Universität Karlsruhe (TH)
Rechenzentrum

HIGH PERFORMANCE SCIENTIFIC COMPUTING

Scientific
Supercomputing
Center Karlsruhe

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The Scientific Supercomputing Center (SSC) Karlsruhe

The Mission

For the solution of large scientific and industrial problems fast algorithms and advanced computer architectures are necessary. However, much of the performance of even the fastest and most advanced available computer may be wasted — if programs are not properly implemented with respect to the special computer architecture.

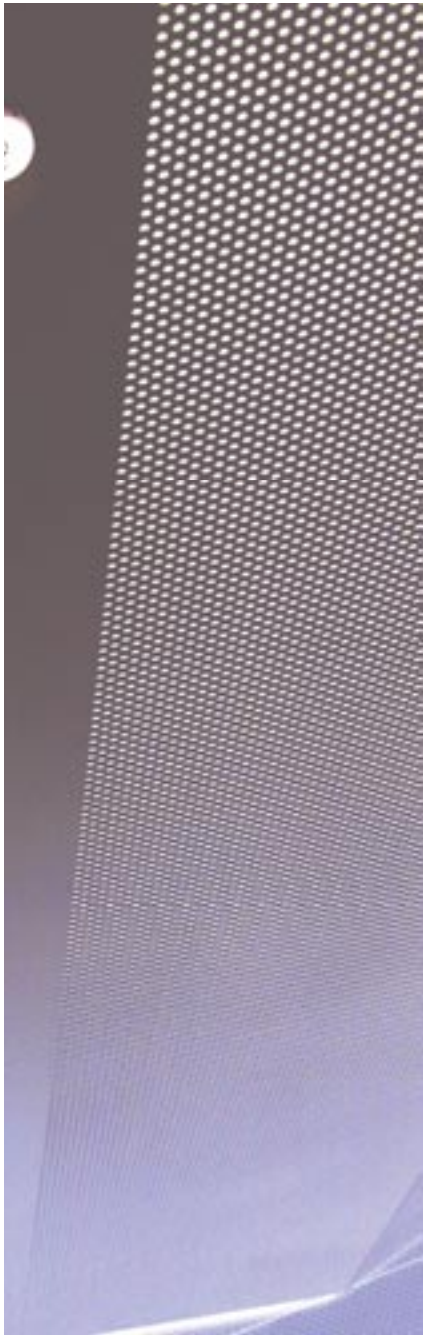
The SSC Karlsruhe (Scientific Supercomputing Center Karlsruhe) will provide support as well for experts as for novices in parallel computing. Our goal is to help our customers in all problems related to scientific supercomputing. Our services are not only confined to advice on how to use supercomputers efficiently but you will also get qualified help if you are looking for appropriate mathematical methods or simply having problems to login. The SSC Karlsruhe is the service unit of the university's computing center that cares for supercomputer customers.

Competence and Experience

Since the first supercomputer (CDC Cyber 205) was installed in Karlsruhe in 1983 the computing center of the university has been continuously engaged in supercomputing. Besides the operating of the machines Karlsruhe always has been establishing expert groups for scientific supercomputing.

In the 1980s and 1990s experts of the Computing Center in Karlsruhe tuned numerical libraries for Siemens/Fujitsu and IBM supercomputers. From this time on close cooperations with other institutes of the university and industrial companies have been initiated, among them: Siemens AG (München), NAG (Oxford), Böhringer (Ingelheim) — to name only a few.

At the SSC Karlsruhe you will find experts for problem solving environments and some of these developments have been even initiated here. At the Computing Center black-box solvers for arbitrary systems of nonlinear partial differential equations and iterative linear solvers have been developed. Thus, the experts at the SSC Karlsruhe know about the needs and problems of their customers from their own experience.



Consultation and Support

According to the mission of the SSC Karlsruhe you will have support on different levels:

- **helpline**
  The SSC Karlsruhe has set up a helpline where you rapidly get support from Monday to Friday, 9:00 to 17:00. Simply call +49(0)721/608-8011. If your problem cannot immediately be solved, it will be pursued by our experts. You can contact us as well by e-mail: contact@ssc.uni-karlsruhe.de.

- **basic support**
  For parallel computers there are rules that should be obeyed in order to get efficient codes based on the hardware design. We will provide you with all our knowledge how to use massively parallel and vector computers efficiently.

- **standard solutions**
  At the SSC Karlsruhe you will find experts who know both: the application software packages and the necessary libraries you need to solve your problem. This means that you obtain double assistance from the beginning in selecting your appropriate solution and later in using it.

- **Individual solutions**
  If you want to solve your particular problem for the first time with the aid of a high performance computer, then you will find at the SSC Karlsruhe experts for modelling and state-of-the art solvers. This unique feature is highly considered by all our customers.

Computing Resources at the Computing Center of Karlsruhe University

IBM RS/6000 SP

The Karlsruhe University Computing Center operates a powerful supercomputer and offers this system to academia and the industry. The present system was installed in autumn 2000 and upgraded at the end of 2001. It consists of 112 Winterhawk-2 thin nodes with 2 POWER3 processors running at 375 Mhz and 2 GB of main memory per node and 4 Nighthawk-2 high nodes with 8 POWER3 processors (375 Mhz) and 8 GB main memory per node, 870 GB external disk space for the parallel high performance file system GPFS and 1.7 TeraBytes for the user file system. The theoretical peak performance of this system is 384 GFLOP/s with a total main memory of 256 GB. The advantages of this system configuration with Symmetric Multi Processor (SMP) nodes are:

- a platform for „shared memory“ parallelized programs and
- also a platform for the hybrid parallelization according to the „shared memory“ and „message passing“ paradigms.

Parallel Computer IBM RS/6000 SP

The nodes of the system are interconnected by a low latency, high bandwidth SP switch capable of transmission speeds of about 140 MB/s at the application level. The integration of the machine into the computer environment of the Computing Center is depicted in Figure 1.

Also, the system is integrated into the „Virtuelles Rechenzentrum (VRZ) Karlsruhe“ (Virtual Computing Center Karlsruhe) and the „Höchstleistungsrechner für Wissenschaft und Wirtschaft (hww) GmbH“ (High Performance Computers for Science and Industry).

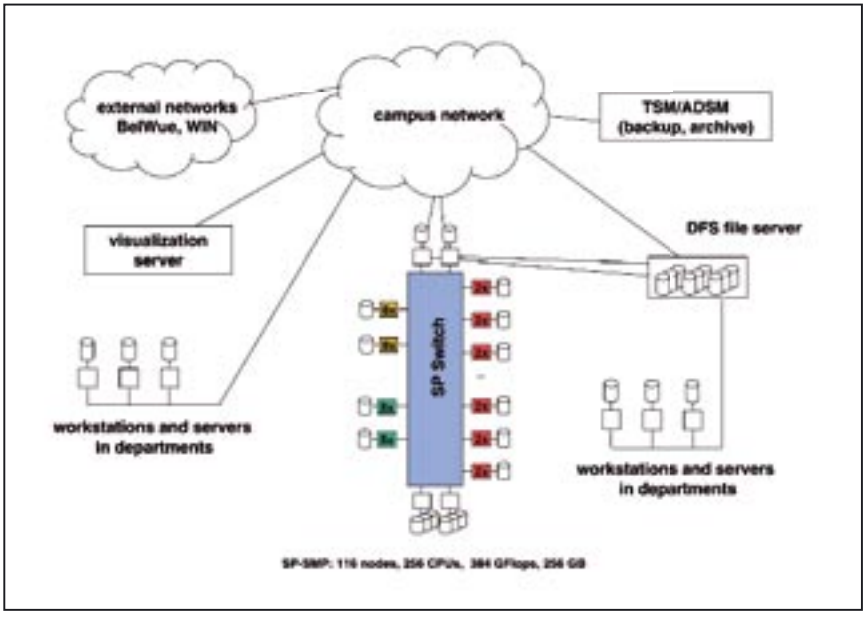


Fig.1: Logical structure and usage of IBM RS/6000 SP at the SSC Karlsruhe

Configuration

Reflecting the diverse requirements from different application areas, the IBM RS/6000 SP contains nodes with various memory sizes and local disk configurations. The POWER3 processors are RISC processors with 64-bit addressing and two cache levels where the second level cache is as large as 8 MB. In the following the different nodes are briefly explained:

- 112 Winterhawk-2 thin nodes with 2 POWER3 processors per node running at a frequency of 375 MHz. The nodes are equipped with 2 GB of main memory and local disk space of 36 GB. The communication within a node takes place via a shared memory segment, while the communication with tasks running on other nodes is done via the SP switch. These nodes are primarily used to run applications that have been parallelized by MPI.

- 4 Nighthawk-2 high nodes with 8 POWER3 processors (375 MHz) and a main memory of 8 GB per node. The processors load/store data from/to the main memory via an internal switch. Each processor card has its own independent path for the data transfer from/to the main memory. By this architecture SMP systems with high numbers of processors are made possible. These nodes are mainly used for serial applications with

high memory requirements, for “shared memory” parallelized applications with up to 8 processors and for applications with hybrid parallelization according to the “shared memory” and “message passing” paradigms.

	POWER3 high nodes 375 MHz	POWER3 thin nodes 375 MHz
number of nodes	4	112
number of processors per node	8	2
memory size	8 GB	2 GB
peak performance per node	12 GFlop/s	3 GFlop/s
total peak performance	48 GFlop/s	336 GFlop/s
utilization	compute nodes	server & compute nodes

Tab. 1: Configuration of SP nodes

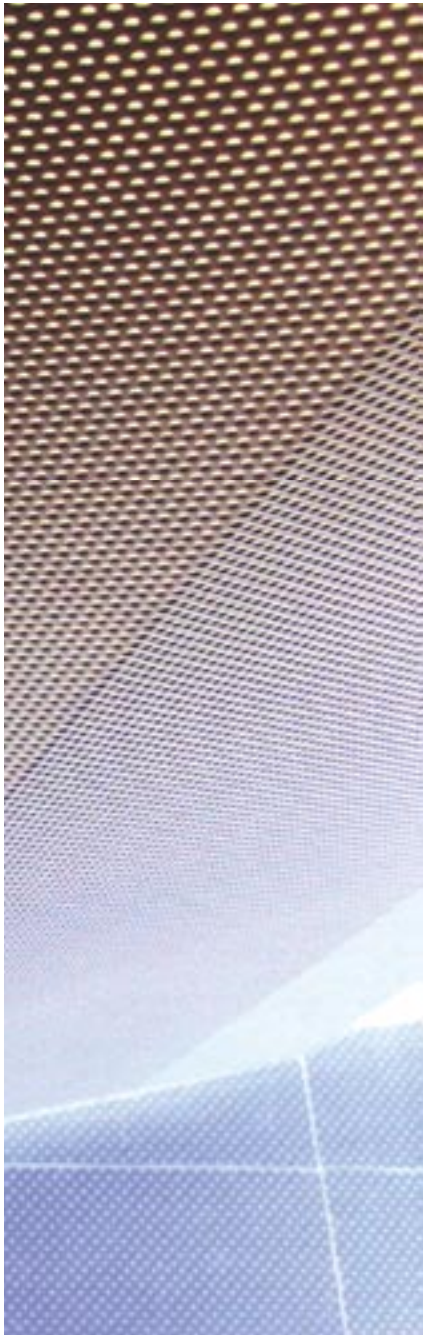
The most important characteristics of the IBM RS/6000 SP besides the high number of nodes are the large local memories of individual nodes and the flexible I/O configuration with large local disk capacities at each node, a global high performance parallel file system and a global DFS file system which holds the users‘ HOME directories.

Software

Each node of the IBM RS/6000 SP is controlled by a full Unix operating system AIX. This enables system administrators as well as users of the SP to utilize the rich set of standard AIX applications and tools which are in most cases also available on the SP.

The Computing Center of Karlsruhe University has been the first site operating an IBM RS/6000 SP with the Distributed Computing Environment (DCE/DFS) resulting in a higher security and giving access to the well scaling Distributed File System (DFS). The SP is fully integrated into the local DCE cell and has access to the various DCE and DFS servers on the campus.

On top of the operating system the Parallel System Support Programs (PSSP) and the Parallel Environment supply the basic infrastructure for the execution of parallel applications on an IBM RS/6000 SP.



The natural programming model for a distributed memory system like an IBM RS/6000 SP is the message passing programming paradigm which gives the application programmer full control over the parallelization of the program. Within the Parallel Environment this programming model is efficiently implemented via the Message Passing Interface (MPI), which is the de facto standard for this type of applications. Other programming environments on the SP include Parallel Virtual Machine (PVM) and High Performance Fortran (HPF) which are both implemented on top of MPI. Additionally, OpenMP is an option for the use of shared memory parallelization.

Because of the very flexible software structure of the IBM RS/6000 SP additional parallel programming environments which are available on networks of workstations can easily be ported and adapted if this has not been done so far. The distribution of workload among the nodes of the SP is handled in a flexible way utilizing IBM's batch system LoadLeveler. It has been enhanced in several ways to simplify user interface and administration and to allow small serial background jobs to fill up the gaps which cannot be utilized by parallel applications. So a very high overall system utilization can be obtained while the serial programs do not restrain parallel applications from using the hardware resources.

For the development of parallel programs powerful tools are essential. The program development environment on the SP includes optimizing compilers for Fortran 90, C and C++, parallel debuggers like TotalView and performance analyzers like xprofiler and Vampir which show the run-time behavior of parallel applications and give valuable hints how to improve the performance of the program.

Application Software

As each node of an IBM RS/6000 SP runs its own copy of the AIX operating system, standard serial AIX software, i.e. application programs, tools and libraries, is readily accessible on the SP.

At the SSC Karlsruhe this includes well proven numerical libraries like NAG Libraries and VNI's IMSL Fortran and C Libraries as well as Linear Algebra Package (LAPACK) and other specialized libraries. Detailed information is always available via the Web based information service of SSC Karlsruhe. Highly optimized codes from many areas of numerical mathematics are supplied by IBM's ESSL library which also contains basic routines like BLAS (Basic Linear Algebra Subprograms) being the building blocks for more complicated numerical algorithms. These programs are optimized to use efficiently the specific features of the SP nodes. These serial libraries can be invoked in serial programs as well as in single or all tasks of parallel applications.

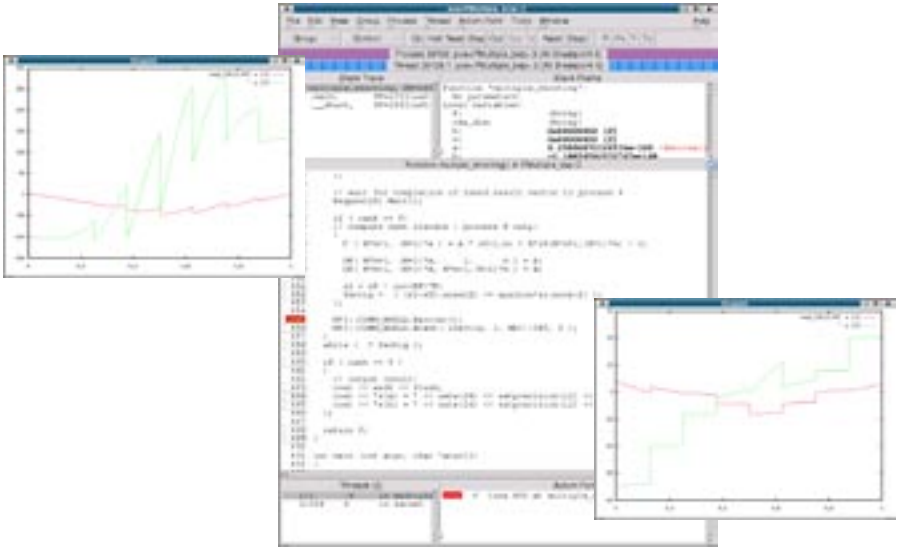


Fig. 2:
Snapshot of some TotalView windows during debugging a parallel program

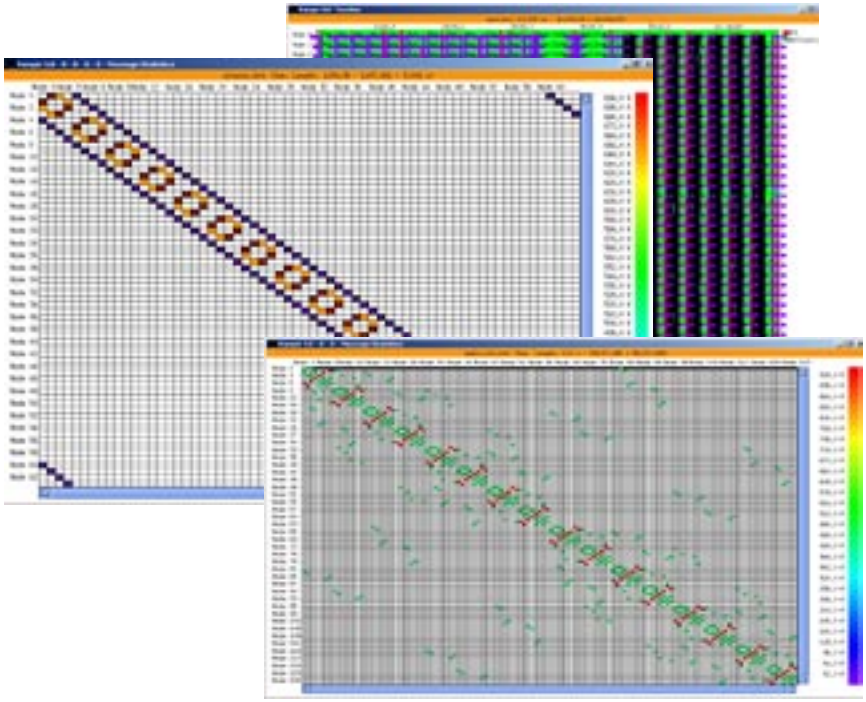


Fig. 3: Snapshot of Vampir windows

On the other hand parallelized subprograms can improve the development of parallel applications significantly. Parallelized libraries on the SP include Scalable LAPACK and IBM‘s PESSL which comprise most areas of Linear Algebra for dense and sparse matrices and which have been successfully used at SSC Karlsruhe for large eigenvalue problems from solid state physics. Other libraries are LINSOL , VECFEM and FDEM which have been developed at the Computing Center of Karlsruhe University. Parallelized application codes on the SP include programs like PERMAS, ABAQUS, NASTRAN, STAR-CD, FLUENT and TURBOMOLE. Other packages can be made available on request.

Visualization and pre- and postprocessing software on the SP includes packages like Patran, AVS, Uniras and PVWave.

Fujitsu / Siemens VPP

The Fujitsu Siemens VPP 5000 vector parallel supercomputer is jointly used by the University of Karlsruhe and the Research Center Karlsruhe.

This system as well as the IBM RS/6000 SP is integrated into the Virtual Computing Center Karlsruhe and is operated by the Computing Center of the Research Center Karlsruhe while the user support for customers of Karlsruhe University is done by the staff of the SSC Karlsruhe.

The vector parallel computer Fujitsu Siemens VPP 5000, in the foreground the SUN Noble RAID Disk System

In May 2000 the VPP 5000 was the first installation of such a system in a German public research utility; this supercomputer provides an opportunity to the scientists to run serial applications on a single processor with the worldwide highest peak performance at its installation time (9.6 GFlop/s). In summer 2001 the VPP 5000 was upgraded to a system with 8 processing elements.

Each processing element (PE) contains a high performance scalar processor (1.2 GFlop/s), a vector processor (9.6 GFlop/s) and 8-16 GB main memory. The single PEs are connected by a communication network implemented as a crossbar (bidirectional 1.6 GByte/s). The whole system has a scalar peak performance of 9.6 GFlops, an overall peak performance of 76.8 GFlops and 80 GB of main memory. The structure of a PE of the VPP 5000 is depicted in Figure 4.

All functional units of a single vector processor are implemented as 16-track pipelines; thus 16 results per cycle can usually be delivered. If the multifunctional pipeline performs a compound operation with one addition and one multiplication like e.g. a contracting linked triad that can be implemented in Fortran as the following loop

```
DO i = 1, n
  a(i) =a (i) + s * b(i)
END DO
```

the theoretical peak performance of 9.6 GFlop/s will be obtained nearly on a single PE.

The operating system of the VPP 5000 is UXP/V V20 featuring the Flexible and high Performance File System (FPFS). The amount of data to be transferred is used for the decision of the file system, if the data are buffered internally or are transferred directly between the application program and the disks. Thus it combines the advantages of traditional file systems and special file systems like e.g. VFL-FS of the earlier VPP 300 for large I/O-intensive applications. Therefore FPFS is suitable for a broader range of applications as many other file systems. By the use of Noble RAID Systems of SUN and the Fiber Channel port transfer rates of 80 MByte/s are achieved that can be still increased by the parallel usage of different RAID systems.

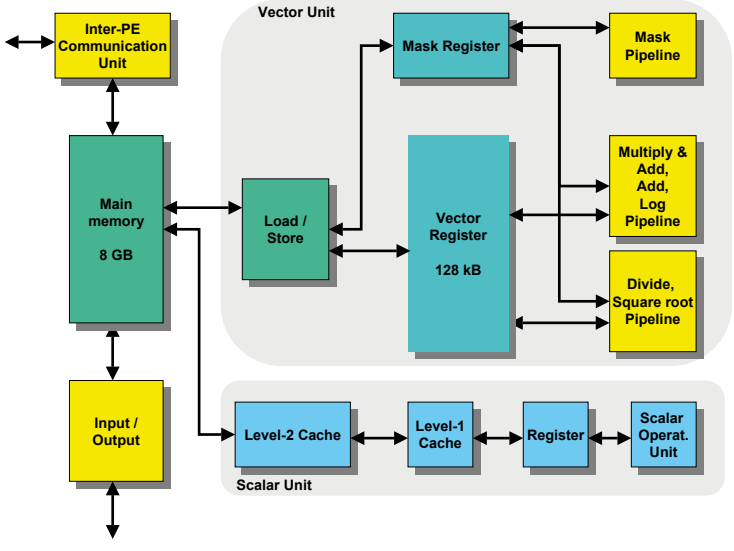


Fig. 4: Block diagram of a processing element of a VPP 5000

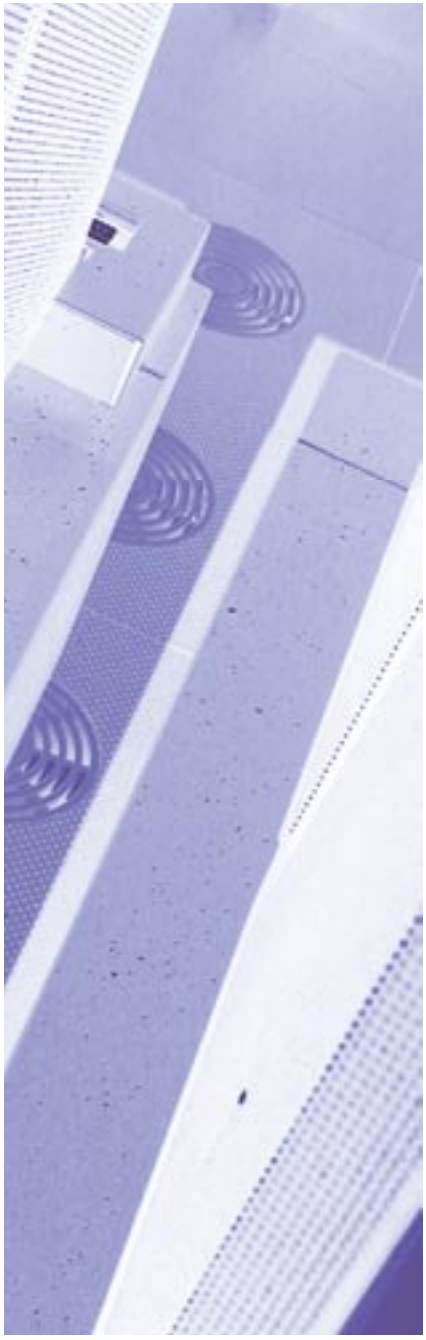
The software development environment on the VPP 5000 includes vectorizing compilers for Fortran 95 as well as for C and C++. As communication library for parallel applications MPI can be used. MPI is implemented according to the specifications of MPI 2.0; thus it also contains MPI-IO and one-sided communication. As further tools the debugger TotalView 3.9 for the application development and Vampir for the runtime analysis of parallel programs are available. Numerical libraries as BLAS, ScaLapack, Lapack, LINSOL, IMSL and NAG are available on the VPP systems.

For parallel applications high transfer rates of more than 500 MB/s for unidirectional and more than 900 MB/s for bidirectional data transfers have been measured on the VPP.

Because of the vector processing hardware the VPP system is best utilized by applications containing operations on long and contiguous vectors. The VPP is intensively and efficiently used by applications from computational fluid dynamics, solid state physics, meteorology and geophysics that achieve a sustained performance between 25% and 50% of the peak performance.

Silicon Graphics Origin 2000

An Origin 2000 with 8 MIPS R10000 Processors, 3 GB of main memory and 142 GB of local disk space is operated by the Computing Center of Karlsruhe University as a serial compute server running applications like ABAQUS, ANSYS, DYTRAN, FIDAP, MAFIA, MSC/NASTRAN or PERMAS. There is limited interactive access to this system which is fully controlled via the batch system NQS.



Laboratory for Graphics, Visualization and Media Services

The Laboratory and its team of specialists at the Computing Center of the University of Karlsruhe was established in spring of 2000. The aim of the Lab is to give the various departments of the University a multimedia environment platform, where a wide range of projects can be carried out in the fields of civil engineering, fluid dynamics, medicine, architecture, physics, robotics and geo science.

The fundamental concept is to provide services in the form of software solutions, hardware, presentation and working rooms, last but not least, specialized advice for:

- Content and methodical support
- Introduction into the various visualization and virtual reality scenarios
- Optimizing and developing new solutions together with the departments
- Presentation know-how and techniques
- Attaining monetary and organizational synergy effects

Our specialists together with other departments in the Computing Center offer support in the following areas:

- Visualization of numerical results by use of high performance computing, 3D techniques, virtual reality and presentation environments
- Global multimedia infrastructures consisting of digital video production and streaming, computer based training (CBT) scenarios, video conferences and teleseminars
- Input and output of graphics and print media

The GVM (Graphics, Visualization, Media Services) laboratory is situated in the generously spaced basement of the computing center building and is split into four main cells:

Media pool of the Computing Center

Planning of a factory hall

Town planning
Software: REALAX *Source: artemedia*

- The Media Point is the cell for presentation, virtual reality scenarios, 3D visualization, animation and large screen video conferencing. Here is also the central location for the multimedia control.

- The Media pool is the cell for project work, planning advanced multimedia and graphic techniques. Also virtual reality scenarios, 3D visualization and animation.

- The Video laboratory is the cell where video production and video animation is created.

- Print media is the cell which houses the laser high speed printing machines, color laser print system and the large format high resolution color printers.

The pulse of the Lab is a SGI Onyx2 Infinite Reality 2 Group Station.

Planning of an observation satellite
Software: REALAX
Source: DaimlerChrysler Aerospace

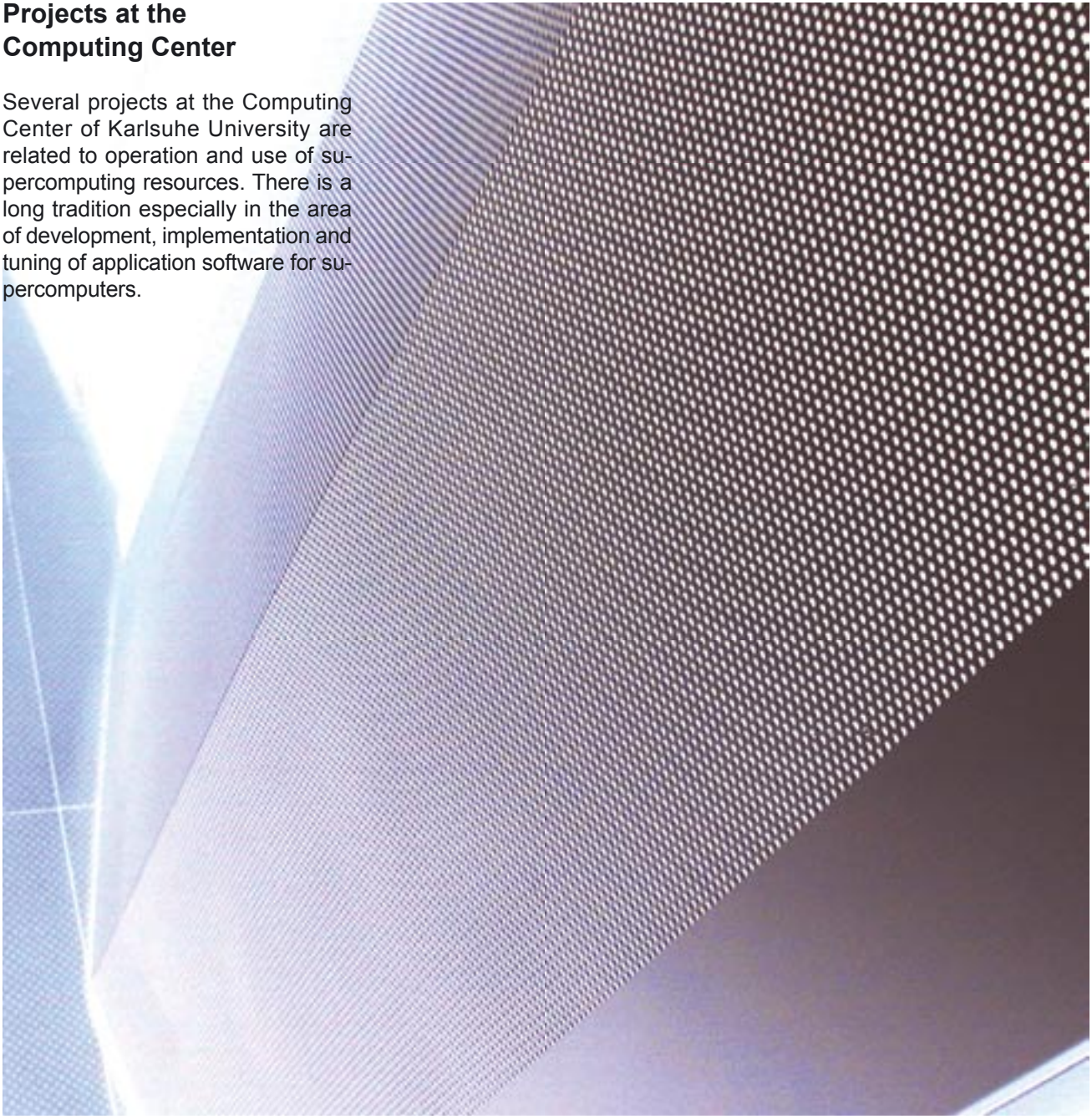
Working with a stereoscopic model in front of a projection screen

SGI Onyx2

Media Point in the Computing Center

Projects at the Computing Center

Several projects at the Computing Center of Karlsuhe University are related to operation and use of supercomputing resources. There is a long tradition especially in the area of development, implementation and tuning of application software for supercomputers.



Virtual Computing Center (VRZ) Karlsruhe

The Virtual Computing Center Karlsruhe is a joint project of the University of Karlsruhe and the Research Center Karlsruhe. At the beginning of 1996 both partners decided to establish a joint virtual computing center. `Virtual' means that each partner keeps its own real computing center, its independence and its structure. The very close and trusting cooperation of both institutions found expression in a shared ownership of the IBM RS/6000 SP and the Siemens (Fujitsu) VPP 300 which were installed at that time. Four of the 16 PEs of the VPP 300 belonged to the university, although they were located at the computing center of the Research Center Karlsruhe and were operated there together with the other 12 PEs. On the other hand, 28 of the 256 nodes of the former SP belonged to the Research Center Karlsruhe, but they were located and operated at the Computing Center of the university. These high performance computers and the campus networks were linked by a fast ATM connection. So from an end users' point of view the response times are independent of the physical location of these systems.

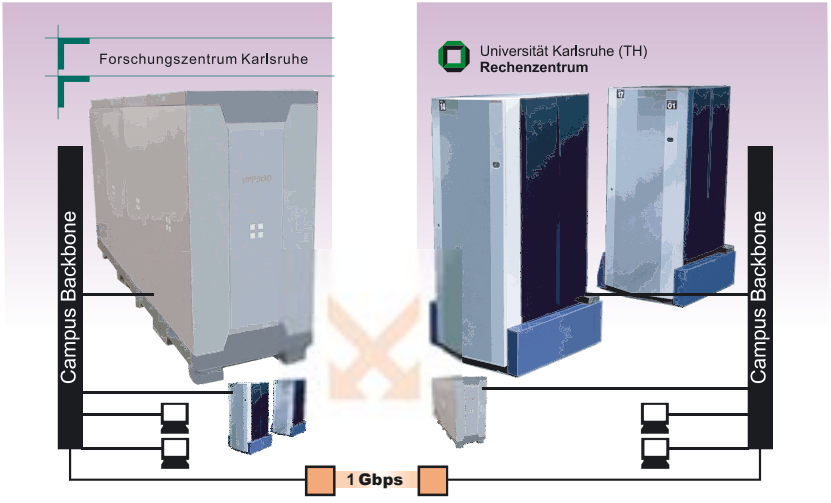


Fig. 5: Configuration of the Virtual Computing Center Karlsruhe

The cooperation in this Virtual Computing Center still continues since its foundation very successfully and as a result of it scientists and students of the university and the research center are enabled to use that supercomputer architecture - RISC based or vector processor based - which is best suited for their needs.

To have an easy migration from one system to another one within the Virtual Computing Center common administrative procedures have been introduced and both sites have set up a shared DCE cell extending over both campuses which are nowadays connected by a 1 Gbit/s ethernet link.

In a sense this Virtual Computing Center Karlsruhe has been an early realization of many concepts which came up only recently in the worldwide movement of GRID Computing.

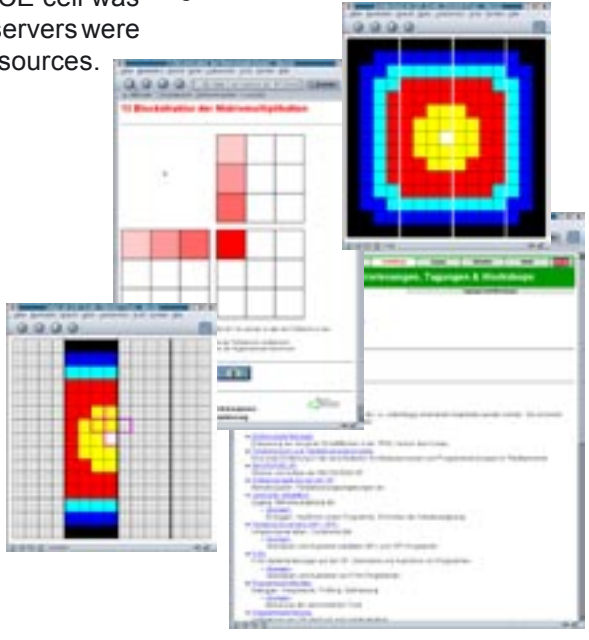
DCE/DFS on IBM RS/6000 SP

The Distributed Computing Environment (DCE) is the basic tool set for development of applications using resources on distributed computing systems. The DCE security service holds a central user database and allows the same login on all DCE machines and protects resources from unauthorized access.

The most important application of DCE is the Distributed File System (DFS), a global file system which has great advantages concerning reliability, security, data protection and performance compared to other more traditional file systems. At the Computing Center of Karlsruhe University DFS is used to hold the HOME directories of all users of several workstation clusters and of the IBM RS/6000 SP as well as large filesets containing application software packages and libraries. The latter ones are stored in read-only filesets so that they can be replicated to increase reliability and performance.

When the predecessor of the IBM RS/6000 SP was installed, major parts of the SP software were not able to cooperate with DCE and DFS. In close cooperation with local IBM staff implementations of DCE/DFS support for the batch system LoadLeveler, the backup and archiving system ADSM and the parallel execution environment have been developed. The reliability and scalability of these implementations have been proved during more than two years of SP operations now. In the next step the DCE cell was extended, and more personal workstations and departmental servers were integrated in order to have a unified access to distributed resources.

Fig. 6: Some examples from SP training course



Online Training Course for SP Users

The efficient usage of supercomputers requires that end users have a detailed knowledge of architecture, programming and operation environment. Therefore operation of a supercomputer must always be accompanied by training and support services. The SSC Karlsruhe offers online training materials using the well established techniques of the World Wide Web. These materials include documentation in form of comprehensive user guides describing the most important aspects of using the SP at University of Karlsruhe Computing Center as well as interactive lessons explaining in a step-by-step manner those topics that are important for efficient usage of the SP. This includes lessons on the architecture of the SP, operating environments, batch and interactive

usage, program development tools and program optimization. All lessons are supplemented by exercises and programming examples.

Education in Parallel Programming

In addition to the online educational training material the SSC Karlsruhe also offers courses in Parallel Computing for interested students and staff members. These courses cover many aspects of parallel programming such as the architecture of parallel systems, parallel programming environments such as MPI and OpenMP and parallel numerical and nonnumerical algorithms and their implementation in Fortran 95 as well as in C/C++. In order to make the lectures as practical as possible, laptop computers running Linux with a software environment for parallel computation are used. These laptops are connected via wireless LAN to form an ad hoc Linux Cluster right in the classroom. This makes it possible to run parallel programs live during the lecture, to make immediate changes and modifications and to try different variants of parallel algorithms on the fly. Also students can take control of this ad hoc cluster to demonstrate their own solution variants. This hands-on approach is very efficient and has been quite popular among participants.

UNICORE

The SSC is also an active player in the development of cutting-edge GRID Computing resources. As an early participant in the German UNICORE project from its very beginning back in 1997 and in its successor UNICORE+ the SSC was contributing important parts of the project in the form of UNICORE plugins for end user applications like FLUENT, STAR-CD and MSC.NASTRAN. Using these plugins a user of UNICORE can run the applications remotely on many different platforms by use of a unified and easy platform independent interface from his WEB browser. UNICORE is free software for academic use and commercially available for industrial use. In April 2003 it has been adopted as GRID middleware from the Japanese National Research Grid Initiative (NAREGI).

The FDEM (Finite Difference Element Method) Project

In a project supported by the German Ministry of Education and Research (BMBF) “Enhancement and Application of the Finite Difference Element Method (FDEM) Program Package for the Solution of Partial Differential Equations” in cooperation with the Institute for Metal Forming Technology (IFU) of the University of Stuttgart and with the manufacturers Bosch, IWKA and Freudenberg industrial problems are solved for which up to now there exists no standard application software. The basis of the project is the FDEM program package that has been developed at the Computer Center of the University of Karlsruhe and that solves partial differential equations by a difference method of high consistency order on an unstructured grid. An estimation of the discretization error is computed with the solution. The code is fully parallelized for distributed memory parallel computers.

Together with the manufacturer IWKA (Industriewerke Karlsruhe-Augsburg) the numerical simulation of the manufacturing of metal bellows is treated, the IFU contributes the material laws for stainless steel sheets.

Together with the manufacturer Freudenberg the diffusion of oxygen in fuel cells is simulated. Freudenberg produces fleece material for fuel cells whose transport properties for oxygen should be investigated.

Together with the manufacturer Bosch the numerical simulation of the lubrication gap in high pressure Diesel injection pumps is treated. By the influence of the extremely high pressure and by heat stress on the pump housing the lubrication gap is deformed. FDEM permits the global treatment of domains that are composed from subdomains with different differential equations. To be able to treat the Bosch problem, FDEM had to be extended to domains that move relative to each other, and to non-matching grids. Thus a global coupled solution for housing, lubrication gap and piston is possible.

The FDEM project runs from January 1, 2001 to June 30, 2003. It is executed in the project group “Numerical Research for Supercomputers”, directed by Prof. Willi Schönauer.

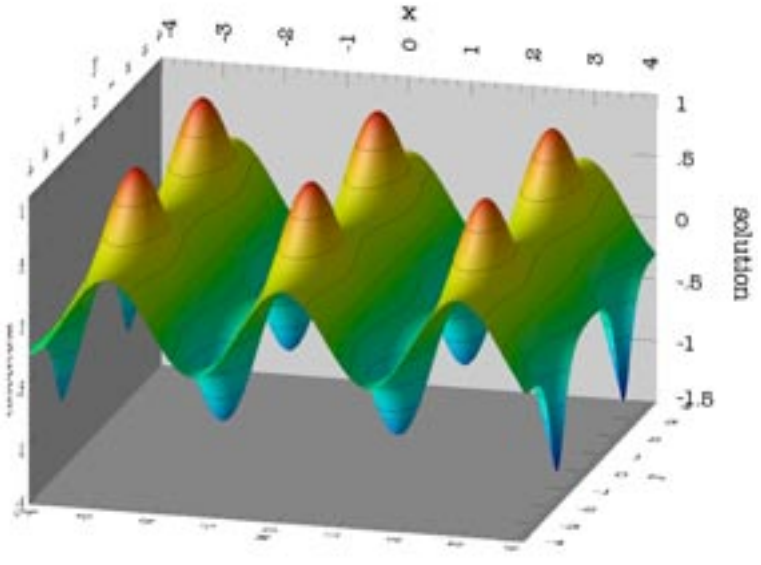


Fig. 7: Graph of the solution of a test problem for FDEM.

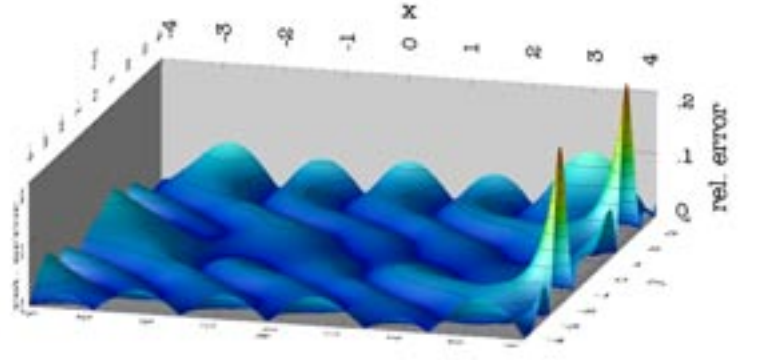


Fig. 8: Graph of the error of the FDEM approximation of the solution of the test problem.

The Parallel and Portable Linear Solver Package LINSOL

LINSOL solves huge linear systems. LINSOL is adapted to the application of sparse matrices, but can be efficiently applied to full matrices, too. As the usage of main memory strongly increases applying direct solvers to sparse matrices, iterative algorithms are employed. Implemented methods are: PRES20, BCG, Bi-CGSTAB, Bi-CGSTAB(2), CGS, BICO, QMR, CGNE, CGNR (ATPRES), GMERR and the classical CG-algorithm. If the just mentioned iterative algorithms do not converge, a direct solver with the Gaussian algorithm as underlying method optimized for sparse matrices can be hooked up. The direct solver is embedded as preconditioner into the iterative algorithms and can be controlled by two parameters. According to the choice of the parameters all graduations between the complete LU decomposition leading safely to the result in one iteration step and a weak approximation of the complete decomposition (incomplete LU) are possible. LINSOL is designed in such a way that two interfaces can be used. Using the standard interface the user has to define parameters in a file controlling the program flow of LINSOL. The matrix can be stored in Harwell/Boeing- or LINSOL-format. The second user interface is useful for the integration of LINSOL into an application program.

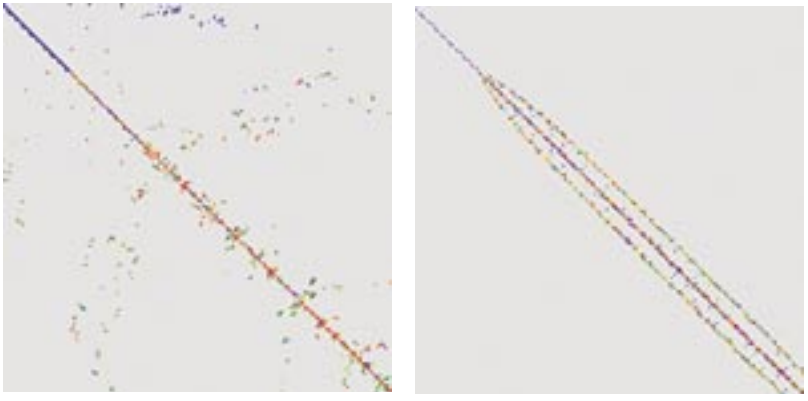


Fig. 9: Discretization matrix resulting from a fluid dynamics problem before and after bandwidth optimization

Important features of this program package are

- robustness
- portability
- flexibility
- and efficient implementation for workstations, vector computers and parallel computers.

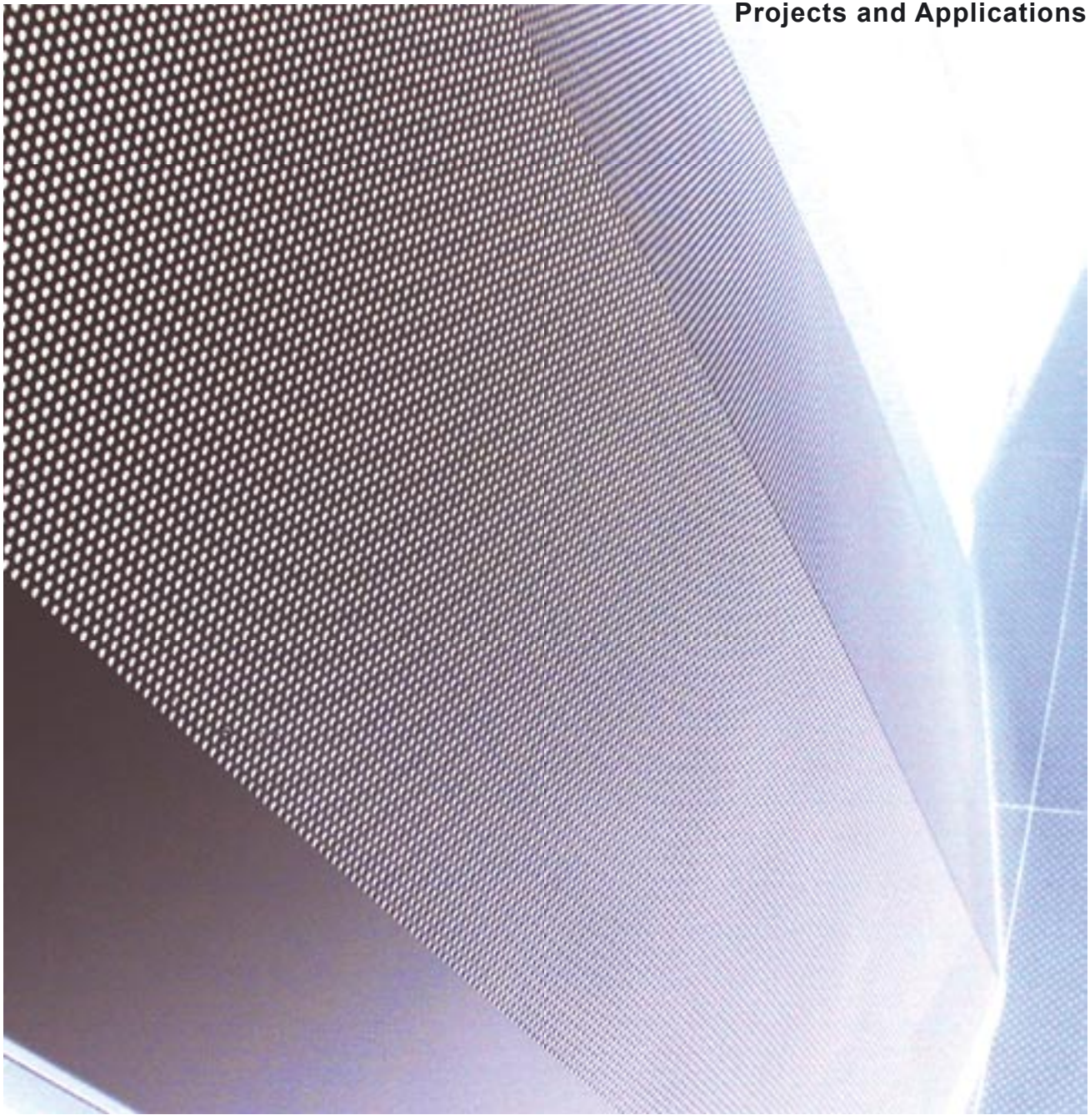
The robustness is basically obtained by two implementation features. The first one is an adaptive method selection called polyalgorithm. It chooses the optimal algorithm from many iterative methods and automatically switches to a better converging method, if the convergence deteriorates. The second one is the embedding of the direct solver into the iterative algorithms; it can be used as convergence accelerator or as „emergency exit“, if the iterative methods converge too slowly or do not converge.

To obtain portability and flexibility of the code the „message passing“ paradigm is used on parallel computers; beyond that, an own, minimal „mes-

sage passing“ interface is defined enabling the user to put in all available „message passing“ libraries in the link step of the program package.

Flexibility with respect to the integration of the program package into an application is obtained by the support of many common storage patterns for sparse matrices. In all, eight storage patterns are provided to the user; the most important are: diagonal, row, column - always full and packed. It is allowed to compose the matrix of the linear system from several storage patterns. For example it is possible to store the main diagonal of the matrix in the storage pattern „main diagonal“ and to store all other elements in the storage pattern „packed row“ so that a sparse nxn-matrix mostly consists of n+1 data types (1 data type of the storage pattern „main diagonal“ and n data types of the storage pattern „packed row“).

LINSOL is optimized for workstations, vector computers and parallel machines. An efficient vectorization leads to a high optimization rate on vector computers. On cache-based systems as e.g. workstations a cache optimization can be switched on. The most important feature on parallel computers is the scalability with respect to the time requirements and to the memory requirements. Further optimizations affect the use of the direct solver; thus a bandwidth optimizer minimizing the „fill in“ of the sparse preconditioning matrix during the factorization can be switched on before the (incomplete) decomposition starts (see Fig. 9); if the matrix is not symmetric and consists of rows with only one non-zero entry, a „pre-forward elimination“ can additionally be switched on shifting entries of the matrix by the use of known solution components to the right hand side and subsequently removing the shifted entries from the matrix.



Large Eddy Simulation of Flow over Rough Surfaces

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Institute for Hydromechanics, Universität Karlsruhe (TH)

In this project the turbulent boundary layer over roughness elements is simulated by means of Large Eddy Simulation (LES). Flows over rough surfaces have considerable engineering interest. In the field of hydraulic engineering, nearly all practical flows are hydraulically rough and the roughness affects the flow above the roughness elements. Moreover, recent research efforts have shown that the turbulent nature of rough wall flows enhance exchange processes with the subsurface pore flow and is responsible for sediment destabilization. The result is a mean velocity profile that differs considerably from the velocity profile over a smooth bed. Furthermore, the flow over rough walls is characterized by the presence of organized (coherent) turbulent structures, which are responsible for the transport of heat and mass as well as momentum across the boundary layer.
The majority of turbulence production occurs when in so-called „low speed streaks“ the fluid particles are lifted away from the wall-layer.

Fig. 1 shows low and high-speed streaks as calculated by LES and visualized with the instantaneous streamwise velocity fluctuations. The blue colour indicates fluid with a velocity smaller than the mean velocity representing low speed streaks; the red colour designates the opposite i.e. high speed streaks.

Fig. 2 depicts the vorticity in a channel whose lower wall is artificially roughened by cubes. This figure clearly demonstrates the effect of wall roughening being reflected in much higher vortical motions in contrast to the smooth upper wall.

The LES calculations are undertaken as part of the German Research Foundation (DFG) project „LES of flow over open channel beds“. Preliminary calculations of the flow over surface mounted cubes were performed on the SP with 8, 16 or 32 processors, respectively, and gave encouraging results. Further computations with different roughness types (spheres) and with inclusion of the subsurface pore flow will be carried out.

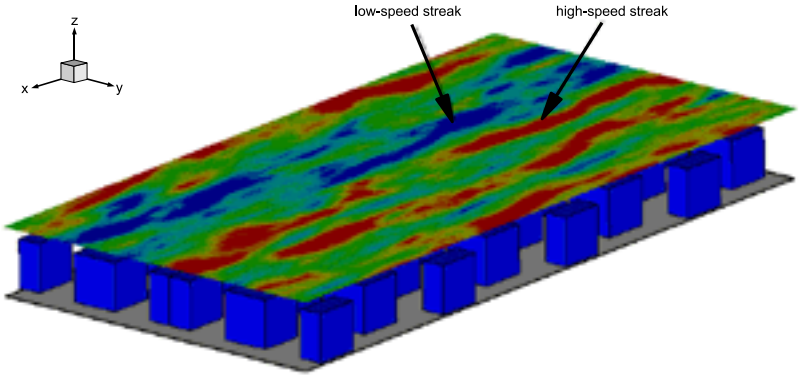

Fig. 1: Low and high-speed streaks as calculated by LES and visualized with the instantaneous streamwise velocity fluctuations.

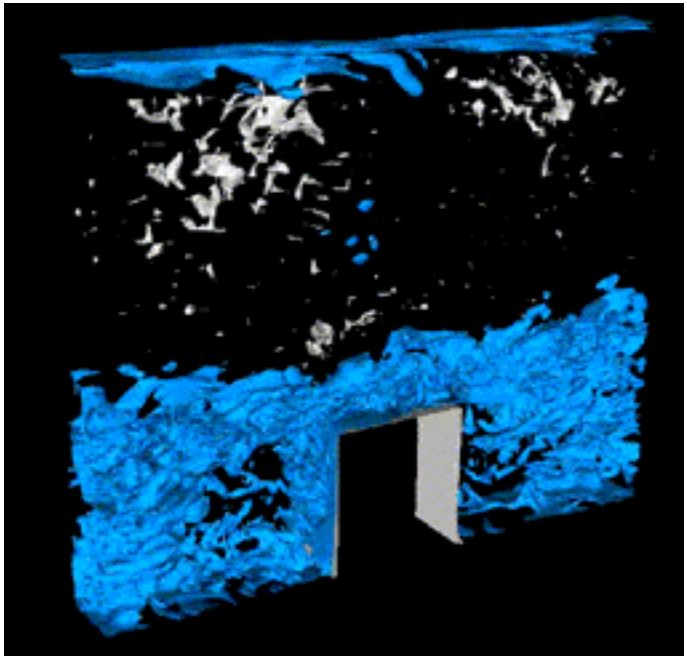

Fig. 2: Depicts the vorticity in a channel whose lower wall is artificially roughened by cubes.

Direct Numerical Simulation of Flow in Turbine Related Geometries

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As part of the German Research Foundation (DFG) project “Periodic Unsteady Flow in Turbomachinery” Direct Numerical Simulations (DNS) are carried out of flow in turbine-related geometries such as turbine cascades and specially shaped channels. Typical for any DNS is that all scales of motion need to be resolved.
In transitional and turbulent flow, motions with scales much smaller than the flow domain are important; consequently, the number of grid points required is huge. The recent increase in the availablity of computational resources makes it possible to perform DNS of Laminar Separation Bubble (LSB) flow and DNS of flow in low-pressure turbine cascades at realistic Reynolds numbers.
The main reasons for performing such expensive DNS is to further the understanding of physical processes associated with flow in complex geometries and to produce data that can be used for the development and improvement of turbulence models. All DNS are performed using a slightly adapted version of the LESOCC code developed at IFH. To achieve a near-optimal load balancing, the computational mesh is subdivided in a number of blocks of equal size that each run on their own processor.
The standard Message Passing Interface (MPI) protocol is used for inter-processor communication. Low Reynolds number calculations of flow in a turbine cascade were performed as an initial test of the accuracy of the code. Fig. 1 shows the shedding of vortices behind a turbine blade at a Reynolds number of Re=1000. The simulation was performed on the SP. Because of the low Reynolds number employed, only 8 processors and 825.000 grid points were required.
A typical DNS, at a more realistic Reynolds number, that is currently performed on the SP is the simulation of passive heat transport in a laminar separation bubble with oscillating oncoming flow. The Reynolds number for this flow problem is Re=60000 and a total of 27.9 Mio. Grid points divided over 60 processors are employed. For the entire simulation at least 200,000 time steps are required. Fig. 2 shows a typical snapshot of the separated boundary layer that is rolling up due to a Kelvin Helmholtz instability. The colours represent the instantaneous temperature.

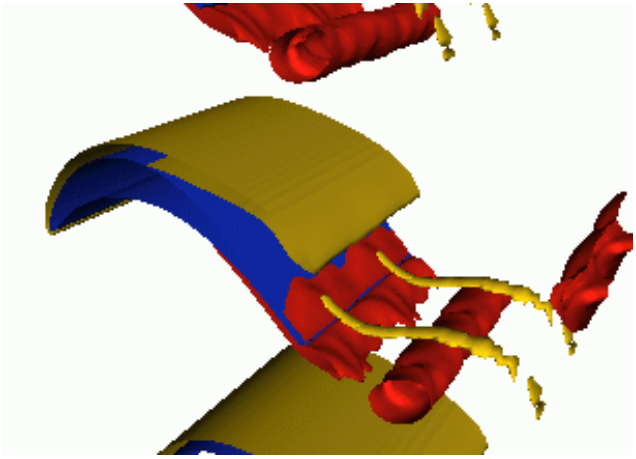

Fig.1: Shedding of vortices behind a turbine blade at Re=1000.

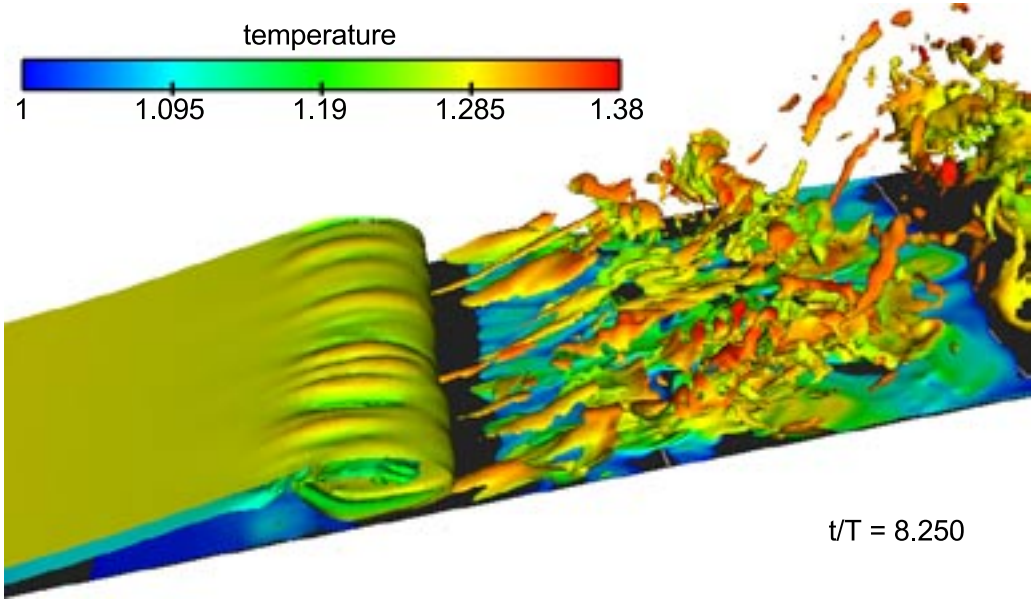

Fig. 2: A typical snapshot of the separated boundary layer at Re=60000.

Large Eddy Simulation of Bluff Bodies

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The computation of turbulent flows is of central interest from a fundamental as well as from a an application point of view.
An important activity of the Turbulence Group at the Institute for Hydromechanics (IFH) is the Large Eddy Simulation (LES) of practical interest flows, in particular bluff body flows. These flows are difficult to treat with other approaches and require the explicit computation of the large vortical structures which is performed with LES.
For this purpose the code LESOCC (Large Eddy Simulation On Curvilinear Coordinates) has been developed at the IFH. It has recently been recoded entirely in Fortran 90 in order to enhance its versatility and flexibility. The code is highly vectorized and has been parallelized for the use of block-structured grids and domain decomposition. The explicit message passing is performed with the MPI library. By the combined use of vectorization and parallelization huge problems can be computed efficiently on a relatively small number of powerful processors. With minor adaptation of the solver the code can also be used very efficiently on a large number of processors as is typical for the IBM SP.

Fig. 1 shows the complex instantaneous vortex structure of the flow around a circular cylinder of finite height mounted on a flat plate at a Reynolds number of 43,000. The block-structured, curvilinear grid contains 6.4 Mio. grid points partitioned into 24 blocks. A total of 100,000 time steps were computed on the VPP5000 to achieve a statisticaly steady state and to accumulate averages.

Fig. 2 displays the flow over a car-shaped body at a Reynolds number (based on the length of the body) of 3 Mio. It shows the streamwise velocity field in a qualitative way. This flow is particularly difficult to calculate due to its physical sensitivity to details of the configuration such as the slant angle at the rear. Therefore it is a well known test case for turbulence modelling. A block structured grid with 214 blocks and 18 Mio points was employed for this computation which was performed on the IBM SP using 64 processors.

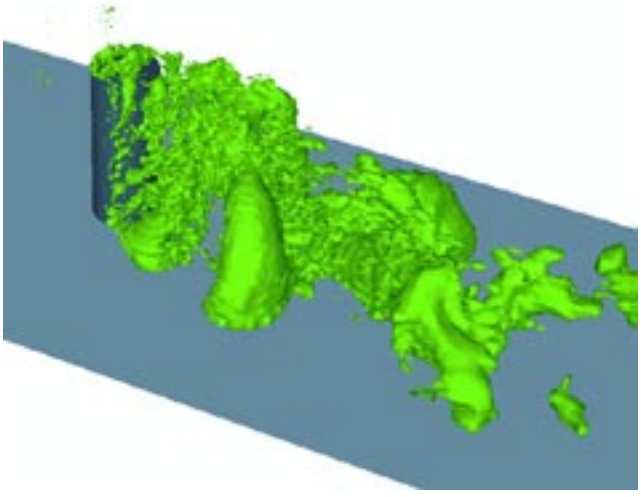

Fig.1: Complex instantaneous vortex structure of the flow around a circular cylinder at Re=43000.

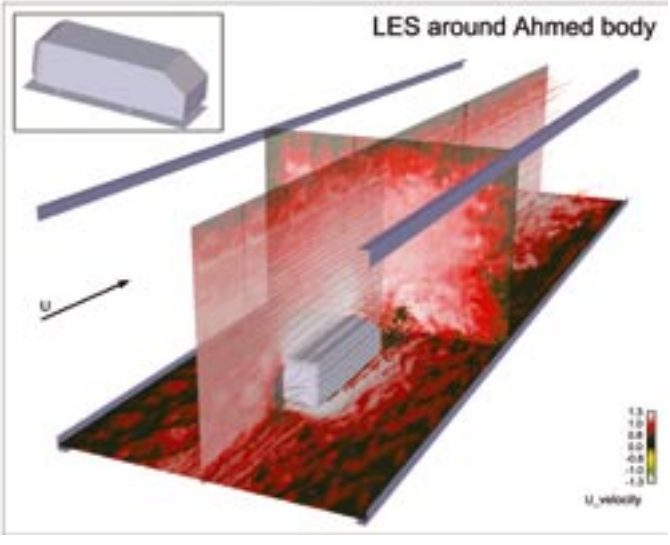

Fig. 2: Flow over a car-shaped body at Re=3-10^6.

FLUENT CFD-Simulation of Loading Fibrous Filter

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Fibrous Filters are widely used, e.g. clean room, HVAC, to remove solid particles form gases at low concentrations. Thereby, collected particles accumulate on single fibers, forming complex deposit structures (Kanaoka 1998) known to alter pressure drop and filtration efficiency significantly. Making general predictions for the increase in pressure drop and filtration efficiency of such filters as a function of dust load has been (and still is) an important but in general elusive goal; partly because flow field and particle deposition must be coupled to obtain realistic structures (Lehmann & Kasper, 2002a). Furthermore, particle bounce/adhesion influences the deposition pattern and must be understood (Lehmann & Kasper, 2003a). Moreover the loading kinetic depends on the “inner” structure of the initial filter medium, as the velocity distribution within the filter and consequently particle deposition are generally determined by the local packing density (distribution) of the filter medium (Lajos 1985, Schweers & Löffler, 1994).

More realistic simulations are now obtained by combining

- (Fig.1) modern techniques for measuring internal structure information of filter media by Magnetic Resonance Imaging (Lehmann & Kasper, 2002b, Lehmann et al., 2003) and CFD-simulations taking into account the three-dimensional information on packing density.
- (Fig. 2) modern FLUENT CFD-simulations, augmented by custom C-routines for particle deposition/bounce and for the effect of the deposit geometry on the flow around single fibers (Lehmann &Kasper, 2001, Lehmann & Kasper, 2003b).

Acknowledgement
Support for the MRI work by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

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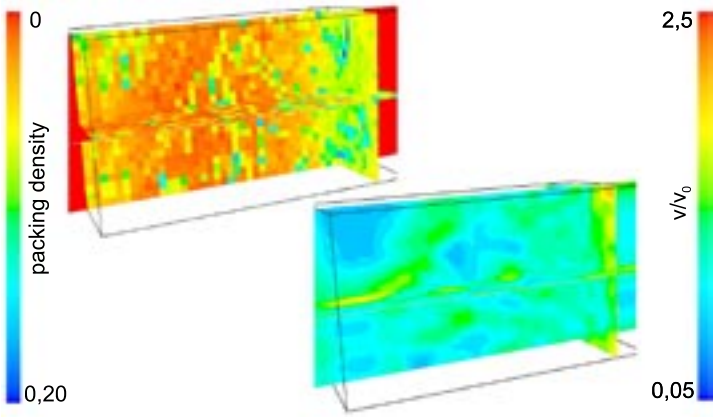

Fig. 1: (left) Local packing density distribution obtained by MRI and (right) with FLUENT calculated velocity of a filter media with thickness 10 mm, mean packing density 0.05, face velocity 1 m/s (contours shown on „inner“ surfaces)

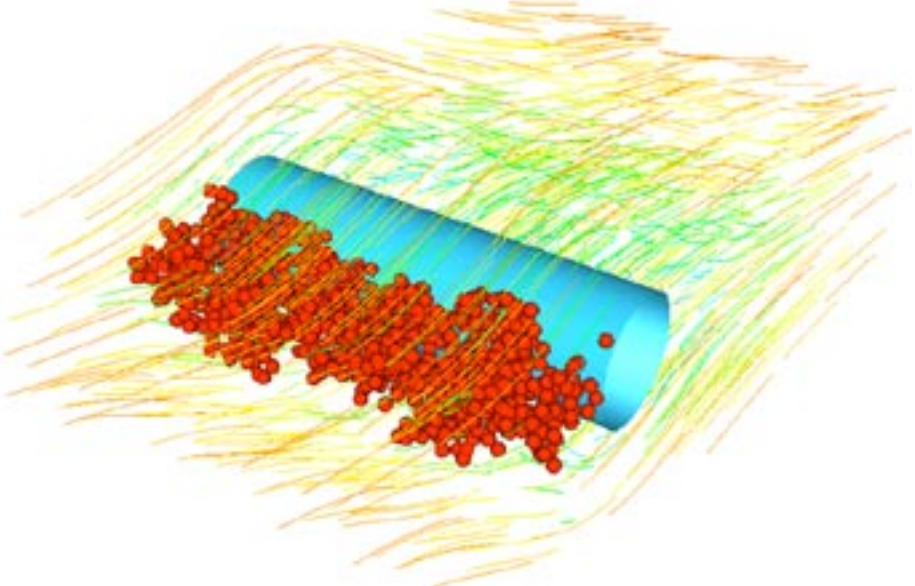

Fig. 2: Flow around a loaded single fiber
(fiber- Ø: 30 µm, latex particle- Ø 3,135 µm, v = 0.46 m/s, Stokes 0.5)

Modelling of Electro-Mechanics in the Heart: Mathematical and Numerical Aspects

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Cardiovascular Research and Training Institute, University of Utah, U.S.A.
Gunnar Seemann, Institute of Biomedical Engineering, Universität Karlsruhe (TH)
Rolf Mayer, Computing Center, Universität Karlsruhe (TH)

Many phenomena in the heart can be described with mathematical methods and reconstructed applying numerical simulation techniques in conjunction with high performance computing. The usage of coupled systems of ordinary differential equations has a long tradition for description of cellular electrophysiology and force development. Partial differential equations and equivalent integrals are employed to describe processes of electrical excitation propagation and passive mechanics. The complexity of these equations increased in the last years resulting from the attempt to incorporate more detailed descriptions, which were elucidated by modern measurement techniques.

Solving of the equations is commonly performed with numerical methods, because analytical methods are inappropriate to handle the complexity. Euler and Runge-Kutta methods are frequently applied to solve ordinary differential equations; finite element and finite differences techniques to solve partial differential equations and equivalent integrals, respectively. Efficiency of the employed numerical methods is a crucial issue, because systems with several hundreds of millions of unknowns can arise. Further complexity is added by anisotropic, non-linear material properties and coupling of phenomena, e.g. cardiac electromechanics, which necessitates the generation of efficient interfaces between the different solvers.

In this work a simulation system is illustrated, which allows the reconstruction of electro-mechanical phenomena ranging from sub-cellular to whole heart level in various species, including human. The system bases on several modules, e.g., anatomy, cellular electrophysiology, cellular force development, electrical mexcitation propagation, and passive mechanics of cardiac tissue. Each module provides interfaces via UNIX IPC, particularly shared memory and message passing. A repertoire of numerical techniques is available for solving the different types of equations. Parallelization of time consuming tasks is possible using OpenMP and MPI. The system is running on variant software platforms, e.g. SGI IRIX, Sun Solaris, Linux, and Apple MacOS X.

An exemplary result obtained with the simulation system is given in Fig 1. The simulated environment was similar to that of the classical Langendorff studies. The simulation represented a cardiac cycle including electrical de-

and repolarization as well as mechanical contraction and relaxation. The ventricle was approximated by crop of two confocal truncated ellipsoids. The ventricle's geometry and fiber orientation was rendered in lattices of 40 x 40 x 50 and 20 x 20 x 25 cubic elements with a length of 0.2 and 0.4 mm, respectively. The macroscopic orientation of myocytes was included by interpolation starting from boundary conditions in three depths of the myocardium. The orientation was set subepicardial to -70°, midwall 0°, and subendocardial 70° reflecting knowledge from anatomical studies. The lattice with high resolution was applied for simulation of cellular electrophysiology, excitation propagation, and force development. The low-resolution lattice served for simulation of passive mechanics. The presented simulation was performed on a shared memory computing server of type SGI Origin 2000 with 8 processors of type R10000 195 MHz claiming 7 processors each for a time 120 h. Parallelization of computationally expensive tasks was achieved on basis of OpenMP.

The simulation revealed characteristic patterns on physiologic excitation propagation and mechanical deformation. In future work various cardiac pathophysiologies will be included, which will allow to gain knowledge of heart disease in humans. This knowledge may be applied to improve clinical diagnosis and therapeutic strategies.

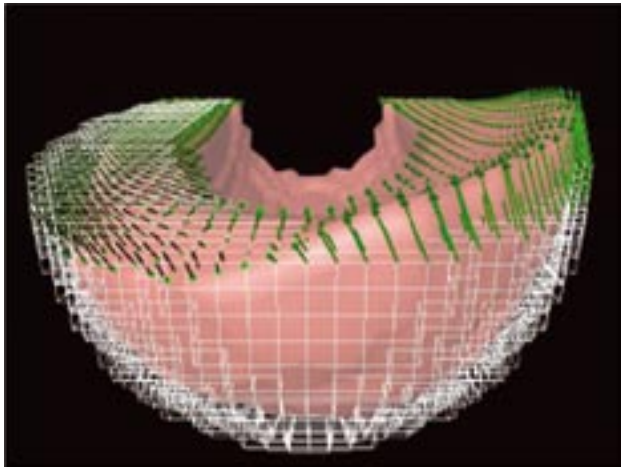

Fig. 1: Simulation results. A hollow half ellipsoid approximates the left ventricle of a small mammal at time of contraction. The ventricle is shown from apex. Green arrows indicate displacements. The white grid depicts the original, non-deformed heart.

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Computer Aided Engineering Methods used by the Institute of Machine Design and Automotive Engineering

Institute of Maschine Design and Automotive Engineering
o. Prof. Dr.- Ing. A. Albers
Universität Karlsruhe (TH)

The Institute of Machine Design uses computational methods to simulate the mechanical behavior of components and systems. Those simulations are the basis for an optimisation of the analyzed structural elements for a given application.The use of computational methods in engineering is also known as Computer Aided Engineering (CAE).
One of the various methods is the so-called Finite Element Method (FEM) which is suitable for the simulation of component behavior such as resultant stresses respectively strains or Eigenmodes and -frequencies at given boundary conditions. As depicted in Fig. 3 the geometry of the analysed mechanical component has to be meshed by means of a generation of finite elements. Those finite elements approximate the original geometry for computation. The colours in Fig. 3 show the value of the calculated stresses at the geometrical position of their appearance. All calculated measurements (e.g. strains, displacements, accelerations, …) can be displayed in such a way.
To simulate the dynamic system behavior the application of Multi Body system Simulations (MBS) is appropriate. MBS-simulations give information about the complete dynamic behavior of the system such as the load-time-history of a specific mechanical component included in the system, for example.
Further CAE-methods are the topology and shape optimization which are based on the finite element method. The shape optimization is suitable to reduce stress peaks caused by geometrical features such as notches. The topology optimization can provide basic design proposals and is often used to decrease material in low-stressed regions of the structure in order to reduce the component's weight. Fig. 1 and 2 show, how the above mentioned methods are combined within the research work of the Institute of Machine Design and Automotive Engineering.The blue component shown in Fig. 1 is embedded in a complete mechanical system in the first step (left upper picture in Fig. 1).
By applying MBS the relevant loads affecting the component can be derived. In a second step the acquired loads are part of the boundary conditions for the FEM-simulation, which is used to determine the resultant stresses. With knowledge of the stresses and the geometrical position of their appearance the topology optimization can be started to reduce the components' weight.

Fig. 2 shows the shape optimization result for a connecting rod in order to reduce the stress-peaks. The resulting FEM model is then used for a modal analysis to determine the Eigenmodes and -frequencies which are then returned to the MBS-model.
The institute also deals with the optimization of springs (Fig. 3). The objectives of this optimization are to improve the mechanical behavior of the springs concerning the stresses and deformation properties and to optimize the springs' cross section with respect to the stress distribution. An important aspect for the simulation of springs is to consider the manufacturing process since residual stresses are caused which influence the resultant stresses.

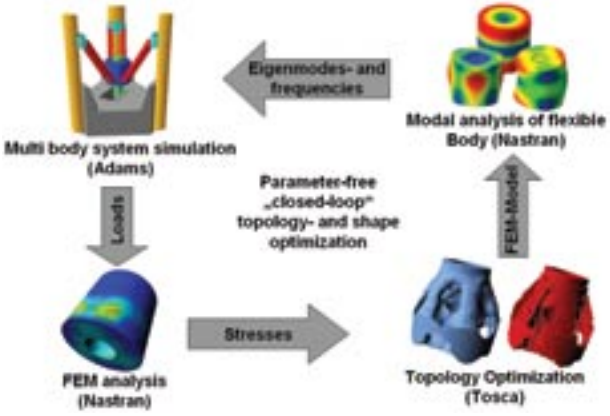

Fig. 1: Parameter-free „closed-loop" topology and shape optimization

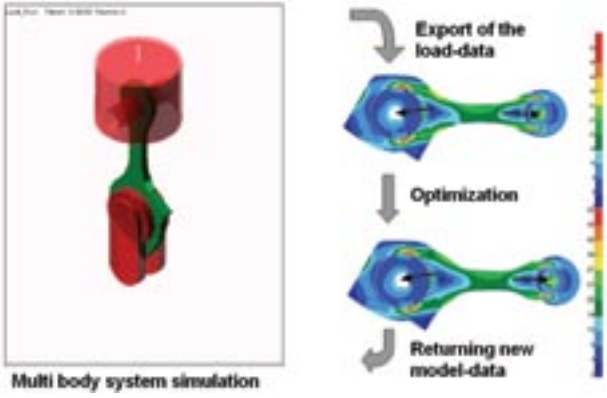

Fig. 2: System based optimization of mechanical components

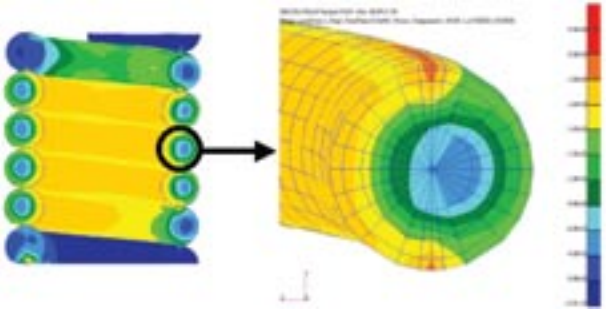

Fig. 3: Optimization of springs

A Goodness-of-Fit Test for Copula Functions

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Description

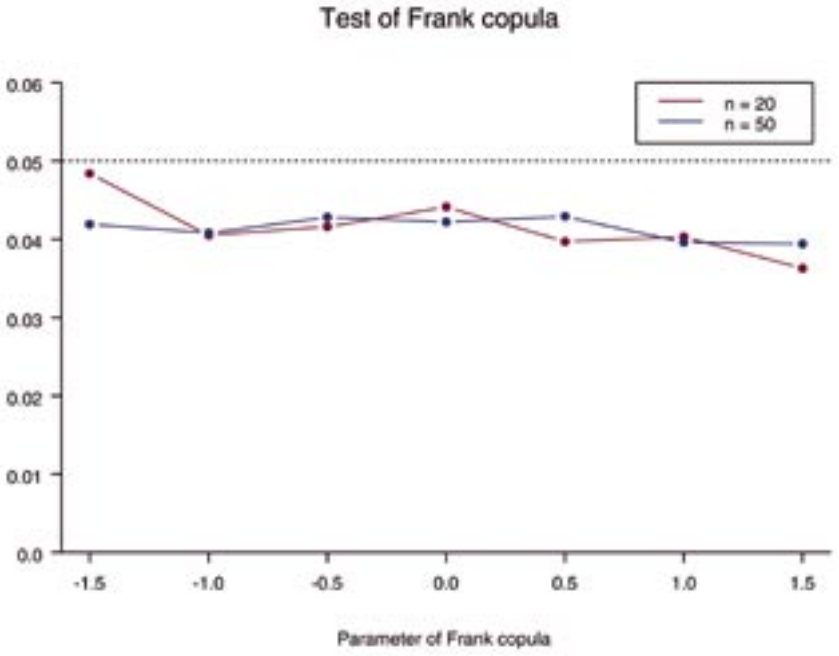
A stochastic model for two-dimensional data consists of marginal distributions (e.g. normal or exponential distribution) and a copula (function). The copula determines the dependence structure of the model completely. So, given a set of data, there is the natural question: Which copula is the “right” one? A statistical goodness-of-fit test addresses the question whether a set of data is compatible with a given family of copula functions.

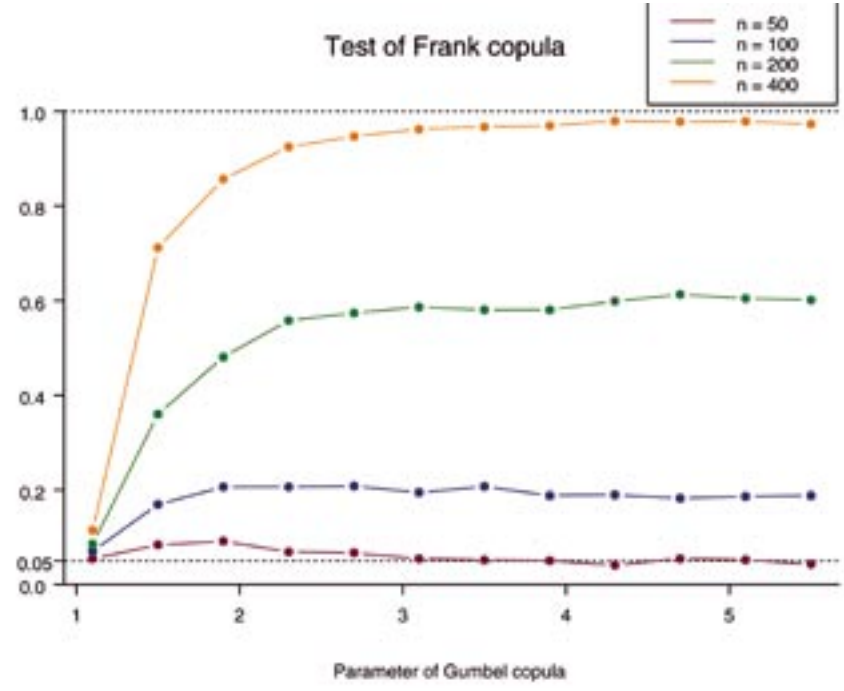
Goodness-of-Fit Test

We consider now the parametric copula family of Frank. As hypothesis H_0 we choose: The “true” copula is a Frank copula. For a growing sample size n the test should maintain a given significance level α (e.g. α=0.05), and it should be consistent. The level α is maintained, if H_0 is true and the probability that H_0 is rejected is at most α for growing n. The test is consistent, if the alternative hypothesis (i.e. no Frank copula) is true and the probability that H_0 is rejected converges to one for growing n. For applications these theoretical asymptotic results were complemented by stochastic simulations on the IBM RS/6000 SP.

Simulation results

The first diagram shows, that the test keeps the level of *0.05* quite well for *n=20,50*. In the situation of the second diagram the “true” copula is Gumbel. We see, that the probability that H_0 is rejected converges to one for growing n.


Test of Frank copula
n = 20
n = 50
0.06
0.05
0.04
0.03
0.02
0.01
0.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Parameter of Frank copula


Test of Frank copula
n = 50
n = 100
n = 200
n = 400
1.0
0.8
0.6
0.4
0.2
0.05
0.0
1
2
3
4
5
Parameter of Gumbel copula

FE-Simulation of Subsequently Piled Foundations

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TU Hamburg-Harburg

Overview

Existing foundations of buildings can be piled subsequently to improve their bearing behavior. The effort of subsequent piling depends on the initial state of soil as well as the load history. Large scale model tests were carried out at the University of Kaiserslautern [3] to study the influencing quantities, especially the initial state of the soil and the installation process, see Fig. 1a.

FE-Model

The tests were numerically simulated with the commercial FE-code Abaqus/Standard 6.2. The mechanical behavior of the soil (sand) was described with a rate-type hypoplastic constitutive model, which considers the dependence of stiffness and strength of soil on the mean stress level as well as on the void ratio. The capacity of this model is documented in many publications and practical projects. In the case of the single-symmetric FE-model eight contact surfaces are modelled with node-to-segment contact for small sliding conditions. The elastic parameters of the hardening concrete piles are introduced time dependent.

In a first step a double-symmetric FE-model, see Fig. 1b, was used for the simulations. A single symmetric FE-model, see Fig. 1c was introduced to enable a measured rotation of the foundation block due to imperfections regarding the eccentricity of the load piston and the initially inhomogeneous distribution of the void ratio of the soil.

Detailed results of the model tests and FE-simulations are published in [3, 1, 2]. Fig. 1d and 1e shows the calculated distributions of vertical stress σ_{33} and vertical displacement u_3 in the soil body for a vertical load of F_3 = 700 kN after the piling process.

Computational Aspects

The simulations were carried out at the SSC (Scientific Supercomputing Center) – University of Karlsruhe – on the SP machine. The single-symmetric FE-model consist of about 30.000 dof. Abaqus/Standard ist a shared memory program, so that maximal eight nodes can be used in parallel jobs. A typical serial job takes about 92 hours wall clock time and requires 2 GByte data and program size for optimal I/O of Abaqus. For parallel jobs a speedup of 2 ÷ 3 could be reached under the given conditions (Abaqus 6.3 shows a better speedup). The relative high wall clock time for the serial jobs is caused by the rate type material model, which have to be integrated carefully on the local level. Faster integration schemes and the application of the explicit FE-code Abaqus/Explicit are part of current FE-projects.

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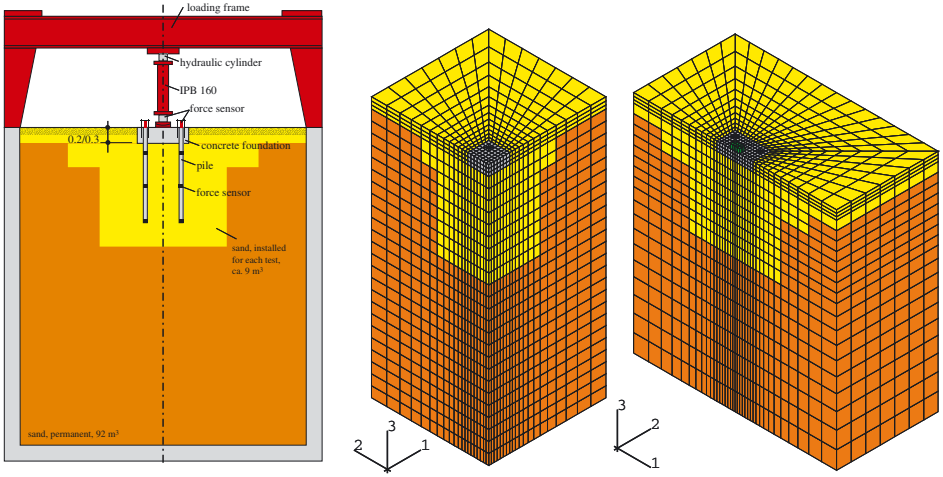
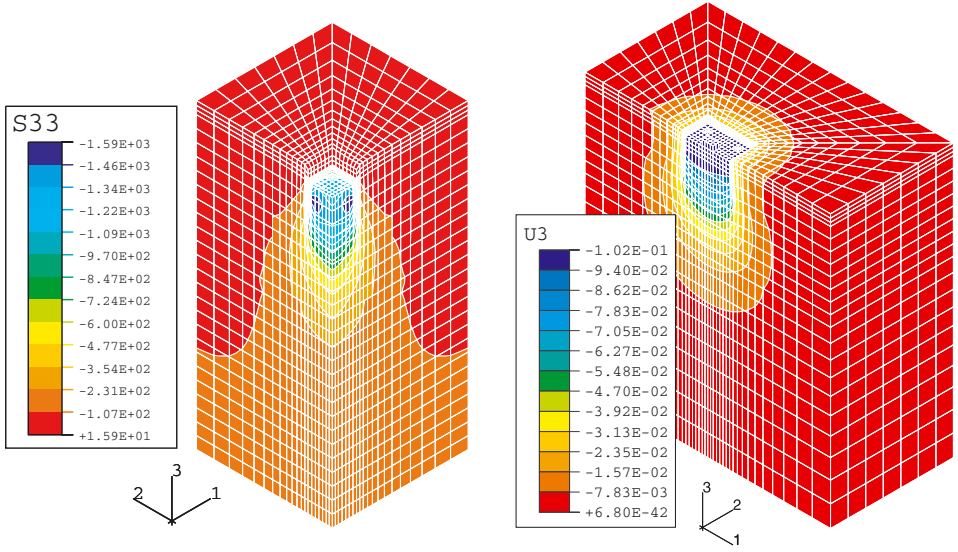


(a) model test (b) double-symmetric FE-model (c) single-symmetric FE-model



(d) calculated distribution of vertical stress σ_{33} (e) calculated distribution of vertical displacement u_3

Fig. 1: FE-simulation of subsequently piled foundations: (a) model test, (b) double-symmetric FE-model, (c) single-symmetric FE-model (colours: orange = permanent sand, yellow = filled sand, grey = foundation, green = loading plate, blue = piles), (d) contour plot of vertical stress σ_{33}, (e) contour plot of vertical displacement u_3

Projects at the Institute for Reliability of Systems and Devices

Institute for Reliability of Systems and Devices
Universität Karlsruhe (TH)

The Institute for Reliability of Systems and Devices (IZBS) is investigating microstructure-property relations of materials. Particular emphasis is placed on the mechanical properties of materials studied by computer simulations. The mechanical behavior of materials is governed by processes on very different time and length scales, and can therefore not be handled by just one computational scheme but requires various computational methods or multi-scale approaches. The consolidation of the information obtained at different scales is the main task in multiscale modelling.
This can be achieved by combining different simulation methods (project LOTF), or by passing information from one scale to the other (Fig.1, project ADD). As an example, engineering simulations of deformation processes at the macro-scale use continuum mechanical techniques like the finite element method (FEM), which require constitutive relations (project MICROCUTTING). Currently, these are empirically adjusted to experimental data. Discrete dislocation dynamics (DDD) simulations can give a physical basis for these constitutive relations. These DDD simulations, however, require information about dislocation-obstacle interaction which is governed by mechanisms on the atomic scale. Molecular dynamics (MD) or Monte Carlo (MC) methods, which can simulate the interaction of many millions of atoms by using semi-empirical atomic interaction potentials (project NANOCONTACT) are used there. Chemical accuracy can, however, not be achieved with such potentials. For problems that require a realistic treatment of the atomic bonding like fracture (project CRACK) or the structure of small clusters (project CLUSTER), one therefore has to resort to ab-initio methods based on density functional theory.
The afore mentioned six projects which are conducted at the IZBS and in close collaboration with other partners will be described on the following pages.

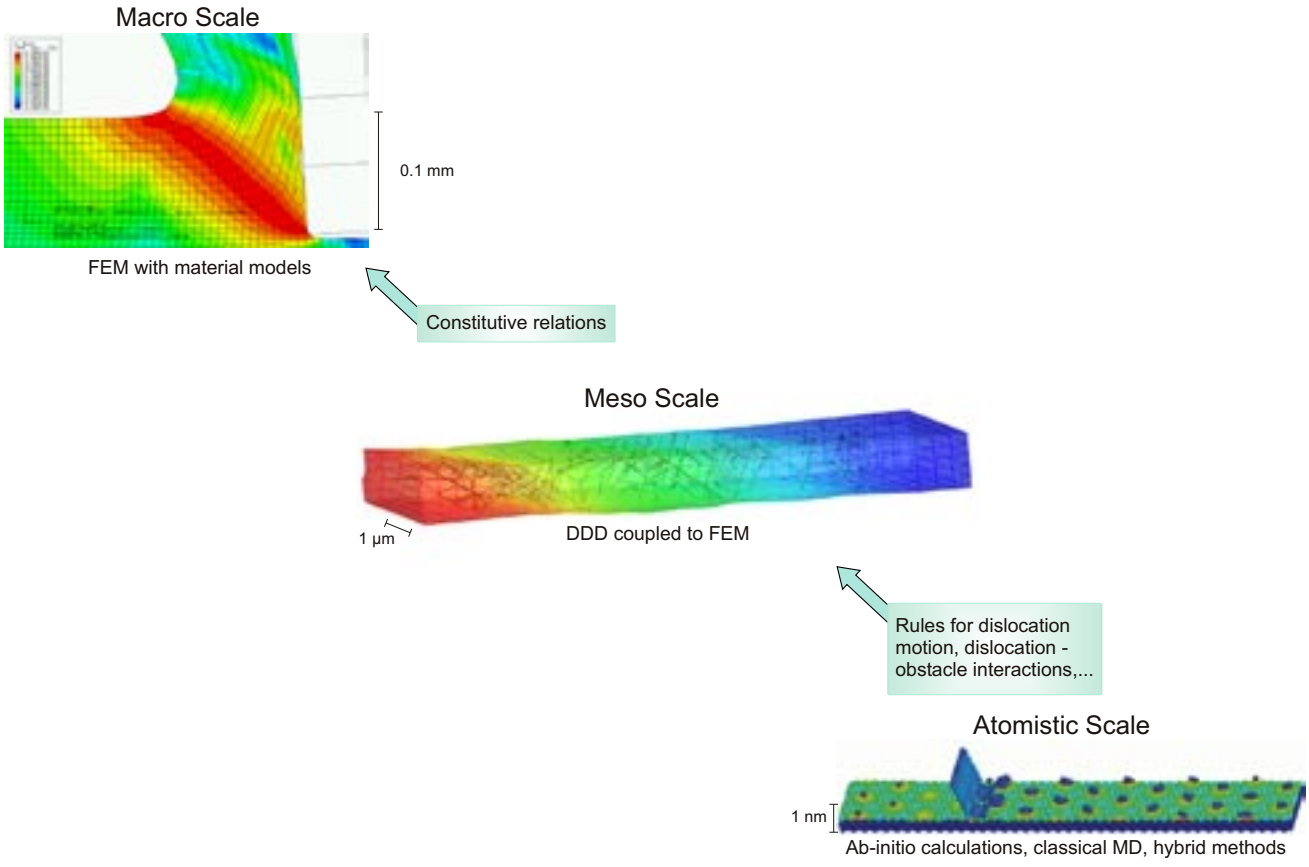


Fig.1: Principle of multi scale modelling applied to the deformation of ductile metals and alloys.

Molecular Dynamic Studies on Dislocation - Obstacle Interactions

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The deformation of materials consists of a well understood elastic contribution and a permanent plastic contribution. The plastic deformation is mainly carried by dislocations, line-defects of the regular crystal lattice. When a dislocation moves through the crystal, it shears the crystal along its plane of motion by a well-defined displacement vector. A quantitative description of plastic deformation in crystalline solids requires knowledge of how an assembly of dislocations evolves under stress. Obstacles which impede dislocation motion can produce dramatic increases in the material's yield strength. Such a strengthening may be caused amongst others by other dislocations (as dislocations strongly interact with each other), alloying elements and interfaces. Insight into the mechanisms of dislocation-obstacle interaction can not only help in the design of advanced materials, but also contribute to the physical basis for the engineering description of the deformation of materials.

In our atomistic simulations the interaction between atoms is given by semi-empirical embedded atom method (EAM) potentials. These potentials are fitted to reproduce the relevant material properties like the cohesive energy, lattice constant, elastic constants, stacking fault energy, etc. of the model material, in our case nickel. In molecular dynamics (MD) simulations the equations of motion for up to many millions of atoms are integrated with the corresponding initial and boundary conditions. Energy minimization methods like the conjugate gradient methods were used to determine static equilibrium configurations. Dislocations have a long-range stress field, therefore large simulation boxes are needed to minimize finite-size effects. Thus appropriate high performance computing resources are required, especially to conduct parameter studies.

As model system for the study of dynamic effects in the interaction of moving dislocations with localized obstacles a vacancy cluster was chosen. Configurations like the studied ones may be found e.g. in irradiated materials.

The simulations showed pronounced dynamical effects which significantly lower the critical passing stress for obstacle passing at room temperature compared to static simulations (Fig. 1). These observations could be explained by including the (relativistic) inertia of the dislocation in a line-tension model. Up to now such inertial effects have been neglected in the modelling of dislocation dynamics.

As other type of obstacles interfaces have been studied in the thin film geometry. The increased yield stress of metallic thin films can be explained partly by the energy required to deposit dislocations at the film-substrate interface (Fig. 2). The interactions of these dislocations with the interface can be very complex, e.g. reactions with misfit-dislocations (Fig. 3), transmission of dislocations and failure initiation at dislocation pile-ups can take place. These processes affect the mechanical properties of nanostructured materials and have an impact on the reliability of multilayer components and micro electro-mechanical systems (MEMS).

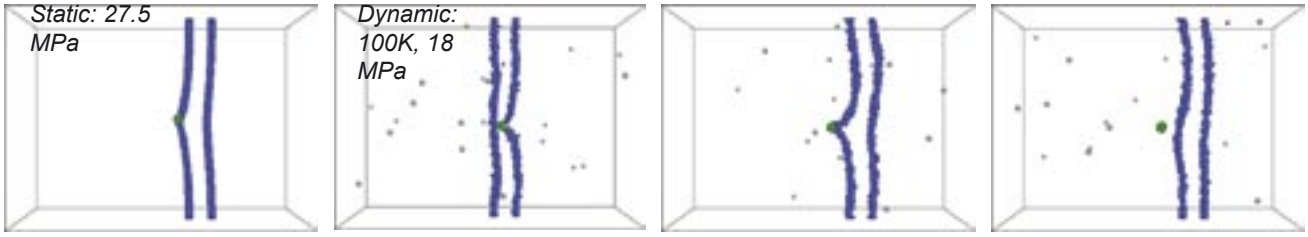

Fig. 1: An edge dislocation split into two partial dislocations is interacting with a vacancy cluster. The critical stress in the dynamic case (snapshots on the left) is much lower compared to static simulations (on the right). This inertial overshooting has up to now been neglected in the simulation of dislocation dynamics. In the above pictures the defects are identified by the atomic coordination number.

Fig. 2: Upon deformation dislocations are deposited at the interface between a thin metal film and a substrate. TEM picture by G. Dehm, MPI f. Metallforschung Stuttgart, MD simulation by E. Bitzek.

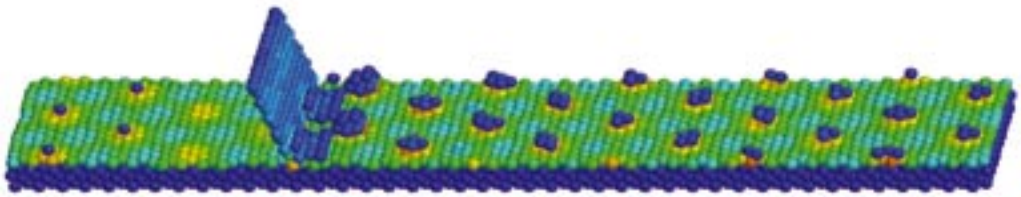

Fig. 3: A deposited dislocation can react with the misfitdislocation network that forms at a semihomogeneous interface to accommodate the lattice mismatch. Only atoms belonging to the substrate and the film atoms which have an increased potential energy are shown.

Simulating Micro-Cutting of Steel with ABAQUS/Explicit

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One main tendency in technology is the miniaturization of devices and components. Micro-fluidic, micro-mechanic, micro-optic and micro-electronic devices are combined as micro-systems allowing for new products for example in bio and medical technology, information and communication technology as well as in automotive industry. For a major breakthrough of micro-technology an economical processing is of vital importance. At the present time most manufacturing processes are adapted from the semiconductors industry. Therefore these are only economical for very high lot. Furthermore these lithographic processes strongly restrict the producible geometry. Micro-cutting has the potential to overcome these problems and to offer new fields of application to micro-technology.
The miniaturization of cutting tools and chipping depth, however faces some problems itself. Together with the “Institute for Materials Science and Engineering (iwk I)” and the “Institute for Machine Tools and Production Science (wbk)” - both at the University of Karlsruhe - the “Institute for Reliability of Systems and Devices (izbs)” works on a shared project investigating size effects in the chip formation. This project is funded by the central public funding organization for academic research in Germany, the “Deutsche Forschungsgemeinschaft (DFG)”, in a nation wide program on scaling of processes (SPP-Prozessskalierung). When the cutting-depth tends to be of the order of micro-meters some unexpected phenomena appear which for example concern the needed cutting force or the quality of the produced surface. These phenomena, not foreseen by conventional scaling used for dimensioning in cutting technology, are summed up as so-called size effects. These size effects can be of different nature. Some of them are of geometric or kinematic nature, as for example the cutting edge can no more be regarded as infinitely sharp. A second kind of size effects originates from the materials behavior which can be inherently size-dependent in small dimensions. This can be for “obvious” reasons, as when the microstructure can no more be regarded as homogeneous, or more hidden in a materials behavior that is depending on the plastic strain rate. The high plastic strain rates occurring in micro-cutting result in the need of modelling complex thermo-mechanical behavior with the materials behavior depending on both, temperature and strain rate. Increasing temperature leads to a softening and increasing strain rate leads to a hardening of the material and thus these two effects compete resulting in the domination of the one or the other depending on parameters like for example cutting speed, cutting depth and cutting angle.

The advance in hard- and software now makes it possible to simulate even such highly dynamic processes with common FEM-programs like ABAQUS, whereby we implement the needed complex material behavior in an own user subroutine (VUMAT).
Simulations allow for insights into the material during the process, which are not accessible via experiments or in situ measurements. As an example you can see the plastic strain rates occurring during the chip formation in Fig. 1 and the corresponding van Mises equivalent stress in Fig. 2. At the moment we are working with an idealized two-dimensional model (orthogonal cutting). To be able to calculate with sufficient accuracy already this 2D calculations require a total of over 4000 elements and of several 100000 time steps. The planned 3D calculations will raise the number of elements significantly. We therefore need fast super computers to be able to do these calculations in an acceptable time.

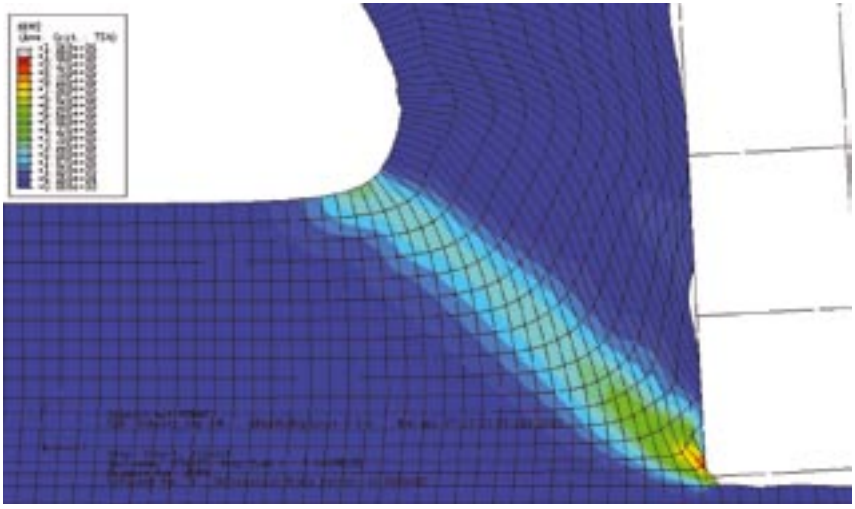

Fig. 1: Contour plot of the equivalent plastic strain rate [1/s] in the workpiece.

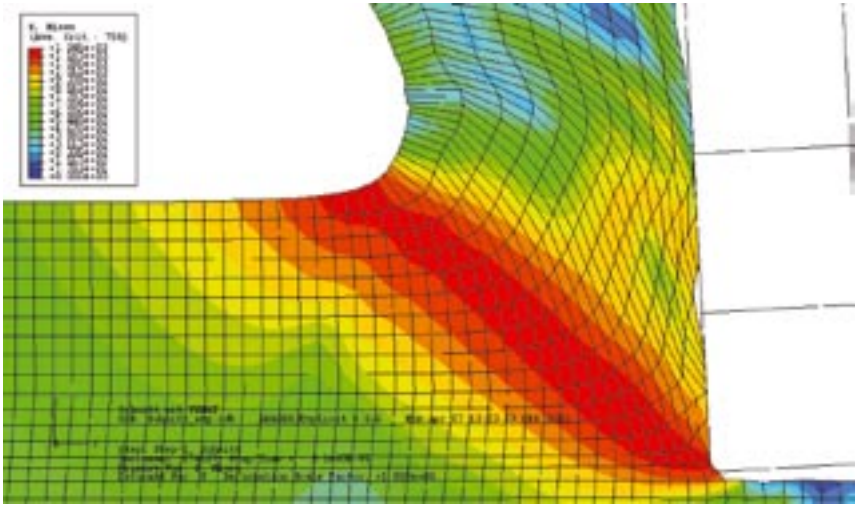

Fig. 2: Contour plot of the von Mises equivalent stress [MPa] in the workpiece.

Atomistic Aspects of Brittle Fracture: Cleavage Fracture of Diamond

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The mechanical properties of materials are ultimately determined by events occurring on the atomic scale. In the case of brittle fracture, this connection is obvious, since the crack in a perfectly brittle material must be atomically sharp at its tip. The crack moves by breaking individual bonds between atoms and can therefore be regarded as a macroscopic probe for the atomic bonding. Atomistic modelling of cracks is a rather complicated problem because both the long-range elastic interactions and the short-range chemical interactions are needed for a correct description of the problem. From atomistic point of view, resistance to crack propagation should be characterized by the forces needed to separate bonds successively. Thus it is critical to examine this phenomenon at the atomistic scale with a method that provides chemical accuracy. Crack propagation in semiconductors has been studied by simple empirical interaction models but recent studies [R. Perez and P. Gumbsch, Phys. Rev. Lett. **84**, 5347 (2000) and references therein] show that first principle calculations are needed to obtain a correct description of theses systems.

We are doing ab initio simulations of a crack tip in diamond. For centuries, people involved in the handling and shaping of diamond have been aware of the tendency for diamond crystals to cleavage quite easily to certain planes. Despite significant theoretical and computational effort [see R. H. Telling et al, Phys. Rev. Lett. **84**, 5160 (2000) and references therein] there are many open questions and the physic of this process is not well understood yet.

We are using the state of the art ab initio methods in material science: density functional theory (DFT) with a plane wave basis set and ultrasoft pseudopontentials. This calculation allows to simulate the system with the required high accuracy. We do this work with one of the best codes available: CASTEP 4.2 [M. C. Payne et al, Rev. Mod. Phys. **64**, 1045 (1992)]. As we have commented above this method is very precise but it demands lots of CPU-time so we need fast parallel supercomputers in order to obtain results in an acceptable time.

Our first results show directional anisotropy in the cleavage fracture of diamond. This means that the fracture process depends on the crack plane and on the crack front direction. We have found that a crack in the (110) plane propagating in the [-110] direction (Fig. 1) presents lattice trapping. Lattice trapping causes the crack to remain stable and not to advance until a criti-

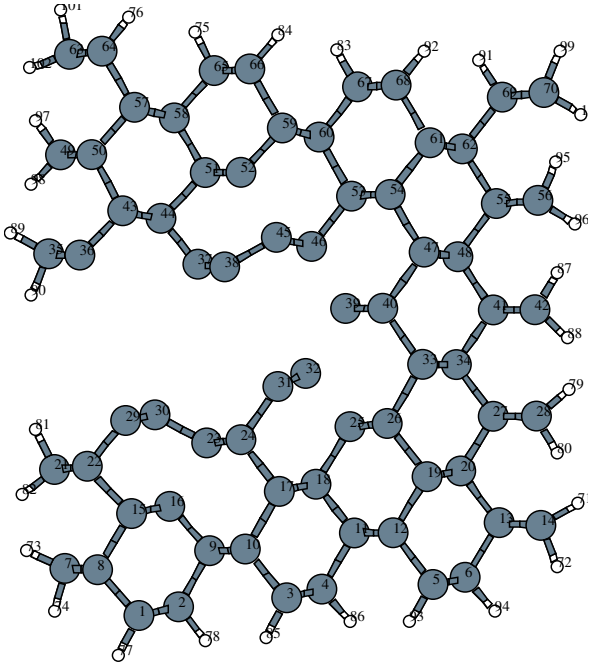

Fig. 1: Carbon crack tip. (110) plane [-110] direction.

cal load that are somewhat larger than the Griffith load K_G (obtained with the traditional analysis of brittle-fracture processes) are reached. We have also observed hysteresis when the crack is opening or closing. Cracks in the (110) plane but in the [110] direction will propagate easier (Fig. 2). The results for the crack in the (111) plane also show "easy" propagation.

All these results confirm that an atomistic description is essential in the fracture study: lattice trapping effect, anisotropy and hysteresis cannot be determined by classical studies.

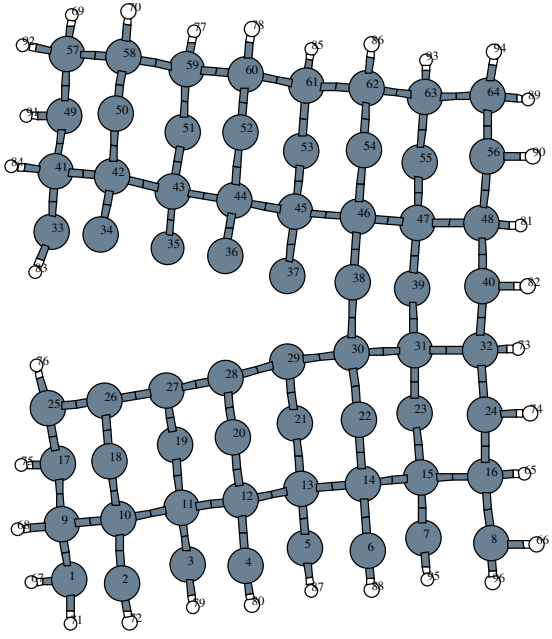

Fig. 2: Carbon crack tip. (110) plane [110] direction.

Large Scale Molecular Dynamic Simulations of Metal Nanocontact Formation

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A nanocontact is a small constriction of the order of nanometers. In its ultimate form, it is just a chain of atoms. At these small dimensions, macroscopic laws, like Ohm's law for the conductance break down and the laws of quantum mechanics take over. A good knowledge about this different behavior is of special interest to the semi-conductor industry in its search for further device miniaturization. Furthermore, nanocontacts play a very important role in friction and wear between two metals as well.
Experimentally, a nanocontact can be obtained by indenting and retracting two small electrodes. After making contact, the electrodes are pulled apart and a nanocontact will form. Using a Scanning Tunneling Microscope (STM) set-up, the indentation-retraction process can be performed in a controlled way. The tip that serves as one of the electrodes is indented and subsequently retracted into a substrate that serves as the other electrode.
During the indentation-retraction process described above, the electrodes will deform. Deformation can be composed into an elastic and a plastic contribution. As opposed to elastic deformation, plastic deformation causes defects like dislocations in the lattice. In order to get more insight into the atomic processes going on during an indentation-retraction processes, a molecular dynamics study using semi-empirical (EAM) potentials is performed.
Since dislocations involve long range stress fields, the simulation box must be large enough to minimize finite size effects. Therefore, our simulated system, that is composed of a tip and a substrate, has dimensions of 27 x 27 x 30nm and consists of about 800.000 atoms (Fig. 1). Experimental conditions like a low working temperature and low tip-sample approaching speed are best approached by simulating quasi-statically. This means that the system is relaxed after each change in position of the tip with respect to the substrate. Quasi-static simulations at these dimensions are computationally expensive and hence large computing power is indispensable.
Up to now, most of the time the experimentally studied material was gold. In our study, the material used is tungsten. Because of the differences in electronic structure, different conduction behavior can be expected for tungsten. Moreover, the different electronic structure is responsible for a difference in structure: tungsten has a BCC structure whereas gold has

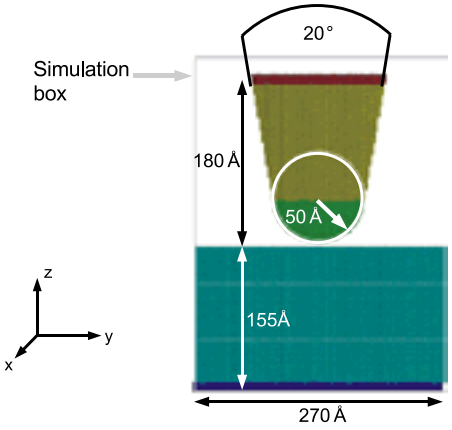

Fig. 1: The initial configuration. The tip is a cone with an opening angle of 20 degrees, a height of 180Å and a radius of curvature of 50Å. The slab has dimensions of 270 x 270 x 155Å. The total amount of atoms in the system is about 800.000.

a FCC structure and these different structures exhibit different deformation mechanisms.
In Fig. 2 some pictures of the result of a simulation are shown. Only atoms that have an increased potential energy are visualized. That is, dislocations and atoms at the surfaces of tip and substrate. The blue lines of atoms that appear are dislocation loops that result from plastic deformation. Next to giving information about the deformation processes, the structural information can be related to the electronic conductance through the contact. Thanks to the close collaboration with the Eindhoven University of Technology, where the experimental work is performed, this structural information can be directly related to the experimentally obtained conductance curves.

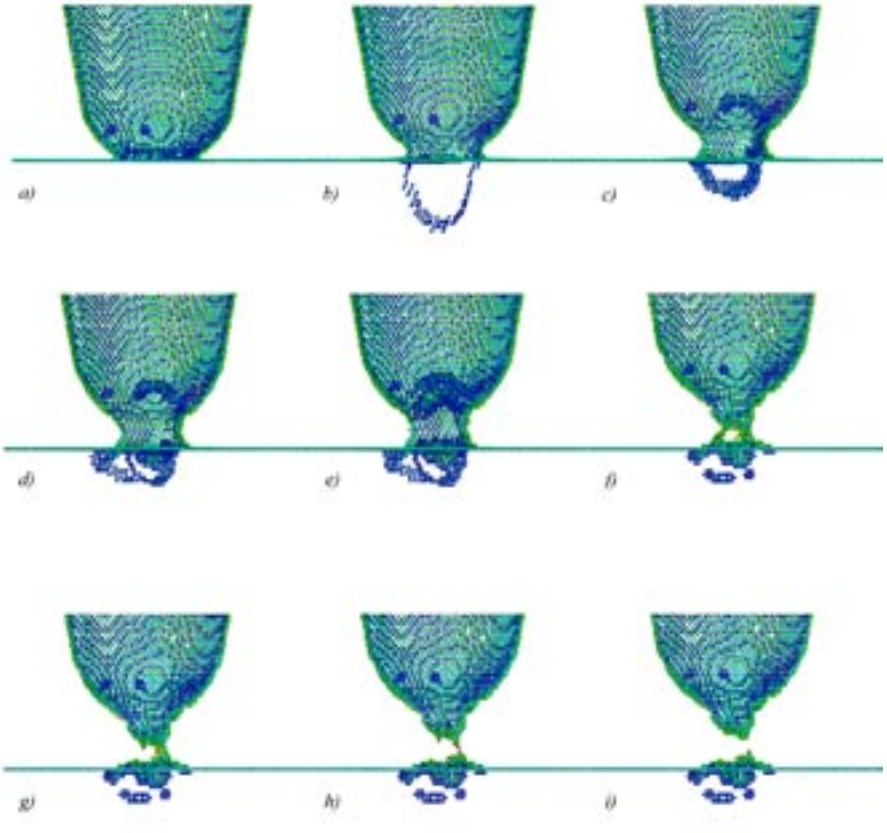

Fig. 2: The pictures a) - i) illustrate the retraction part of the simulation showing nanocontact formation. Only atoms that have an increased potential energy are visualized.

The SKaMPI Benchmark

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While developing programs for parallel computer, software engineers are confronted with several problems. First of all their programs have to be fast, which often requires several expensive and time consuming development cycles during the development process. On the other hand their programs are supposed to be portable. Not only technically i.e. with simple recompiling of the code, but also without too much loss of effciency. MPI tries to help the programmer in this respect and provides not only simple point-to-point communication operations but also more complicated collective ones. One of course hopes that these are implemented more efficiently than the application programmer could do due to his lack of detailed hardware knowledge and especially because he is usually not allowed to access low-level system interfaces. Unfortunately not all MPI implementations are as optimized as one would expect.

It is therefore crucial to know about the different aspects of an MPI implementation and SKaMPI can help in that respect. SKaMPI is an abbreviation for “Spezieller Karlsruher MPI-Benchmark”. It measures the effciency of an MPI implementation. While other benchmarks try to express the computing power of a machine with a single number, SKaMPI supports the application programmer with more differentiated information. Every single MPI operation is accurately measured and a report generator written in Perl automatically fits this data together in to a detailed report. This report can help the programmer to make the right design and implementation decisions. SKaMPI started as a diploma thesis of Ralf Reussner and has been continuously enhanced since then. The major changes of the recent version 4 is a noticeably improved measurement method for collective operations, which gives more accurate results than any other benchmark known by us. An example is given in Fig. 1. It shows the relation between number of nodes and the time for an MPI Barrier operation on the IBM SP in Karlsruhe measured with the old and the new method. The results of the new method show more regularity and a lower overhead. Of course the relative overhead in this explicitly chosen example is higher than it would be for an operation with larger message length.

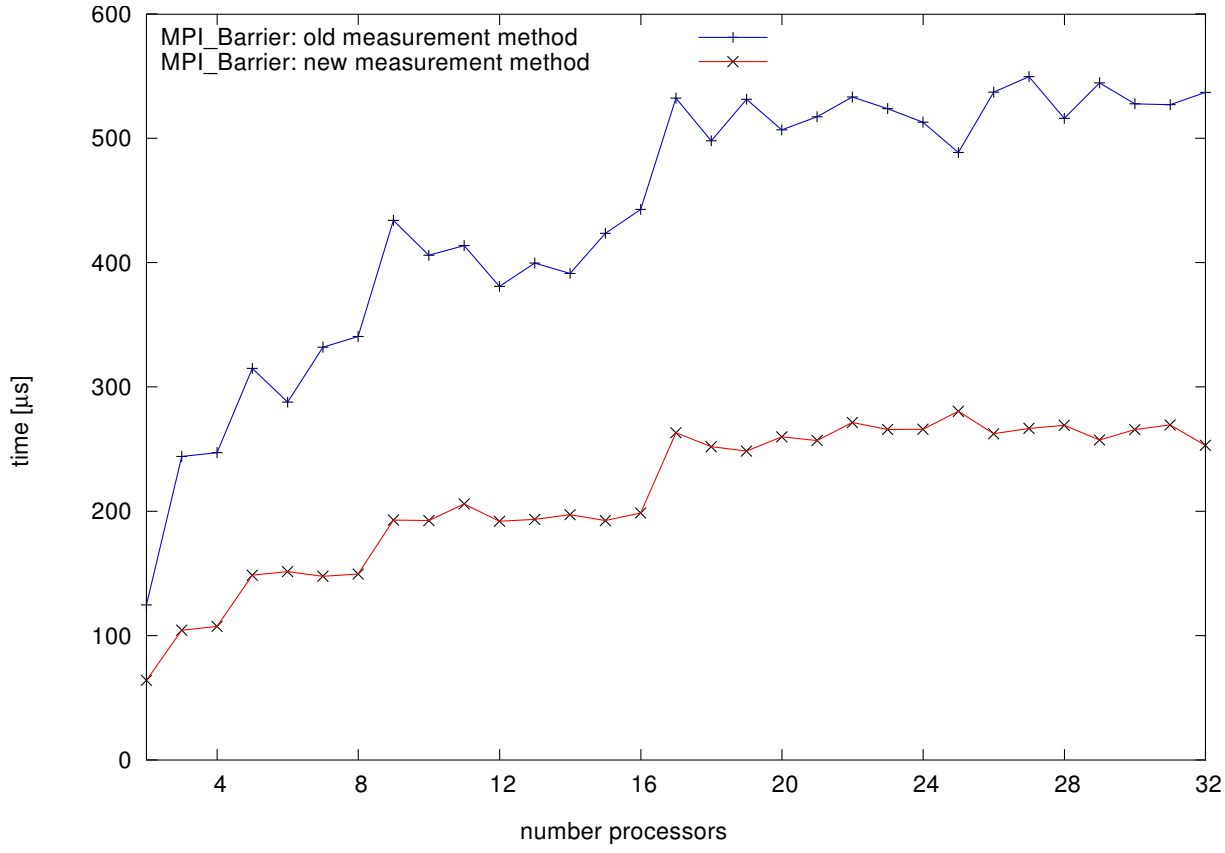

Fig. 1: The source code of SKaMPI (released under the GPL), additional information and access to a database to compare SKaMPI's results on a lot of different parallel computers are available on the SKaMPI homepage: http://liinwww.ira.uka.de/~skampi/.

Fluid-Structure Interaction in the Human Aorta

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Death caused by heart diseases is the most common one in the western industrialized nations. In the Year 2000 over 400,000 people died in Germany due to diseases of the cardiovascular system. The KAHMO (KArlsruhe Heart MOdel), initialized by the Institute of Fluid Mechanics at the University of Karlsruhe, tries to assist medical diagnostics by numerical prediction of the fluid mechanics and its effects on the circulatory system within the human body. One important part of KAHMO is the the numerical simulation of the heart valves and the large vessels in their vicinity. An important aspect of this task is the coupled problem of the elastic walls of a blood vessel and its interaction with the bloodflow.

The simulations are carried out with commercial software packages, which could interact on grid based coupling software. The incompressible Navier-Stokes-Equations are solved for the fluid mechanical part of the problem by using STAR-CD. The structure mechanics are handled by PERMAS. The structure of the vessel were simplified as an isothropic material. For comparison with experimental results, which originate from LDA-measurements in a silicone aorta, the material properties of silicone were applied. The coupling is done by using the Mesh-based parallel Code Coupling Interface (MpCCI), which were developed by the Fraunhofer Institute for Algorithms and Scientific Computing (SCAI). It works on non-matching grids and derives a previously defined exchange quantity. In case of a fluid-structure interaction nodal forces are transmitted from the fluid-mechanical side to the structure mechanics, which return a nodal displacement to CFD.

Time dependent mass flux is specified at the inlet. For modelling the peripheral resistance of the circulatory system, porous media is implemented downstream the coupled computation domain and fixed pressure boundaries are set at the outflow regions. The heart beat is 71 bpm and is equivalent to the heart beat rate of a adult person in resting position.

The figures show contour lines of the velocity magnitude and the streamlines of the flow for four points in time of one single heart beat. The initial condition is shown in figure 1. The velocity is zero, the aorta is in its initial geometry. After T/4 of the cycle, the flow velocity is rising up to a peak of 0.5 m/s and the elastic walls of the aorta are deformed by the rising pressure. With the increasing volume of the aorta it represents a fluid mechanical compliance, which lowers the peak pressures downsteam. At T/2 the flow velocity decreases and the aorta has reached its largest expansion. At T/3 appear regions of backflow, especially at the inner radius of the bent vessel. After one cycle the velocities are reduced to a minimum. The flow

is not clearly directed, which can be seen by the streamlines. The elastic aorta reduces its deformation and returns in the initial state.
In the next step of the project the model will include the aortic valve. With the expansion, it will be possible to analyze the effects on the flow of different sorts of pathological aortic valves.

t=0

t= ¼ T

t= ½ T

t= ¾ T

Density Functional Theory Studies on Clusters

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The study of clusters, i.e small aggregates of atoms or molecules, is an increasing field in modern physics. A reason for that are the enormous possibilities to use clusters in technical applications. An example is the use of deposited clusters on surfaces as a catalyst.
For a better understanding of these complex processes and thus an improvement of the applications it is needed to compare experimental results with quantum mechanical calculations. Even in the framework of density functional theory these electronic structure calculations make great demand on computer power and can often only be handeld with parallelized supercomputers.
In this project we have studied the thermal photoelectron spectra of free anionic sodium cluster with an ”ab initio” density functional method.
Photoelectron spectroscopy is a frequently used experimental method to extract electronic binding energies from atomic, molecular and condensed matter systems. In the framework of this project we compared the density of states of thermal molecular dynamic simulations to experimental measured photoelectron spectras.
In contrast to the structure of molecules, clusters do not have one certain geometrical arrangement. Many different stable structures exist with different total energy. As a first step we determined the structure with the lowest total energy, the groundstate (GS) structure. In Fig. 1 one can see the calculated GS structures of the $Na\text{-}_N$ clusters (N=4-19).
Starting from the W-shaped pentamer and ending with $Na\text{-}_{11}$ a growth pattern can be identified, i.e., the topology of the $Na\text{-}_N$ cluster derives from $Na\text{-}_{N\text{-}1}$ by replacing an atom with a dimer ($Na\text{-}_6$, $Na\text{-}_7$ and $Na\text{-}_{11}$) or by capping a facet ($Na\text{-}_8$, $Na\text{-}_9$ and $Na\text{-}_{10}$). Interestingly, our search for the GS structures of the midshell clusters $Na\text{-}_{12}$ and $Na\text{-}_{13}$ resulted in two energetically quasidegenerate GS isomers with clearly different shapes ($Na\text{-}_{12}$: triaxial oblate vs. triaxial prolate; $Na\text{-}_{13}$: axially symmetric prolate and oblate).
A comparison of the experimental photoelectron spectra (measured at room temperature) with the electronic density of states (DOS) of our thermal molecular dynamic simulations in Fig. 2 shows that only the oblate isomer appeared in the experiment. In the 1st and 3rd column of Fig. 2 the experimental photoelectron spectra of $Na\text{-}_4$ to $Na\text{-}_{19}$ (thin solid black curves) is compared with the Gaussian broadened DOS of our GS clusters (thick solid curves) and in the 2nd and 4th column to the DOS histograms from our thermal simulations (represented by the red stickspectra). As one

cansee there is an overall good agreement between the measured spectra and the thermal simulation spectra. In many cases, the Gaussian broadened DOS of the GS clusters already provides a reasonable description of the measured spectra (see e.g. Na_5, Na_6, Na_{11}, Na_{13} oblate and Na_{16}). For other clusters, several details in the spectra are not well reproduced and some are even absent whereas the thermal simulation spectra describes many details as e.g the thermal splitting of degenerated electronic states for the Na_7 and Na_9.

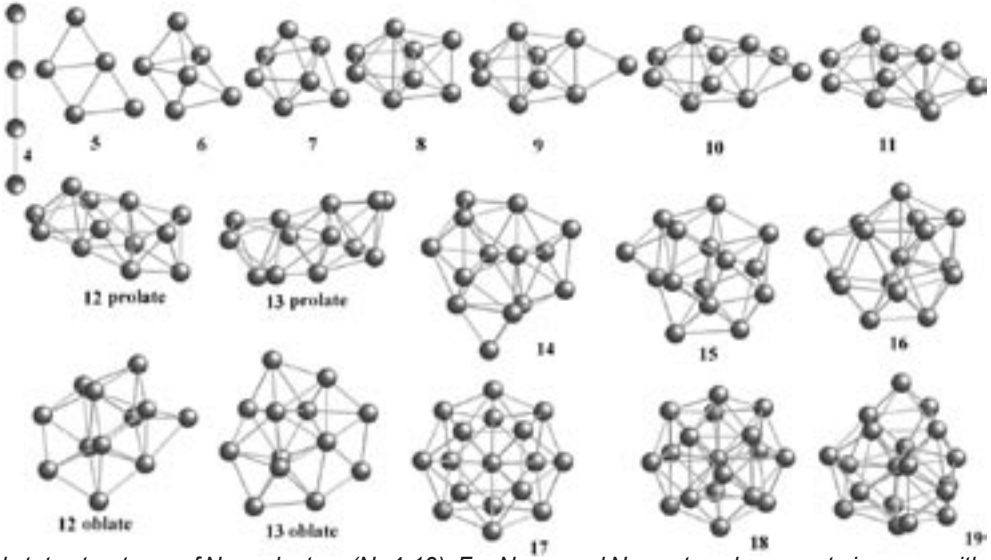

Fig. 1: Ground state structures of Na_N clusters (N=4-19). For Na_{12} and Na_{13}, two degenerate isomers with different shapes occur, labeled as "prolate" and "oblate".

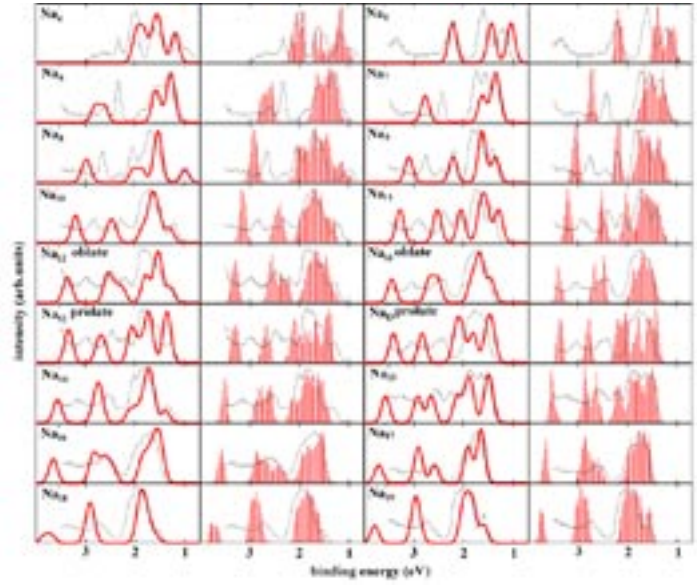

Fig. 2: Experimental photoelectron spectra of sodium cluster anions (thin solid curves) are compared to the ground state density of states with artificial Gaussian broadening (thick solid curves in 1st and 3rd column) and to the thermally broadened density of states of the simulated Born-Oppenheimer trajectory (histograms in 2nd and 4th column).

Hybrid Simulation in Material Science, Application to the Brittle Fracture in Silicon

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In spite of their successes obtained in material science simulations, purely quantum or purely classical methods remain insufficient to tackle some important classes of problems. These limitations concern mainly large systems (over few thousands of atoms) that are practically untractable within pure quantum methods and in which some chemical reactions are expected to occur locally. Because of the complexity of these reactions, it is not always possible to build a classical potential able to describe accurately all the regions of the system. In these cases, QM/MM hybrid simulation schemes are required to afford the problem. The dynamic crack propagation nicely illustrates this situation. First, a large system size is needed to take into account the slowly decaying elastic field and the elastic energy stored in the whole system. Simultaneously, the description of the system at the quantum level is also mandatory to accurately simulate the bond-breaking processes in the crack tip region.
Experimentally, brittle fracture can be obtained in diamond silicon by pulling along [111] or [110] directions when the crack fronts are respectively oriented along [1-10] and [001]. In each case, the final surfaces ((111) and (110)) are clean and flat. A different behavior is observed for the (110)[1-10] geometry, in this orientation the crack does not open clean (110) surfaces but rather turns by 35 to open (111) facets.
To attack this problem of crack propagation in silicon we used an original hybrid method first developped by Alessandro De Vita (University of Trieste) that is mainly based on the concept of adaptable classical potentials. In this method the system is described at every time *t* by a single classical potential form. However, the potential parameters are not constant over the whole system and are allowed to vary in space and time. They have a local and instantaneous meaning and they are updated when and where it is needed to fit the forces given by a more refined quantum model. In pure silicon we use a Stillinger-Weber form for the classical potential and the quantum forces are calculated on some selected atoms within the embedded cluster approximation. In this approximation, a cluster is carved out of the system around each atom of interest and is chemically terminated with hydrogen atoms. Then, the force on the central atom is simply obtained from a separate quantum calculation (tight-binding or ab initio). From the computational point of view the CPU time scales linearly with the number

Fig. 1 : (111)[1-10] orientation, hybrid calculation

of the quantum atoms and the scheme is particularly convenient for parallel applications since the clusters can be distributed on different processors and calculated separately.
In our application to crack propagation we only calculate the quantum forces on a few hundreds atoms in the crack tip vicinity every ten time steps (1 time step = 20 a.u.) while the reference forces for the rest of the system were evaluated by a Stillinger-Weber potential.
After several successful tests on small clusters and silicon surfaces we performed dynamic simulations of about 7 picoseconds long on the (111)[1-10] and (110)[1-10] crack systems. When a tight-binding approximation is used for the quantum model each series of calculation approximatively takes 2500 hours monoprocessor. The calculations were repeated under few different loading conditions for each orientation.
Some of the results obtained untill now are shown on Fig. 1 and 2. Fig. 2 shows the final configuration obtained on the (111)[1-10] crack system one model opening for a loading condition that corresponds to a large density of elastic energy (elastic released energy rate, I 4 × surface energy). We can see that the final opened surfaces are rather clean and flat with a low rugosity in close agreement with the experimental results. Interestingly, some dynamic surface reconstructions were observed during the hybrid simulations and highlight the importance of electronics effects.
Fig. 2 displays the final configuration for the (110)[1-10] crack system on high loading conditions. In this case the initial crack tip splits into two open (111) facets. This dynamic behavior indicates, consistently with the experiments, that the straightforward propagation of this crack is unstable. With respect to the purely classical picture our hybrid calculation of dynamic crack propagation represents a significant progress in the description of the problem. This can be be verified on Fig. 3, 4 that were obtained with pure Stillinger-Weber model. The opened surfaces are rough and the crack tips are large, round and disordered. No surface reconstruction are observed in the (111)[1-10] crack system while the (110)[1-10] crack progress straightforward and does not show any (111) facets.
At the moment we are carrying on new calculations to study the behavior of the (110)[1-10] for lower loading energies.

Fig. 2 : (110)[1-10] orientation, hybrid calculation

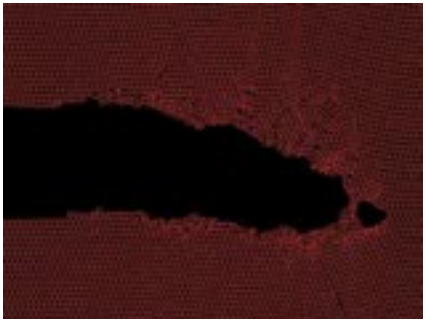

Fig. 3 : (111)[1-10] orientation, Stillinger-Weber

Fig. 4 : (110)[1-10] orientation, Stillinger-Weber