systems FOKUS
- Secure Information Technology SIT
- Software and Systems Engineering ISST
- Telecommunications, Heinrich-Hertz-Institut, HHI (associated member)

Prof. Dr. Dieter Rombach
Chairman of the alliance

Prof. Dr. Matthias Jarke
Deputy chairman

Contact
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Communication Technology Alliance (ICT-Alliance)
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Phone: +49(0)30 72615-660

www.iuk.fraunhofer.de

THE FRAUNHOFER-GESELLSCHAFT

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

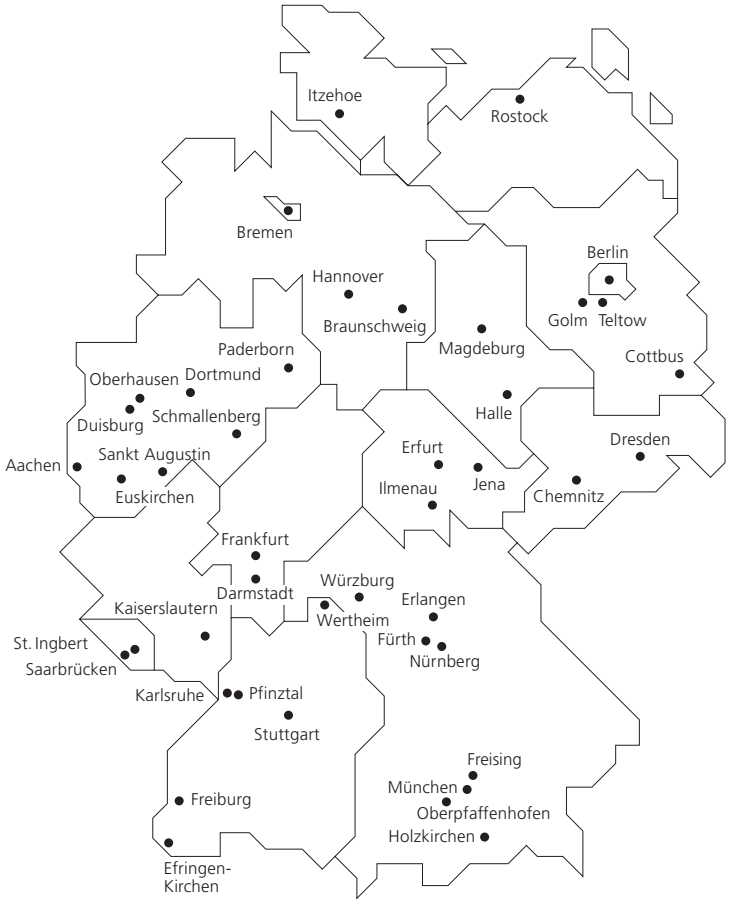
Applied research has a knock-on effect that extends beyond the direct benefits perceived by the customer: Through their research and development work, the Fraunhofer Institutes help to reinforce the competitive strength of the economy in their local region, and throughout Germany and Europe. They do 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 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 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.



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»Computer simulation accelerates the design of products and helps to optimize processes. This reduces time for development, saves real experiments and leads to better constructions of prototypes – in short: it reduces costs.«

Johannes Linden

SIMULATION ENGINEERING

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Klaus Wolf, Dr. Anton Schüller, Dr. Carsten Dehning and Dr. Johannes Linden (from left)

The department of Simulation Engineering develops numerical tools, algorithms and software solutions for complex applications in science and engineering. The emphasis is placed on multiphysics simulation and on high performance and Grid Computing.

In the multiphysics area, we currently focus on coupled simulations such as

- fluid-structure-interaction,
- thermal coupling in fluid dynamics and structural analysis,
- or magneto-hydrodynamics and plasma processes.

For the efficient and cost-effective solution of multi-physics problems, we have developed the coupling software MpCCI. It enables the user to directly couple codes from different application fields. MpCCI represents a multiphysics simulation environment which includes set-up and control of simulation runs, exchange of data between simulation codes, the mapping of computational meshes, efficient neigbourhood search and interpolations. MpCCI runs with most of the leading simulation codes for fluid dynamics and structural analysis. With more than one hundred licences sold, MpCCI has established itself as a solution accepted worldwide in the growing multiphysics community.

Our services include software support and consulting. In joint projects with research partners and customers we also develop tailored solutions, ranging from the physical modelling to computations on the institute's high performance computers.

High performance and Grid Computing have been core competencies of the department for many years. Our traditional focus is on the development of efficient algorithms, on the porting and optimization of software to various cluster systems and architectures.

In Grid Computing, the department is involved in many research projects on the national and European level. Within these projects the development of a distributed simulation platform which supports the collaboration in a virtual organisation is of particular importance for our work. This development is the central part of a joint research project with the German Aerospace Center and partners from the shipbuilding industry.

In 2006, the »Computational Chemical Engineering Group« was started with the department of Bioinformatics. The goal of this group is to improve and accelerate commodity design by way of molecular simulations. To overcome the general problem that many different length and time scales are involved, we utilize and develop efficient multi-scale methods. The current emphasis is on modelling polymer systems such as polystyrene melts.

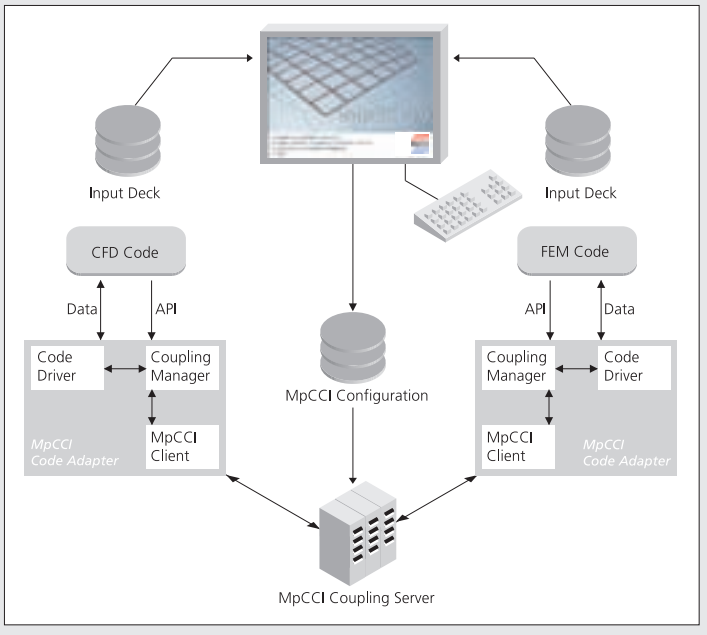
The following pages describe selected products and projects. More information about our grid projects can be found on page 34 ff.

Multidisciplinary simulation through code coupling with MpCCI

There is an increasing need for multidisciplinary simulations in various research and engineering fields. Fluid-structure interaction, magnetohydrodynamics, thermal coupling, plasma computations or coupled manufacturing processes define only a subset of recent multi physics activities.

There is a common feeling in the community that in most cases not a single (proprietary) simulation system can provide all necessary features but that coupling the best codes of each discipline will enable more flexibility and simulation quality to the end user.

The MpCCI interface has been accepted as a »de-facto« standard for simulation code coupling. MpCCI (Mesh-based parallel Code Coupling Interface) provides an application-independent interface for the coupling of different simulation codes. MpCCI is a software environment which enables the exchange of data between the meshes of two or more simulation codes in the coupling region. Since the meshes belonging to different simulation codes are not compatible in general, MpCCI performs a suitable interpolation. In case of parallel codes MpCCI keeps track of the distribution of the domains onto different processes. MpCCI allows the exchange of nearly any kind of data between the coupled codes; e.g. energy and momentum sources, material properties, mesh definitions, or global quantities. The details of the data exchange are hidden behind the concise interface of MpCCI.



MpCCI's modular architecture

Within the MpCCI 3.0 system the code adapters establish a direct connection between the MpCCI Coupling Server and the codes themselves. The adapters make use of the APIs of the commercial codes and thus (in most cases) need no modified versions of these codes. A code adapter is a library which is linked to the code either statically or dynamically. Any code adapter consists of two modules – the Coupling Manager and the Code Driver. Additionally, there are specific scripts for each code to scan the model input data, to start the codes and finally to stop the codes properly.

The MpCCI environment supports the codes ABAQUS, Ansys, Fluent, Flux3D, ICEPAK, MSC.Marc, Permas, StarCD, and RadTherm. Adapters for further codes like the 1D pipeline code Flowmaster are under development.

MpCCI 3.0 provides many new features for the coupling of simulation codes. Together with the MpCCI code adapters a complete toolbox for multidisciplinary simulation is now ready for use. Around 100 licensed users world wide demonstrate the applicability of this concept and the valuable outcome for the end users.

mpcci.de

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3-code coupling improves calculations of underhood car component temperatures

With the help of Fraunhofer SCAI´s coupling platform MpCCI, DaimlerChrysler was able to solve complex thermal calculations of underhood car components. The new trilateral partitioned approach, combining structural analysis, fluid dynamics and radiation, delivers accurate numerical results.

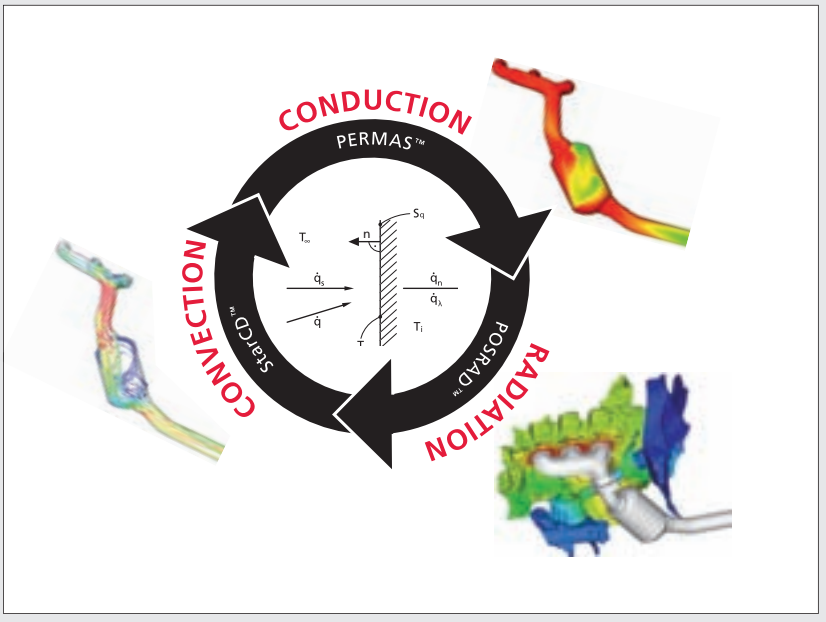
Thermal protection is of vital importance for the development process of passenger cars. Underhood component temperatures are sensitive to all three modes of heat transfer: conduction, convection and radiation. The calculation of underhood component temperatures of passenger cars requires the combination of three different disciplines: structural analysis, fluid dynamics and radiation. For the simulation of thermal conduction and convective heat transfer, a coupled fluid-structure environment is needed. With regard to the whole car geometry, radiation also plays an important role in the overall heat management calculation.
In areas with relevant fluid flows (e.g. engine compartment, gear box or exhaust system) convective heat transfer and radiation need to be calculated in a coupled environment.

DaimlerChrysler has started to use a fully coupled 3-code environment based on StarCD, PERMAS and POSRAD (a radiation code from CD adapco) to solve such thermal management applications. MpCCI was chosen as the coupling platform to realise this complex simulation approach. The standard MpCCI product version already provides an application independent interface for the coupling of two different simulation codes.

However, to solve the requirements of this specific application, MpCCI was extended to allow a coupling of 3 codes at the same time. The inner surface of the exhaust system is computed by coupling StarCD, PERMAS and POSRAD iteratively. For the outer surface PERMAS and POSRAD are coupled iteratively while the convective heat transfer is read in from include files.

This trilateral partitioned approach has demonstrated its capability to deliver accurate numerical results, with minor effort with respect to runtime and set up overhead. The new approach fulfils accuracy and runtime demands within a development process for passenger cars. In the near future this approach will be used to compute component temperatures in an entire car underhood, e.g. in case of »thermal soak«.

scai.fraunhofer.de/mpcci.html



A fully coupled 3-code simulation environment

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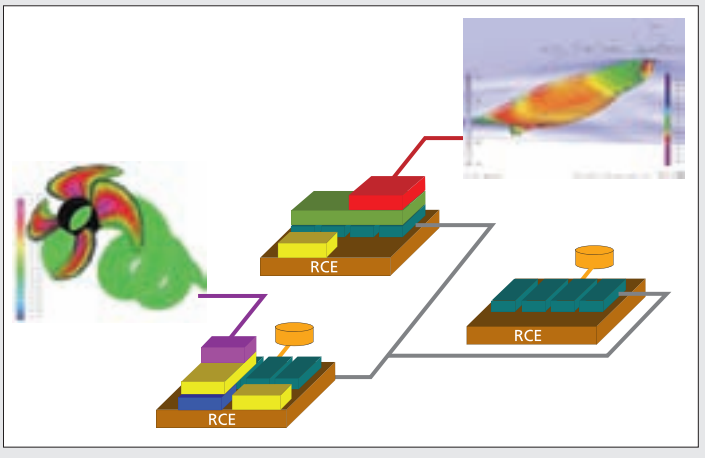
Reconfigurable computing environments speed up design processes in shipbuilding

The »Reconfigurable Computing Environment« RCE is a service oriented software infrastructure to manage collaborative engineering processes. It hides the complexity of heterogeneous and distributed IT systems behind common user interfaces and hereby enforces security in the access of data and services.

Concept

RCE is designed as an open system, which can be easily extended by application specific plug-ins. It is based on OSGi (Open Services Gateway initiative), the industry standard for modular dynamic java applications; therefore the RCE platform is independent and portable and can be used on any architecture from laptops up to mainframes.

Services are integrated as plug-ins, the central mechanism known from the Eclipse universe. Non-java codes, like C or Fortran decks, can be integrated via wrapper technologies, which were developed to integrate existing codes. This approach allows the re-use of existing software, thus saving earlier investments.



The distributed architecture of RCE.

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Communication between the components is realized via a generic interface. Various implementations realize data transfer depending on the distance of the partners and their security needs. RMI realizes communication in the same compute node, CORBA is used for intranet communication and WebServices pass firewalls between company domains.

RCE has an integrated user rights management, protecting the access to resources and services. The basic philosophy is that the owner fully controls his access to data or code. He has to explicitly grant access rights to other users or user groups. This is inevitable in collaborative industrial environments, where intellectual property rights have to be preserved.

Applications

Due to its open architecture, RCE can be applied to various application scenarios. In joint projects with German shipyards (Flensburger Schiffbau Gesellschaft and Lindenau GmbH Schiffswerft und Maschinenfabrik), RCE is used to integrate the ship design processes of the ship yard, their consultants and suppliers. The resulting »Ship Design and Simulation System« (SESIS) is based on RCE. It integrates the individual data bases of the companies, which are involved in the construction of a new ship. Grid technologies in SESIS provide simulation and optimization tools to all partners. Overall, SESIS significantly improves the design process of ships, which have to be constructed in a short time frame involving deep know-how of a large number of partners.

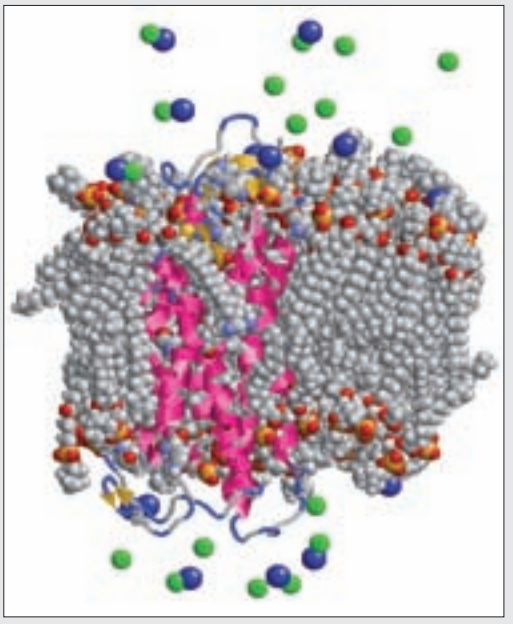
DLR and Fraunhofer SCAI are planning to establish RCE as a service oriented platform for future projects in other application areas. The integration of engineering processes in the automotive and aircraft industries is in preparation.

RCE is a joint project with the German Aerospace Center DLR in Cologne.

Chemical engineering by means of multi-scale simulations

Material and drug development involves the deep understanding of the microscopic behaviour and mechanisms of the investigated systems. Computer simulations linked at different length and time scales deliver the information needed for successful commodity design.

Many properties of chemical systems can only be understood by a thorough investigation of their microscopic details. To derive all relevant information, computer simulation is, in principle, an appropriate and efficient way. Due to the broad range of time and length scales involved, however, not all questions can be dealt with at the atomistic level in which all atoms are contained explicitly. The detailed treatment of degrees of freedom that govern small scales computationally prohibits the consideration of the longer modes that determine macroscopic properties. Coarse graining approaches side-step that problem: at a mesoscopic level, system-specific »superatoms« composed of up to ten atoms replace complete chemical repeat units. Mapping back and forth between the scales makes the computational task of deriving the interesting chemical and physical properties feasible, and hence, helps designing new commodities.



Membrane-embedded receptors, like the prototypic rhodopsin shown at left, are pharmaceutically most interesting. The aim is to gain control over cellular response by designing new drugs

SCAI scientists target both polymer and protein systems

In recent years, the above methods have proven to be robust and reliable, i.e. experimental data could be qualitatively reproduced and new insight could be gained. Scientists are now able to derive properties of a great variety of chemicals in different system states by means of multi-scale simulations. Industry can directly benefit from computationally gained knowledge in order to optimize production, to steer key developments in a better direction, or to execute whole series of experiments which would not be feasible otherwise. Typical system examples are polymers in melts or solution (e.g. polystyrene or polyacrylic acid), polypeptides in water, low-molecular liquids (e.g. solvents), and mixtures. Researchers are capable of studying surface adsorption effects, system annealing and quenching, gas permeation effects, or calculating transport coefficients like the thermal conductivity or shear viscosity. To do so most efficiently and to be able to constantly utilize the latest scientific developments, Fraunhofer SCAI collaborates intensively with world-renowned academic partners, like the Max-Planck-Institute for Polymer Research Mainz, the Technical University of Darmstadt, and the University of California, Davis.

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»The great challenge of the future is the combination of interactive simulation with robust design, which has been made possible by extremely efficient, scalable solver technology.«

Clemens-August Thole

NUMERICAL SOFTWARE

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Dr. Klaus Stüben and Clemens-August Thole

The use and the impact of numerical simulation for virtual product development and for the understanding of product properties are continuously growing. A reduction of product cycle time, for example in the automotive industry, is not possible without an increase in the use of numerical simulation. For the exploitation of oil fields, it is only through numerical simulation that knowledge pertaining to the processes occurring in the interior of an oil reservoir can be obtained and that hence an analysis of the various recovery strategies in order to guarantee optimal exploitation can be made. As before, it is the creativity and experience of the engineer which determines the quality of the product. However, he will be able to enhance his abilities to the degree to which

- simulation software is more strongly integrated into optimization processes,
- the precision of the models involved is increased,
- simulations can be carried out interactively.

Here, however, current numerical simulation often reaches its limits. Thus, necessarily, the typically long run times of the simulations must be substantially reduced. In addition, various tools for a detailed analysis and reuse of the simulation results are not available.

Core Activities

The development of methods and software which, as indicated above, enable a more efficient use of industrial software is the focus of our activities.
On the one hand, this is the development of highly efficient software for the optimal and scalable solution of large systems of linear equations, as they occur at the heart of typical simulation packages. The focus is centered on modern hierarchical approaches (products SAMG and HLIBpro).
The analysis of data and design optimization, especially with regard to robust design, also belong to our main fields. 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.

Possibilities and Perspectives

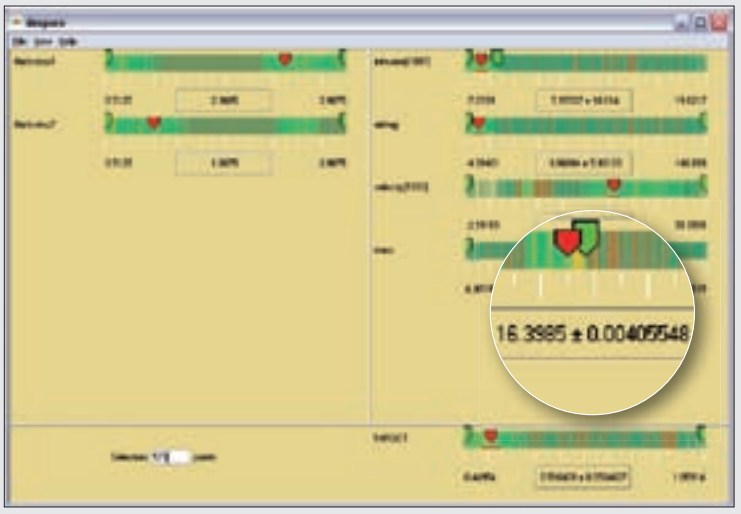
Most of the technologies and methods mentioned are already available as individual products suitable for industrial use. The strong interest expressed by many companies, especially in the oil and automotive industries, documents the relevance of these developments for numerical simulation.
The great challenge of the future is, however, the combination of interactive simulation with robust design, which has been made possible by extremely efficient, scalable solver technology. Interactive simulation – i.e. push a button for alternative models, in real time, analyzed and evaluated – this is what the strategic work in NUSO is oriented towards.

DesParO – Interactive environment for the optimization of design parameters

In contrast to existing automatic optimization tools, DesParO allows the user to interactively explore the whole space of design variables and to find the optimal region with respect to multiple design objectives.

DesParO provides the user with a global view of the design space, reveals a full set of alternative solutions, and allows the user to find a truly optimal design. Consequently, DesParO is free of common drawbacks inherent to automatic optimization tools, such as a solution stuck at a local optimum, which is typical for differential methods, or exhaustive numerical experimentation required by Monte-Carlo-like strategies.

The underlying optimization algorithm has been successfully evaluated in a number of real-life multidimensional problems (in particular, from automotive design), characterized by a high number of design variables (up to 100) and a high number of design objectives (up to 50). DesParO is available as standalone application for Windows and Linux platforms and as a documented SDK for integration into other optimization software.



Graphical User Interface – the zoom shows the visualization of tolerances.

Optimization with DesParO

In addition to the convenient exploration capabilities, DesParO offers the following unique features:

- Robust tolerance prediction: DesParO predicts not only the value of the design objective, but also the tolerance limits on the objective. In case of noisy objectives constraints can be satisfied in a safe manner, including the tolerance, and the optimal design can be obtained.
- Global correlation analysis: DesParO automatically recognizes a pattern of interdependencies between the optimization criteria and design variables and represents it as an easily readable colour-coded diagram. The diagram indicates most influencing design variables, most sensitive optimization criteria and shows also a sign of dependency: increase, decrease or non-monotony.
- Interpolation of FEM data: DesParO also provides interpolation of bulky data, such as FEM data files containing the results of numerical simulation, to the values of design variables specified by the user. This allows the visualization of a full solution immediately and to inspect in detail the obtained optimal design.

Solution of an optimization problem in DesParO proceeds through the following steps:

- Set a desired region for optimization criteria. This causes a corresponding range of design alternatives in parameter space to be displayed.
- Evaluate the design alternatives, taking tolerances into account.
- Identify the optimal design.

scai.fraunhofer.de/desparo.html

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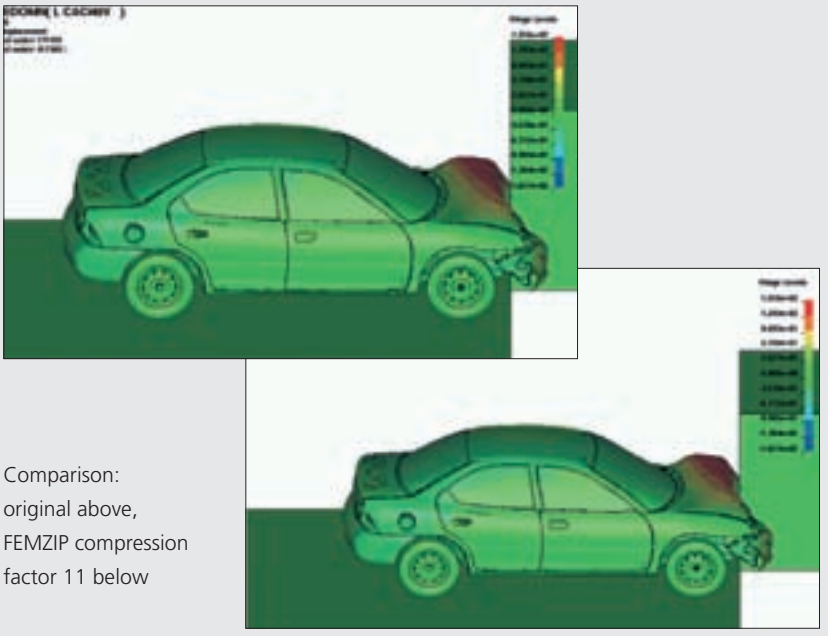
FEMZIP – Making extra-large data archives manageable

Simulation programs open new vistas for product development and strike terror into the hearts of IT managers responsible for archiving the resulting terabytes and petabytes of data. SCAI has developed compression tools to alleviate this problem.

In engineering, the hunger for ever more data storage is by far outstripping the capacity increase of archiving hardware. We have developed specialized tools in several areas to compress this data. One example is the lossless compression of meteorological data, where data archives reach 5 petabytes, but we are also active in the other engineering fields. In particular, in the field of crash simulation, we have developed a tool, FEMZIP, now more or less an industry standard, which not only reduces archive sizes drastically, but in the newest versions also accelerates access to the data for visualization, one of the main uses of the data in this field. This tool is specialized for the compression of LS-DYNA (FEMZIP-L) and PAM-CRASH (FEMZIP-P) results. It reads and reconstructs the native data formats. With the high compression rates of FEMZIP, storage and backup resources can be reduced by a factor of about 10. Additionally these high compression rates allow a fast exchange of compressed files via data networks.



Comparison: original above, FEMZIP compression factor 11 below

How does it work?

Crash simulation results are usually stored in a 32 bit floating point representation. Due to numerical approximation errors and the inaccuracy in the model description itself, the 32 bit floating point representation is usually far too accurate. FEMZIP allows the user to specify his accuracy preferences in a parameter file. Mathematically speaking, 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.

The compression and decompression modules of FEMZIP 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 shorter than opening an uncompressed crash result file.

scai.fraunhofer.de/kompression.html

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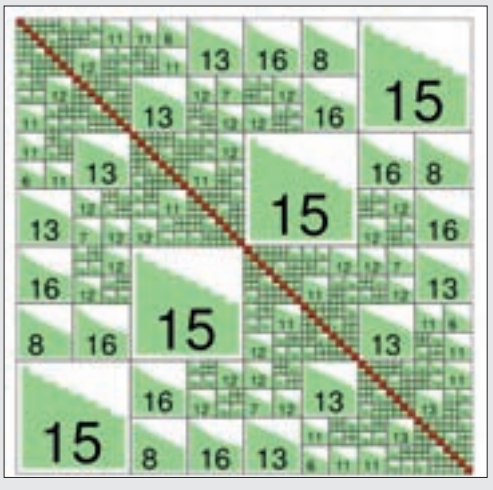
HLIBpro – Efficient solution by means of hierarchical matrices

Modern advanced simulation systems require highly efficient numerical solution strategies to yield answers in an economical time frame. The technique of hierarchical matrices provides a means to solve many large applications in a (nearly) optimal way.

HLIBpro is a software library by which large applications with nearly optimal performance can be solved. It is especially suited for the numerical solution of integral and elliptic partial differential equations, in particular those corresponding to exterior domain problems. By now, the underlying technique has been successfully used in micro structure and electrical circuit simulations (automotive industry), population dynamics, particle methods for incompressible flows, cognitive neuroscience (medicine) and induction heating. For advanced electrical circuit simulation problems, for example, the discretization matrices are so huge that they cannot be set up and stored on a computer. HLIBpro provides a means to tackle even such problems and solve them with (nearly) linear complexity.



An exemplary H-matrix structure for a 1000 x 1000 matrix. The numbers represent a parameter related to the reduction of the matrix dimension (»low rank approximation«).

HLIBpro is being jointly developed by the Max-Plank-Institute for Mathematics in the Sciences (MPI MIS) in Leipzig and the Fraunhofer-Institute SCAI. The main focus is on industrial applications, the target group being software houses as well as industrial companies developing their own simulation software and requiring particularly efficient numerical solvers.

Hierarchical Matrices (H-Matrices)

HLIBpro is based on the theory of hierarchical matrices. This theory, first introduced by Wolfgang Hackbusch from MPI MIS in 1999, provides a technique to represent various types of – even full – matrices in an effective data-sparse format, and a special way to perform matrix arithmetic. Based on this, matrix-vector multiplication, matrix-matrix addition and multiplication as well as matrix inversion can be performed with almost linear complexity. Even matrix equations can be solved with similar complexity. HLIBpro provides all necessary routines for the construction of hierarchical matrix structures, arithmetic algorithms that perform certain approximate matrix operations (such as addition, multiplication and inversion), as well as algorithms for decomposing matrices, e.g. LU- and Cholesky-factorizations. Finally, various solvers for solving linear equation systems, direct as well as iterative ones, are included.

Many types of sparse and dense matrices arising in practical applications (in particular, discretized integral equations or elliptic boundary value problems) can very well be approximated by hierarchical matrices.

scai.fraunhofer.de/hlibpro.html

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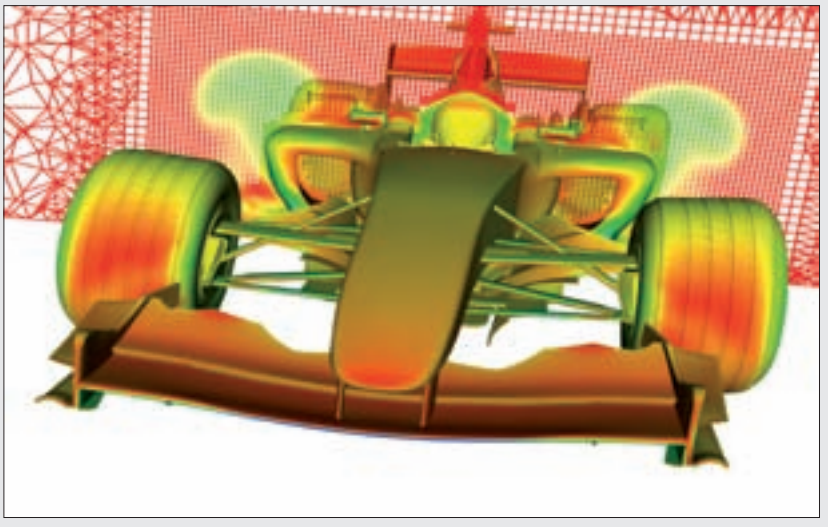
SAMG – Dramatic performance improvements by using algebraic multigrid methods

In many application areas, the computational time required to solve huge, sparsely populated linear systems of equations is today's major bottleneck in the practicability of numerical simulation. Therefore SAMG has become a well-established tool for important software providers and major oil companies.

Algebraic multigrid (AMG) is becoming increasingly popular as an advanced technique for the highly efficient solution of important types of large and sparsely populated linear systems of equations, both in scientific development and industrial application. SAMG is an advanced software library based on this technique with the main focus on industrial applications.

While ever-increasing problem sizes and increasingly complex geometrical structures have highlighted the limits of classical solvers, SAMG's major advantages – numerical scalability and ease-of-use – have become the driving forces behind its growing success in industrial use. SAMG is currently being used in such diverse areas as fluid flow, structural mechanics, oil reservoir and ground water simulation, casting and moulding, process and device simulation in solid state physics, electro-chemistry, and circuit simulation. In particular, in oil reservoir simulation, SAMG has become a well-established tool for important software providers as well as major oil companies.



Cross section of a highly complex mesh for the simulation of exterior flow around a racing car (courtesy of Fluent and Sauber-Petronas)

Numerical scalability: a requirement for advanced solvers

Scalability requires hierarchical algorithms which, mathematically speaking, ensure a rapid reduction of both short and long range error components. A breakthrough, and certainly one of the most important advances in numerical development, was due to the (geometric) multigrid principle. Algebraic multigrid solvers attempt to combine the advantages of geometric multigrid – based on the efficient interplay between smoothing and coarse-grid correction - with those of easy-to-use plug-in solvers. However, while geometric multigrid explicitly requires and exploits grid structures, AMG operates directly on the linear system of equations, obtained through a discretization process. As a consequence, AMG-based solvers are easy to integrate into existing simulation packages – one of the major reasons for their industrial success.

During the last years, systematic extensions of the classical AMG approach have been investigated and realized in the SAMG package. In particular, SAMG is not just a solver but rather a highly flexible multilevel framework which can be adapted to specific requirements of various problem classes.

scai.fraunhofer.de/samg.html

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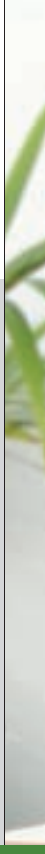

»Data mining technologies play a pivotal role in all industries that are based on knowledge. Having all relevant information at hand is a pre-requisite for rational decision making. We serve knowledge driven research & development through cutting edge technology for automated information extraction – with a particular focus on the life science industries and the publishing industry.«

Martin Hofmann-Apitius

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The Department of Bioinformatics at the Fraunhofer Institute SCAI conducts applied research and development in the field of:

- Information Extraction/Semantic Text Analysis
- Applied Chemoinformatics
- Grid Computing

In compliance with the general mission of a Fraunhofer Institute, the Department of Bioinformatics works closely with industrial partners – including small and medium size enterprises – to enhance their competitiveness through mediating knowledge and technology transfer from academic research to industrial application. Collaborative research and development projects of the Department of Bioinformatics deliver solutions to the pharmaceutical and biotech industry and to the publishing industry. Positioned at the boundary between pure commercial and pure academic research we maintain strong links to both communities. Two products have been developed which are both solving problems prevalent in the management of information in the pharmaceutical and publishing industry:

ProMiner, a system for the detection and disambiguation of biomedical named entities such as gene names, protein names, disease names and drug names in text. ProMiner has been developed together with industrial partners and has been successfully evaluated in BioCreative 2004, an international critical evaluation of text mining solution in molecular biology.

chemoCR, a system for the reconstruction of chemical information from chemical structure depictions. This tool has been developed to make one of the largest sources of chemical information accessible: the information communicated through images containing chemical structure depictions. Although communication of chemical information through 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 tools are addressing the issue of making information hidden in scientific text and image sources available for improved retrieval, information extraction and knowledge discovery. Our industrial partners use our tools for indexing of large document collections, normalization of named entities in scientific literature and data interpretation of high content data. Together with our grid research team we are working on making these tools available in distributed information management environments.

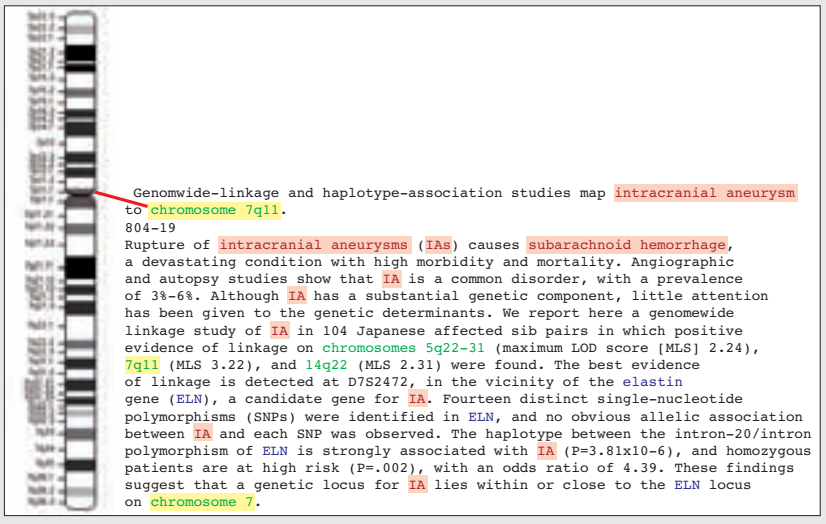
The department takes part in the education of students of the Life Science Informatics curriculum of the Bonn-Aachen International Centre for Information Technology (B-IT) and we participate actively in various national and European research initiatives. Currently, the Department comprises 16 scientists including 6 PhD students.

Finding the names of genes and proteins in scientific literature

The software package ProMiner extracts information from scientific texts. This identification is based on automatically generated lexica. The performance of ProMiner for the recognition of gene and protein names in text has been demonstrated in BioCreative.

Problem description

Up to date information about biomedical entities like genes, proteins, diseases or drugs is often not found in structured databases but rather in scientific text. For specific information retrieval or information extraction the recognition of these terms and their normalisation to database entries (e.g. gene names to ENTREZ-GENE) or structured vocabulary/ontologies (e.g. GO/MESH/UMLS) is a prerequisite. The need of normalisation implies the usage of dictionaries generated from these sources and the inclusion of direct mappings. As databases and ontologies are evolving rapidly, automated updating and processing is needed to generate comprehensive and specific dictionaries.



ProMiner automatically recognizes biomedical entities and their spelling variants in texts.

The high ambiguity of terms and acronyms used in the Life Science domain complicates precise recognition further.

Technology

ProMiner is a tool developed for the identification of biological, medical or chemical named entities in scientific text. The entity recognition in ProMiner is based on a dictionary approach and can work with voluminous dictionaries, complex thesauri and large controlled vocabularies derived from ontologies. Automated generation, curation and updating is followed by an automatic and manual evaluation process. ProMiner addresses several fundamental issues in name 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

The impressive performance of ProMiner for the recognition of gene and protein names in text has been demonstrated in BioCreative I where an F-score of 0.8 could be reached for fly and mouse and an F-score of 0.9 for the yeast organism.

Technical Specification

ProMiner is available for UNIX/Linux and Microsoft Windows. ProMiner can be used as stand alone software for indexing purposes or integrated in larger processing pipelines (e.g. as a pre-tagging module for information extraction systems). The software is already integrated as an annotator service for named entities in the Unstructured Information Management Architecture (UIMA) framework.

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The computer recognizes chemical structures in text

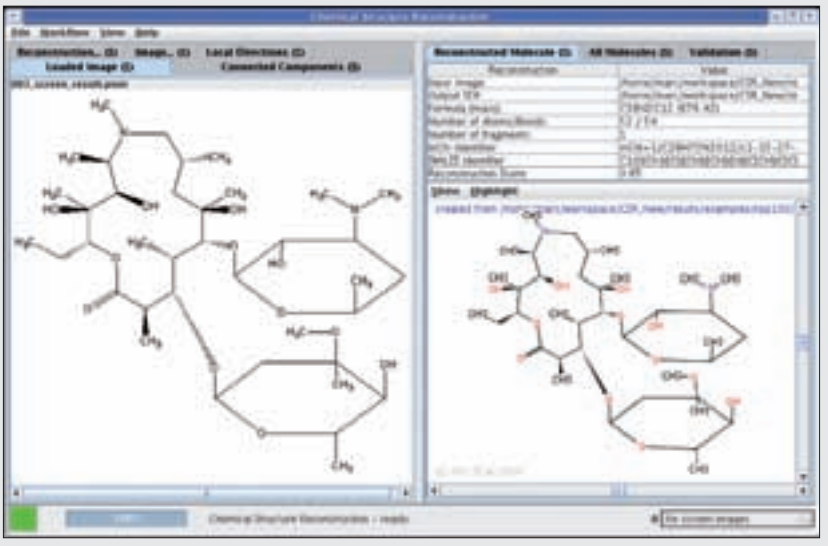
ChemoCR, tool for Chemical Structure Reconstruction, extracts chemical structural formulas and their chemical structure depictions from scientific literature. The software package converts the structure depictions into a format the computer can use to process the information contained in the depictions.

Problem description

Chemical entities can appear in scientific text as trivial and brand names, assigned catalogue names, or IUPAC names. However, the preferred representation of chemical entities is often a two-dimensional depiction of the chemical structure. Depictions can be found as images in nearly all electronic sources of chemical information (e.g. journals, reports, patents, and web interfaces of chemical databases). Nowadays, theses images are generated with special drawing programs, either automatically from computer readable file formats or by the chemist through a graphical user interface. Although drawing programs can produce and store the information in a computer readable format (i.e. the connection table), chemical structure depictions are published as bitmap images (e.g. GIF for web interfaces or BMP for text documents). As a consequence, the structure information can no longer be retrieved by chemical search engines or used as input to chemical analysis software packages. To make published chemical structure information available in a computer-readable format, images representing chemical structures have to be manually converted by redrawing every structure. This is a time-consuming and error-prone process.

Technology

To solve the problem of recognizing and translating chemical structures in image documents, our chemoCR system combines pattern recognition techniques with supervised machine-learning concepts. The method is based on the idea of identifying from depictions the most significant semantic entities (e.g. chiral bonds, super atoms, reaction arrows…). The workflow consists of three phases: image preprocessing, semantic entity recognition, and molecule reconstruction plus validation of the result. All steps of the process make use of chemical knowledge in order to detect and fix errors. The system adapts to different sets of input images.



Snapshot of the CSR graphical user interface. In the left panel the input image and the intermediate reconstruction results are shown..

Technical Specification

The chemoCR core functionality is based on platform independent JAVA libraries. It has been tested on UNIX operating systems (Fedora Linux, Sun Solaris) and on Windows XP. External tools can be easily included in the workflow. Our software can be used interactively by a graphical user interface or it can be run distributed in batch processing mode. Our benchmark test set consisting of 8000 images of natural products is processed in about two hours.

scai.fraunhofer.de/chemocr.html

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»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 in the shortest possible 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.«

Ralf Heckmann

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Dr. Ralf Heckmann

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

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

The optimization department acts as an optimization consultant for trade, commercial, or industrial companies. Among the services we offer are the following:

- Consulting/Problem analysis: Evaluation of the solution complexity of a given customer problem
- Specification: Development of mathematical, methodological descriptions of a given problem
- Development of custom-cut solutions: Creation of an optimization software with precise consideration of the problem-specific fundamental and ancillary conditions
- Development and sale of standard products: Alone or together with partners we develop, market and sell products for standard problems (e.g. AutoNester, PackAssistant, CUTPLANNER)
- Maintenance: Based on the wishes of our customers we offer all kinds of maintenance, training and support in order to guarantee best possible life cycles of our solutions
- Further development and customization: We offer further development of our solutions, even after years, as well as customization of our standard products to individual needs.

SCAI has about 20 years of experience in optimization and also a large construction set of optimization methods at its disposal which can be fallen back upon when constructing solutions for new problems. Depending on the problem that needs to be solved we identify and employ the best fitting state-of-the art optimization technique enriched with our special knowledge and improvements and added by problem specific constraints.

Cooperation between SCAI and our customers is performed in many different ways using a wide variety of business models. As an example, a typical development cooperation can start with a first non-binding meeting to discuss the problem solvability. Since many optimization problems are complex the second step can be creating a specification together with a first draft for its solution. In the next step an optimization software or a simulation is developed.

Cutting, packing and arrangement problems

In nearly 20 years of experience, the optimization department has gained a multilayered knowledge regarding effectiveness and suitability of the different optimization methods. The arrangement of objects in one, two or three dimensions are examined and solved.

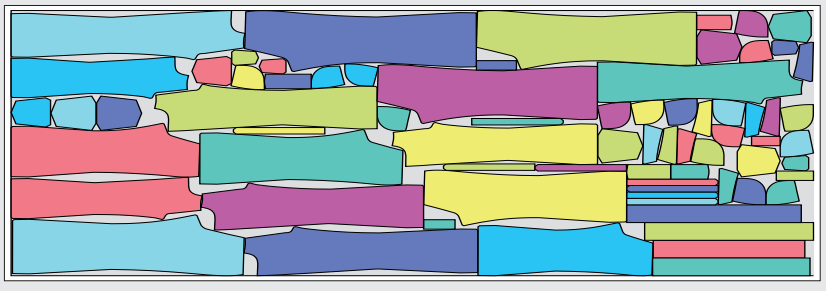
Although arrangement and cutting and packing problems can occur in many variations, they essentially all have the same logical principle. A certain resource (e.g., material, personnel, time, space, money) must be used as optimally as possible by determining an efficient subdivision. The problems get their individual face by the constraints that describe how such subdivisions must happen. These differences in the constraints often require totally different methodical approaches for the solution of such problems. It is possible to prove that nearly all practically relevant problems belong to a class of problems whose mathematical solution is very difficult. In computer science, this class is known as the NP-hard problems. I.e. expert knowledge and experience is needed in order to find good solutions for such kinds of problems.

In spite of progressive automation of production processes, cutting and packing problems in many companies are still solved manually nowadays – partly under considerable effort of time and personnel. The reasons for this are complex. Some companies fight shy of changing their production processes, others don't have the know-how, or unknown interfaces in hardware and software systems make a continuous automation more difficult. But often inherent cutting and packing problems are not recognized as such or it is supposed that – due to their complexity – known cutting and packing problems cannot be solved with the help of a computer. Especially regarding the last two topics, Fraunhofer SCAI has shown in the last years that it is possible to solve difficult and extensive problem settings in leading international countries automatically. The realized solutions have led to significant cost savings and a quality increase in the production process.

Also problems which, at a first glance, do not look like packing problems can possibly be modelled as such and be solved by similar methods. Well-known examples for this are deployment planning of personnel and resources, e.g. the creation of timetables or work plans, load planning of machines or vehicles, job scheduling, and coin changing problems.

Examples of recent and current projects

AutoNester is our flagship product for two-dimensional nesting, i.e. for the automatic creation of the best possible arrangement of cutting patterns on a wide range of different materials. It is available for different branches of industry, e.g. for nesting on textile materials, leather, metal, or wood. We also have developed tailored solutions for special two-dimensional cutting problems, like nesting on coils. The software currently has become an industry standard and is used by many thousands of companies world-wide.

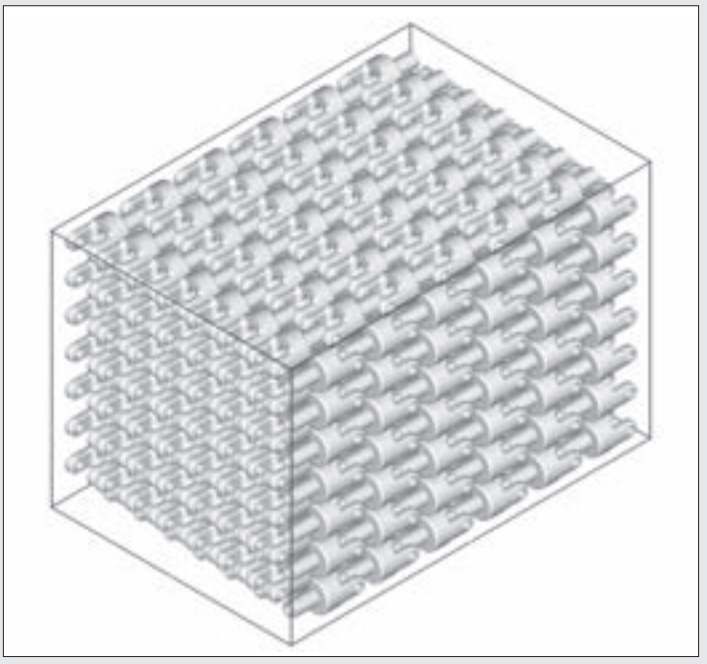


Marker on fabric

Our PackAssistant software calculates the optimal packing arrangement of identical parts in standard containers by using 3Ddesigns (CAD). This also works for parts with complex shapes, as the software will identify and take the individual shape of the object into account.

Making best use of container space can save transportation and storage costs. You simply have to find the right way to arrange the objects to be packed in the available container space. Experienced packing planners usually spend a lot of time meticulously arranging and packing parts with complex shapes and still, in most cases, they will not achieve the same packing density as with PackAssistant.

Also for one-dimensional cutting problems, optimization software can produce significant savings. We developed an optimization software for a steel manufacturing company which deals with the optimal usage of steel profiles. In a two-staged problem, optimal intermediate profile lengths have to be calculated for a set of final lengths ordered by a customer.



Container packed densely with components.

Nests on leather hides

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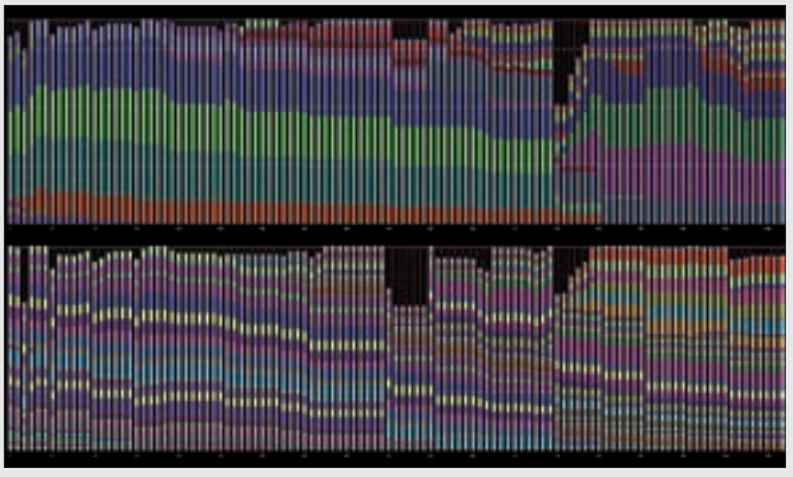
Optimization in production planning

Which assignment of jobs to machines is most efficient? Which garments are the best to be pooled on a single piece of cloth? Which is the best order of production to minimize set-up times? Custom software developed by Fraunhofer SCAI helps to answer such questions.

Today's production systems offer potential for optimization in manifold ways. Those do not necessarily involve investment in new machine technologies that implement the latest developments. In fact, often large improvements in efficiency are possible by using the multitude of information like order books, machine specifications, and cost records – which is almost always available electronically – to optimize the utilization of the existing technologies. Questions can be: Which assignment of jobs to machines is most efficient regarding costs as well as limited capacity and other constraints? Which garments are the best to be pooled on a single piece of cloth? Which is the best order of production to minimize set-up times?



Optimized assignment for 2 out of 30 presses

Often even experienced humans fail to solve these tasks optimally because of the large number of possible (suboptimal) solutions in conjunction with complicated constraints. Custom software developed by Fraunhofer SCAI as well as ready-to-use products for standard problems help to close the gap between the optimal solution and the de facto utilization.

Examples of recent projects

In the project MBOpt, SCAI developed a software for long-term planning of machine assignments in the production of car bodies. Planning more than 10 years into the future is of supreme importance here because the machines involved are among the most capital-intensive. Our partner BMW can use our software to compute the optimized machine utilization in an early stage of product development.

SCAI's software CUTPLANNER provides an optimization for a standard problem that arises in the garment industry one step before marker making. CUTPLANNER decides which garments to be put simultaneously on the cutting table to increase the savings that can be achieved with AutoNester.

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Material flow simulation to increase efficiency of production systems

Computer-aided simulation of production systems supports the strategic, tactical, and operational management in planning and improving layout, logic, and dimensioning of the whole supply chain. Several options can be compared, and advantageous values for parameters can be determined experimentally.

In many cases, the step before optimization of a production system is the identification of bottlenecks and deficits in efficiency. For this purpose we use the means of discrete simulation – as an analytical description is often extremely difficult due to the high level of complexity, the dynamics, and the number of random effects such as machine malfunction and quality. »Field tests« are in most cases far too expensive – or even impossible.

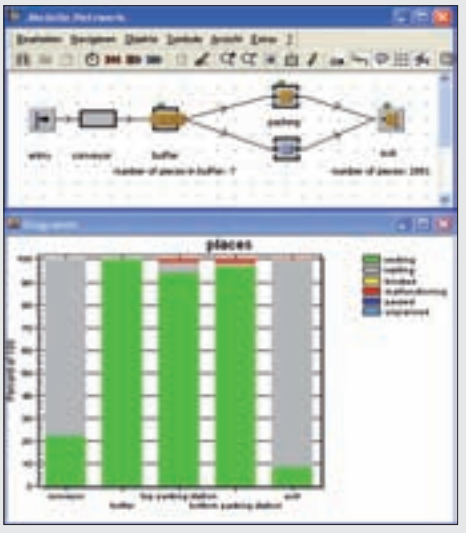
In contrast to continuous simulation, which deals e.g. with the simulation of fluids, discrete simulation features

- model variables that change their values only at certain points in time (discrete in time) and
- well-defined model states (discrete in state).

For processing a part on a machine, for example, only the states before and after processing are simulated but no states in between.
Typically, simulation and optimization of production systems aim at

- the layout (types and arrangement of machines and work benches),
- the logic/controlling (Who carries out which task and when?), and
- the dimensioning (e.g. number of workers, size of buffer).

In a simulation study, we support our customers in modelling their material flows with appropriate simulation tools. Of course, the quality of the study strongly depends on the quality of the database; that is why the process of collecting data deserves our close attention. Another challenge is finding adequate accuracy: reality can only be approximated due to the limited calculating capacity available.
In the next step, we analyse relevant parameters (such as the size of a buffer or the clock of a production line) and identify bottlenecks. While the sole adjustment of parameters can often be accomplished by built-in means, custom-made optimization methods are mostly more appropriate for the mitigation of bottlenecks: if – for example – a set of machines is spotted to be a bottleneck, an optimized assignment of jobs to machines can improve the performance of the whole production system significantly. Based on its long-term expertise in the field of optimization, Fraunhofer SCAI offers to its customers the development of those individual optimization methods for various kinds of problems.



Example for a small production line modelled in the simulation tool eM-Plant.

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»The idea of Grid Computing is to use emerging technologies to provide transparent standardised access to computing resources in such a way that technical details of a system are hidden from the end user. Fraunhofer SCAI is one of the European core institutions transferring Grid know-how from research to everyday use in industry.«

Ottmar Krämer-Fuhrmann

GRID COMPUTING

COORDINATION

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Horst Schwichtenberg, Marc Lob, Dr. Barbara Steckel, Ottmar Krämer-Fuhrmann, Wolfgang Ziegler (from left)

Grid Computing

Continuous advances in computer and network technology offer new opportunities for individuals, science and industry. This leads to a higher demand for computing power. The idea of Grid Computing is to use emerging technologies to provide transparent standardized access to computing power in such a way that technical details of a system are hidden from the end user. Similar to the power grid, high performance computers and software systems will become easily accessible from any computer at home, at work or en-route.

Grid Computing is targeting research communities and distributed developer groups in industry. Both communities use similar software for steering the grid, so-called middleware, but their requirements are significantly different. Hence numerous national and international initiatives and projects are supporting the development of Grid technologies in large research projects and its acceptance in industrial pilots.

SCAI transfers research results into industry

Fraunhofer SCAI engages in research initiatives and industrial projects. Hence SCAI transfers recent innovations in research into industrial use. The main requirements of the industry are security, availability, cost efficiency, and robustness of data and services.

The core competencies of the institute are in numerical simulation, virtual engineering and data technologies. This enables us to integrate Grid solutions into the workplace of engineers and researchers. All phases of product design are enhanced by improved access to databases and computer based simulation and optimization.

Aiming at transparent networking of resources between different companies and research institutes, raises the problem of data security. All partners in a virtual organization must stay independent of each other and their resources must be protected against unauthorized access. Additionally semantic problems occur when different application domains have to be integrated. SCAI engages in these areas with the goal of defining international standards, since Grid Computing can work only between standardized components.

National and international grid activities

Fraunhofer SCAI participates in the setup of a Grid infrastructure on several levels. First of all, SCAI is one of the eight Fraunhofer institutes that established the Fraunhofer Grid Alliance in order to share computational resources and to provide them to the entire Fraunhofer organization, which is distributed throughout Germany.

SCAI is active in building the basic infrastructure and the integration of various research communities in the D-Grid. D-Grid is a Grid Platform that is funded by the German Federal Ministry of Education and Research to carry several national research projects.

Large European integrated projects, partly coordinated by SCAI, integrate national Grids to a large international service infrastructure. The institute is one of the European core institutions transferring Grid know-how from research to everyday use in industry.

Selected Grid projects

@neurIST
@neurIST is focussed on intracranial aneurysms and intends to provide an integrated decision support system to assess the individual risk of aneurysm rupture in patients and to optimize their treatment. A complete IT infrastructure is being developed for the management and processing of the vast amount of heterogeneous data acquired during diagnosis. www.aneurist.org

BEinGRID
18 »Business Experiments in Grid« foster the take-up of Grid solutions in industry. Fraunhofer SCAI is engaged in two of them, enabling engineers in ship building and automotive supplier industries to access Grid resources easily in their daily work. Simulation and optimization facilities help them to improve the product design. www.beingrid.eu

CoreGRID
The CoreGRID Network of Excellence aims at advancing scientific and technological excellence in Grid and Peer-to-Peer technologies. About 300 researchers from 41 institutions integrate their research in knowledge and data management, programming models, system architecture, Grid systems, resource and workflow management, tools and environments. www.coregrid.eu

DEGREE
Dissemination and Exploitation of GRids in Earth sciencE is linking the Earth Science (ES) and grid communities throughout Europe, and focusing in particular on the EGEE II project. An ES applications panel with a range of candidate applications suitable for porting to Grid will make sure key ES requirements on the Grid middleware are identified. SCAI contributes especially on job management and is responsible for data management. www.eu-degree.eu

D-Grid, especially InGrid, IVOM and VO-Management
The German Grid Initiative, called D-Grid, builds a sustainable Grid Computing infrastructure for education and research in Germany. SCAI integrates tools for setting up the management of Virtual Organizations, including authentication and authorisation mechanisms. In the community project InGrid, methods and software components to support engineering processes by Grid technology are developed. www.d-grid.de

DWD.UNICORE
Together with T-Systems, Fraunhofer SCAI offers support for Grid environments based on UNICORE. The main customer is the German National Meteorological Service (DWD), who uses UNICORE as production environment for external partners. The support includes end user and administration support and training courses. SCAI and T-Systems plan to develop additional tools for UNICORE, i.e. to integrate UNICORE into existing HPC environments.

EGEE II
The Enabling Grids for E-sciencE project brings together scientists and engineers from more than 90 institutions in 32 countries to provide a seamless Grid infrastructure. Together with other research centers, the Fraunhofer institutes ITWM and SCAI are running the German Regional Operating Center with professional IT-services to guarantee the functionality of the European infrastructure, especially in Switzerland and Germany. SCAI also collaborates in the Biomed and Earth Science application domains. www.eu-egee.org

EPG
See article in next section.

PHOSPHORUS
Development of new applications to couple scientific instruments, data and high-end computing resources distributed globally. In a European Grid testbed the project will enable on-demand end to end network services across multiple domains with a dedicated quality of service. www.ist-phosphorus.eu

SESIS
Partners from ship building industries and IT develop an open Ship Design and Simulation System. SESIS enables the collaborative design of new ships by integrating the workplaces of engineers at the ship yard and its supplier industries. Both get facilitated to use advanced simulation techniques to estimate the ship's functionality and cost in early design phases. www.sesis.de

SIMDAT
Distributed virtual product development enables improved product quality and faster time to market while reducing costs and risks. It is, however, a complex task: data and processes have to be shared in a secure way and integrated among departments and locations of a company, between different disciplines or across all partners that participate in product development. Grid technology promises to reduce this complexity. The SIMDAT project introduces advanced Grid technology in the automotive, aerospace, pharmaceutical and meteorological verticals. www.simdat.eu

VIOLA
See article in next section.

WISDOM
WISDOM (Wide In Silico Docking On Malaria) initiative aims at demonstrating the relevance and the impact of the Grid approach to address drug discovery for neglected and emergent diseases. It gathers several partners around the world conscious of the urgency of working on these diseases. They are using Grid infrastructure to organize and accelerate their research. They deploy production experiment of virtual screening at a large scale against diseases, called a data challenge. wisdom.eu-egee.fr

Research and development in Grid Computing

Grid Computing basically is about sharing resources and collaborating, resources often being geographically dispersed and collaboration frequently crossing administrative domains. This is a hot topic in scientific environments but increasingly in commercial environments.

Problem description

Making use of distributed resources for applications or services within a single administrative domain or across multiple domains raises a number of topics to be resolved in the middleware layer. These issues include authentication and authorisation, orchestration of resources, mapping of applications to suitable compute resources, management of licenses for commercial software, and service level agreements (SLAs). Today some limited or proprietary solutions for these issues exist – usually only supporting local environments. However, Grids and Service Oriented Architectures (SOA) as evolving technologies for executing applications or services in both scientific and commercial environments will become a real option only if interoperable, standards based solutions will be available.

Grids and Service Oriented Architectures (SOA) are the future of world-wide collaboration.

Developments

Based on more than eight years of involvement and experience in Grid Computing, we are focussing on solutions for the problems mentioned above. Moreover, we already have first results ready for evaluation, described under Solutions below. We develop our solutions in the context of European projects, the German D-Grid and the Open Grid Forum (OGF). Solutions under developments that will become available within the next twelve months are

- Interoperable authentication and authorisation mechanisms (developed in D-Grid)
- Mapping of applications to suitable compute resources (developed in CoreGRID)
- Management of licenses for commercial applications in distributed environments (developed in D-Grid and CoreGRID)
- Negotiation and management of SLAs (developed in the OGF)

We also are working on a solution for text mining in the Grid, leveraging ProMiner, a product of the department, to be efficiently used in Grids. All developments support either the three major Grid platforms (Globus Toolkit, gLite and UNICORE) or are independent of the middleware. As we use web-service technologies, all developments naturally fit into SOA environments.

Solutions

With the MetaScheduling Service (MSS) we currently offer solutions for orchestration of resources, located both in single administrative domains and in multiple domains. The MSS supports advance reservation of resources for complex applications that either need multiple resources at the same time (co-allocation) or with timely dependencies (workflows). The MSS may be used stand-alone. However, we also provide integration into the UNICORE client.

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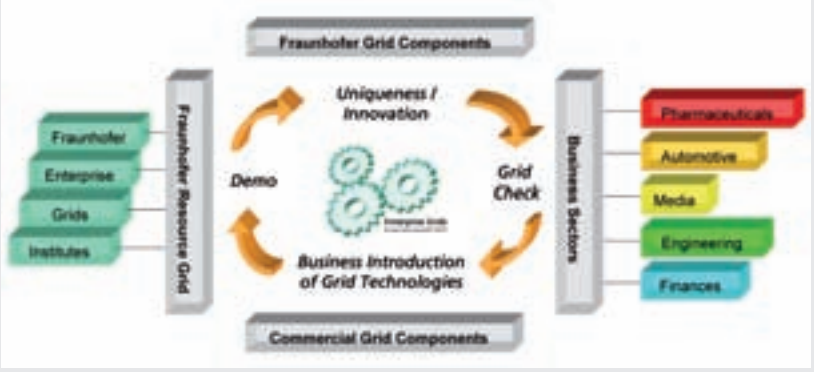
Enterprise Grids – Business solutions for optimized utilization of distributed IT-Resources

Which assignment of jobs to machines is most efficient? Which garments are the best to be pooled on a single piece of cloth? Which is the best order of production to minimize set-up times? Custom software developed by Fraunhofer SCAI helps to answer such questions.

Fraunhofer Enterprise Grids is a cooperation of four institutes – Fraunhofer FIRST, Fraunhofer IAO, Fraunhofer ITWM and Fraunhofer SCAI. Together these institutes can look back on a long history of research and development in the areas of industrial applications, high performance and Grid Computing as well as the management of complex software systems. Within this cooperation, it is the aim of Fraunhofer Enterprise Grids to open up the paradigm of grid computing for industrial use and to support and push the transfer of innovative technologies from science to business and industry. As there are certain business sectors that seem particularly ready for the adoption of grid technologies Fraunhofer Enterprise Grids is concentrating on:

- Automotive industry
- Engineering
- Pharmaceutical industry
- Media
- Financial services

In these business sectors the technological as well as the organizational requirements for an efficient introduction of Grid technologies, such as a high degree of standardization and the need for large amounts of IT resources, are most promising. Fraunhofer Enterprise Grids combines consulting services like a »Grid Check« with its knowledge base on commercial and open-source grid and HPC technologies. On top of that the EPG partners integrate application know-how in the targeted business sectors with their own customized solutions for special purpose tasks.



Fraunhofer Enterprise Grids push the transfer from science to business and industry.

MpCCI in a grid environment

Many of these business sectors necessitate multi-discipline physical simulations. Relevant problems require the solution of two or more distinctive physical subsystems that are tightly coupled like fluid-structure interaction or thermo-mechanical interaction. In most cases a single (proprietary) simulation system cannot provide all necessary features. Coupling of the most suitable codes for each necessary discipline will enable more flexibility and simulation quality to the end user.

MpCCI (Mesh-based parallel Code Coupling Interface) has been developed at the Fraunhofer-Institute SCAI in order to provide an application-independent interface for the coupling of different simulation codes. In the »Enterprise Grid« – Project it will be evaluated and tested if and how a web service based communication can be used for such a coupled simulation. This will ensure that MpCCI could be used as a service resource and could be integrated into modern grid environments.

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Running an optical testbed for advanced network services and large applications

The project VIOLA (Vertically Integrated Optical Testbed for Large Applications in DFN) aims at preparing the next generation of the German research network. Fraunhofer SCAI provides its know-how to both middleware and applications like algebraic multigrid solvers and multiphysics code coupling.

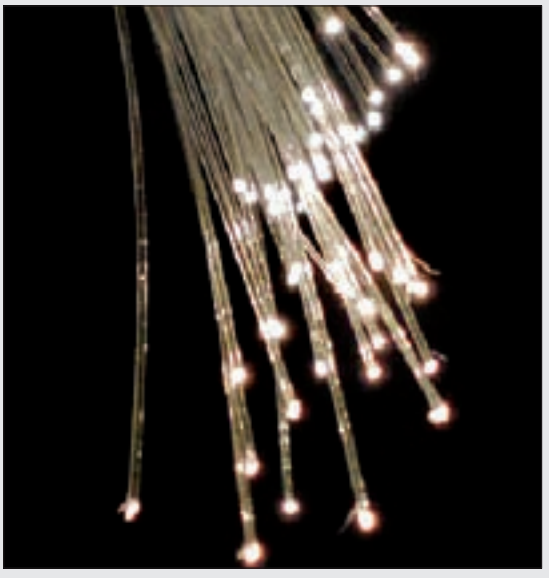
VIOLA started in June 2004 and is now close to its end after three successful years. A consortium of partners from industry, research laboratories, universities and the DFN-Verein has created a German Optical Testbed in the State of North-Rhine-Westphalia with an extension to the State of Bavaria. SCAI operates one of the core sites forming the UNICORE based VIOLA Grid providing a unique environment for scientific and commercial MPI-Applications to be distributed across multiple clusters to achieve increased performance.

The major goals of VIOLA are:

- Test of advanced network equipment and network architectures, compatibility of network equipment from different manufacturers
- Development and test of Grid middleware for the user-driven dynamical provision of bandwidth
- Enhancement and test of advanced distributed applications

SCAI contributed to both middleware and applications: In VIOLA-SUPPORT the Meta-Scheduling Service (MSS) has been developed. The MSS orchestrates compute and network resources for a single application. Together with an implementation of MPI supporting MPI jobs spanning multiple clusters (MetaMPICH developed at the RWTH Aachen University) and a network reservation system (ARGON developed at the University of Bonn), the MSS leverages distributed applications with high requirements for the compute resources and the interconnecting network.

In AMG-OPT the software package SAMGp (a product of SCAI) was enhanced. SAMGp is a numerical and parallel scalable solver for many linear systems which have to be solved repeatedly in many simulation packages. SAMGp has been used extensively for benchmarks within the VIOLA testbed for solving linear systems which are distributed over different compute clusters. It could be demonstrated that the parallel scaling capabilities of the solver carry over when using such an environment.



Fibre optic cables are part of the infrastructure of the project

In TechSim different aspects of the Czochralski crystal growth process are simulated in a cooperation with the crystal growth group of research center Caesar. Multiphysics is done on the Grid by coupling the codes Fluent, CrysVun and Amdis using MpCCI (see page 16). MpCCI takes the part of managing the transfer and interpolation of surface and volume data between codes running on different clusters.

VIOLA is funded by the Federal Ministry of Education and Research (BMBF).

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2006

Bergner, Wolfgang: **Erkennung Domänenspezifischer Terme in biomedizinischer Literatur.** FH Schmalkalden, 2006

Beibei, Han: **Bayesian network modeling for cerebral aneurysm rupture risk and treatment**. Bonn-Aachen International Center for Information Technology (B-IT), 2006

Blanck-Wehde, Nils: **Entwicklung eines grafischen Tools zur Parametrisierung, Generierung und Überwachung von EDG-Jobs zur Durchführung molekularbiologischer Docking-Tests in einer Grid-Umgebung**. Fachhochschule Bonn-Rhein-Sieg, 2006

Galunic, Goran: **Parallelisierung des Galerkin Produkts im AMG Verfahren mit OpenMP.** Fachhochschule Bonn-Rhein-Sieg, Master Thesis, 2006

Gladbach, Katharina: **Partitionelle Verfahren für Probleme der Fluid-Struktur-Wechselwirkung.** Universität zu Köln, 2006

Hülsmann, Marco: **Vergleich verschiedener kernbasierter Methoden zur Realisierung eines effizienten Multiclass-Algorithmus des Maschinelles Lernens.** Universität zu Köln, 2006

Kasam, Vinod Kumar: **Design of Plasmepsin Inhibitors: A Virtual High Throughput Screening Approach on EGEE Grid.** Fachhochschule Bonn-Rhein-Sieg, 2006

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Schadewald, Nicole: **Mutual segmentation – a novel measure for multiscale registration of presegmented MRI brain images**. Universität zu Köln, 2006

Thum, Peter: **Algebraic Multigrid for Navier-Stokes Equations – Studies on Smoothing and Coarsening**. Universität zu Köln, 2006

Valluripalli, Phani Kumar: **Interaktive hierarchische Visualisierung hochdimensionaler Daten mit Hilfe von Cluster-Algorithmen.** RWTH Aachen, 2006

Wang, Wei: **Conceptual Design and Physical Implementation of a Protocol Database for Chemical Image Mining.** Bonn-Aachen International Center for Information Technology (B-IT), 2006

Wolf, Antje: **Jenseits von Consensus Scoring: Qualitativer Vergleich von Docking Tools.** FU Berlin, 2006

Dissertations

Friedrich, Christoph M.: **Kombinationen evolutionär optimierter Klassifikation.** Universität Witten/Herdecke, 2006

Garms, Onno.: **Periodische Verschachtelungsprobleme in $\mathbb{R}$ x [0, w].** Rheinische Friedrich-Wilhelms-Universität Bonn, 2005

Spiess, Holger: **Reduction methods in finite element analysis of nonlinear structural dynamics**. Universität Hannover, 2006

von Öhsen, Niklas: **A novel profile-profile-alignment methode and its application in fully automated protein structure prediction.** Universität München, 2005

TEACHING

Hofmann-Apitius, M.; Kumpf, K.; Ziegler, W.: Seminar »Introduction to Grid Computing«, Bonn-Aachen International Center for Information Technology (B-IT), Wintersemester 2006/2007

Hofmann-Apitius M.: Bio-Database Lecture, Bonn-Aachen International Center for Information Technology (B-IT), Wintersemester 2006

Hofmann-Apitius M.; Friedrich Ch. M.; Fluck J.; Kumpf K.: Life Science Knowledge Discovery Lecture, (B-IT), Wintersemester 2005/2006

Hofmann-Apitius, M.; Zimmermann, M.; Friedrich, Ch. M.; Fluck, J.: Seminar »Current Topics in Applied Life Science Informatics«, (B-IT), Sommer- und Wintersemester 2006

Hofmann-Apitius, M.; Ziegler, W.: Blockpraktikum »Applied Grid Computing«,Bonn-Aachen International Center for Information Technology (B-IT), Sommerschule 2006

Kumpf, K.: Blockpraktikum »Life Scence Databases«, Bonn-Aachen International Center for Information Technology B-IT, Wintersemester 2005/2006

Lorentz, R.: Kompressionsverfahren, Universität Duisburg-Essen, Sommersemester 2006

Lorentz, R.: Datenkompresion, Universität Duisburg-Essen, Wintersemester 2006/2007

Lob, M.: Mathematik 2 für Maschinenbau, Fachhochschule Bonn-Rhein-Sieg, Wintersemester 2005/2006

Lob, M.: Informatik 1 für Elektrotechnik, Fachhochschule Bonn-Rhein-Sieg, Sommersemester 2006

Lob, Marc: Informatik 1 für Elektrotechnik, Fachhochschule Bonn-Rhein-Sieg, Wintersemester 2006/2007

LECTURES

Lob, Marc.: Mathematik 2 für Maschinenbau, Fachhochschule Bonn-Rhein-Sieg, Wintersemester 2006/2007

Nikitin, I., Nikitina, L.: Applied Optimization, Universität zu Köln,Wintersemester 2006/2007

Wienands, R.: Numerische Mathematik I (Vorlesung), Universität Duisburg-Essen, Campus Duisburg, Sommersemester 2006

Wienands, R.: Vorlesung »Konvergenzanalyse von Mehrgitterverfahren«, Universität zu Köln, Sommersemester 2006

Wienands, R.: Übungen zur Vorlesung »Konvergenzanalyse von Mehrgitterverfahren«, Universität zu Köln, Sommersemester 2006

Wienands, R.: Vorlesung »Algebraische Mehrgitterverfahren«, Universität zu Köln, Wintersemester 2006/2007

Wienands, R.: Übungen zur Vorlesung »Algebraische Mehrgitterverfahren«, Universität zu Köln, Wintersemester 2006/2007

Wienands, R.: Praktikum »Entwicklung eines Mehrgittercodes«, Universität zu Köln, Wintersemester 2006/2007

Zimmermann, M.: Blockpraktikum »Computer-Aided Medicinal Chemistry«, (B-IT), Wintersemester 2005/2006 and Wintersemester 2006/2007

Zimmermann, M.; Hofmann-Apitius, M.: Blockpraktikum »Introduction to Computational Chemistry and Computational Biology for CEMBIO Students«, Bonn-Aachen International Center for Information Technology (B-IT), Wintersemester 2006

Lectures held in the research series of Professor Trottenberg

2006

Prof. Dr. Andreas Meister, Universität Kassel: **Ein Fluss-Präkonditionierungs-Verfahren für Strömungen beliebiger Mach-Zahlen**, 11th January, 2006

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Dr. Peter Schwarz: Modellierung und Simulation heterogener Systeme – Arbeiten im Fraunhofer-Institut für Integrierte Schaltungen, Außenstelle für Entwurfsautomatisierung EAS Dresden, 22nd March, 2006

Christof Baeuerle, Altair Engineering GmbH, Boeblingen: **Morphing im Einsatz zur Formoptimierung nichtlinearer FEM-Probleme**, 6th April, 2006

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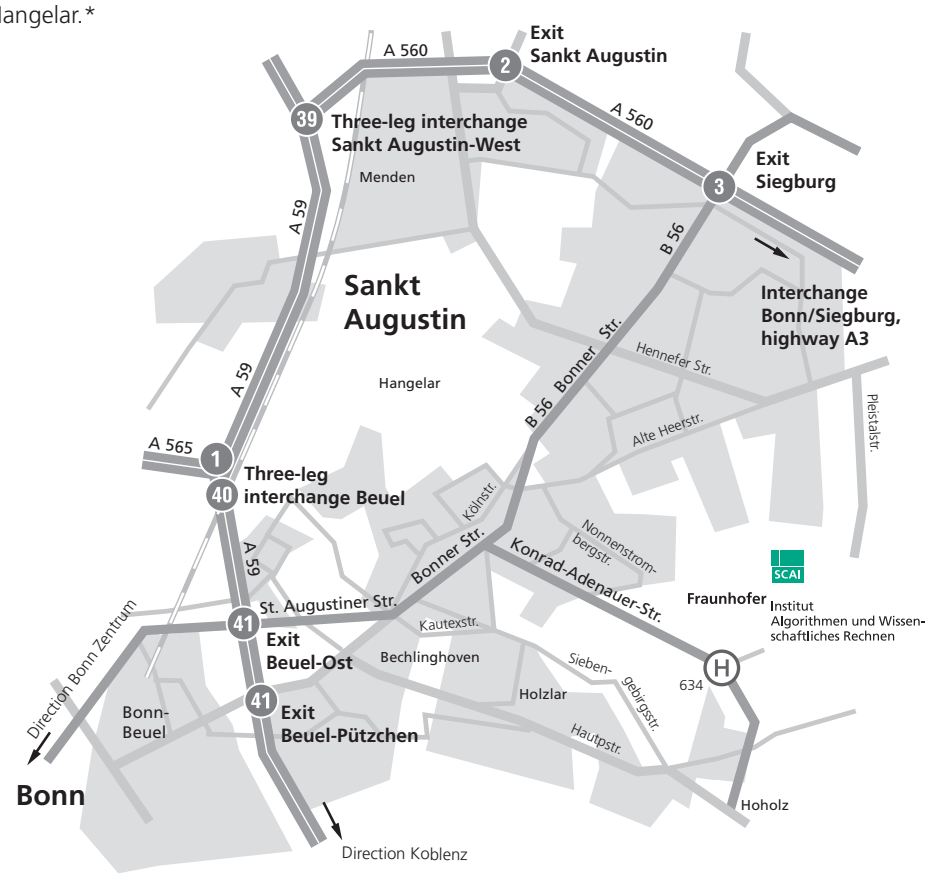

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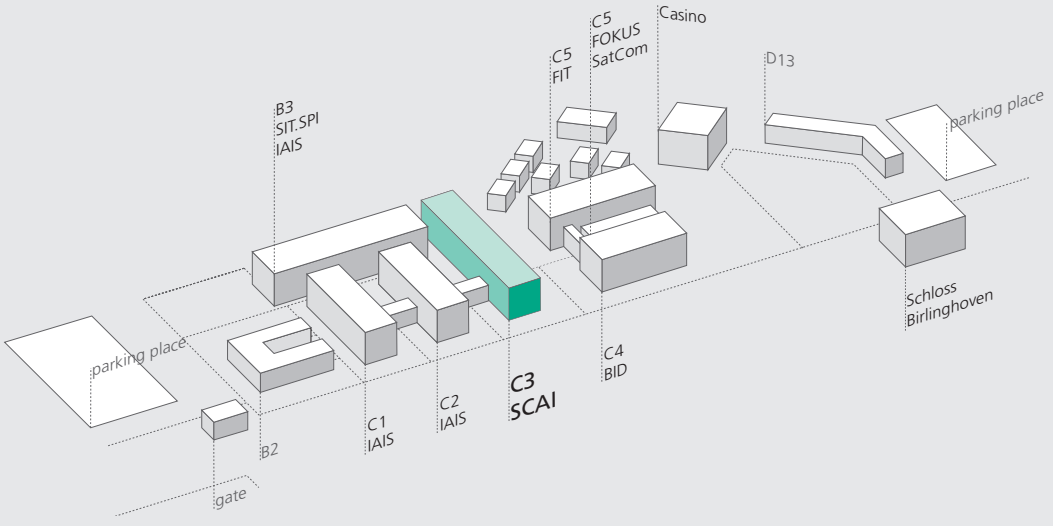

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