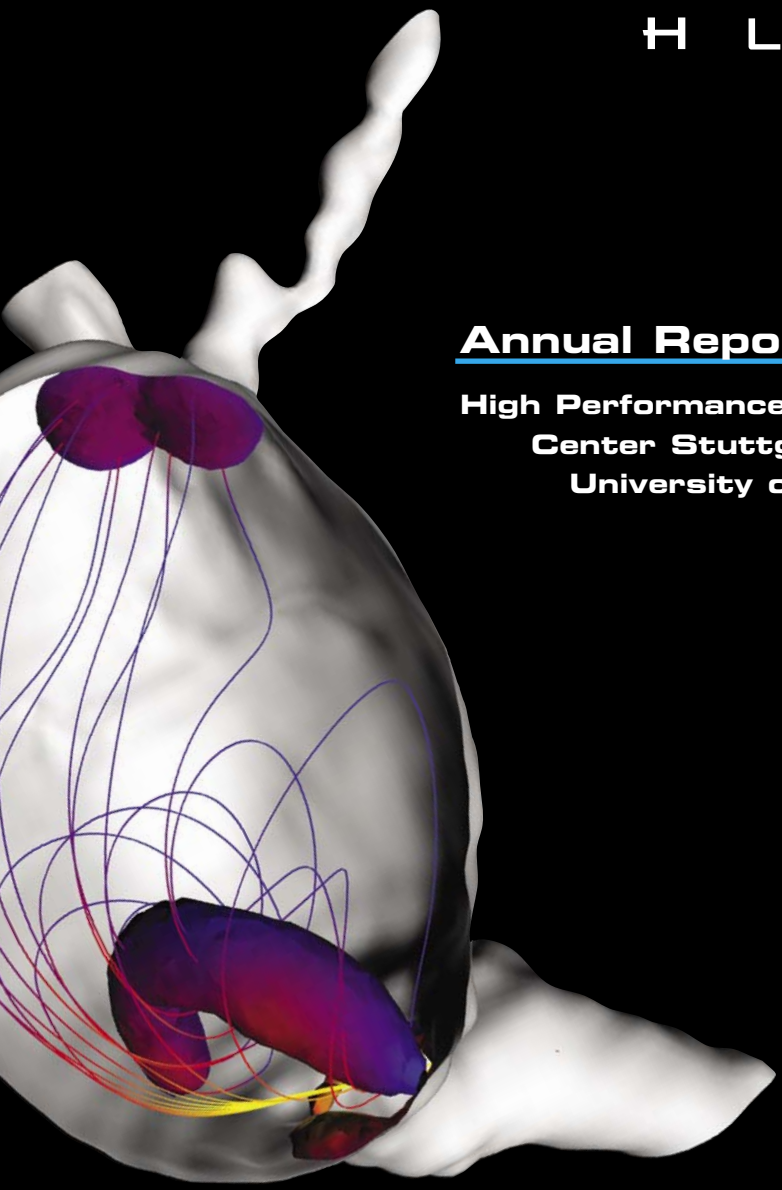
H L R S



Annual Report 2005

High Performance Computing Center Stuttgart (HLRS) University of Stuttgart

Publisher
High Performance Computing Center Stuttgart
Nobelstraße 19 • 70569 Stuttgart, Germany
phone: +49-711-685-87269 • fax: +49-711-68587209
info@hlrs.de • www.hlrs.de

Person responsible for subject matter: Prof. Dr.-Ing. Michael M. Resch
Editor: F. Rainer Klank

Contents

1 Overview

The year 2005 was marked by a number of achievements that had been prepared in the years before. The climax of the year was the inauguration of a new building and a new supercomputer in July by the Minister President of the state of Baden-Württemberg Günther Oettinger and the Federal Minister of Education and Research Edelgard Bulmahn. From a scientific point of view the large number of new projects and especially the leading role that HLRS plays in the German Grid computing project d-grid highlight the strong position of HLRS as a research center. Finally HLRS was able to substantially strengthen its industrial role by convincing Porsche to do all of its simulations for their next generation model (Panamera) at HLRS.

The new building was taken over in April 2005 and is now home for 35 employees of HLRS. As the staff number has grown faster than expected in the last years HLRS is now distributed over three buildings that are within walking distance. Nevertheless planning has started for a building extension to bring all people together in a single environment.

Early in the year NEC started installation of the new supercomputer SX-8. When installed the system was Europe's fastest supercomputer with a peak performance of 12,6 TFLOP/s. It's extremely high level of sustained performance will keep it in the top 3 systems in Europe for applications for the next years. The installation of the systems was accompanied by an intensive co-operation of HLRS and NEC in the field of application tuning and hybrid supercomputer architectures. Bringing together the benefits of vector based systems and clusters hybrid architectures can provide the best in class for every user application.

The collaboration with NEC made it possible to further strengthen the cluster line at HLRS. With its 400 processors the Intel based system more than doubles the available cluster performance. The cluster is in heavy use both by science and industry. A further step to meet the demands of science and industry was the acquisition of a new Cray XD1 system. With these new systems in place HLRS and its users are well equipped to meet the challenges of the next years.

HLRS has also extended its level of co-operation in 2005. It has further deepened its links inside Europe. This report names 10 European projects in which HLRS is involved. Further projects will start early in 2006 with a focus on applications, infrastructure and Grid middleware. The large number of projects reflects the international and collaborative research approach of our center. This is highlighted by the acceptance of HLRS as a new partner in the European infrastructure project DEISA. As much as HLRS is part of an international community it also has strong regional ties. Collaboration with the University of Karlsruhe and the University of Heidelberg were continued in the frame of the Höchstleistungsrechner-kompetenzzentrum Baden-Württemberg (hkz-bw).

Prof. Dr.-Ing. Michael M. Resch

2 Inauguration of the new HLRS Building and the NEC SX-8/576M72

On July 21st and 22nd the new building of the High Performance Computing Center Stuttgart (HLRS) was inaugurated together with the new NEC SX-8/576M72 system. The president of the Universität Stuttgart Prof. Dr. Dieter Fritsch and the director of HLRS Prof. Dr. Michael Resch welcomed the Minister President of Baden-Württemberg Günther Oettinger and Federal Minister of Education and Research Edelgard Bulmahn who came to Stuttgart on July 21st. The presence of both a Federal Minister and the Minister President of the state made clear the importance of the national supercomputing center HLRS both for the state of Baden-Württemberg and Germany. Consequently both Federal Minister Bulmahn and Minister President Oettinger emphasized the close collaboration of state and federal government in pushing the frontiers of science and research and supporting large scale innovations like the new NEC SX-8 system. Minister President Oettinger pointed out the importance of HLRS for the state of Baden-Württemberg both for research and for industry. He made it clear that becoming a European supercomputing center and at the same time keeping its role as a leading partner and provider for industry should be a key goal for HLRS for the next years.

The importance of the installation at HLRS was emphasized also by the attendance of Senior Vice President Masahiko Yamamoto from NEC Corporation, Tokyo. Senior Vice President Yamamoto brought the greetings of NEC president Akinobu Kanasugi and pointed out that the importance of HLRS and the SX-8 installation for NEC is reflected in the close collaboration of HLRS and NEC which will lead to an additional investment of about 8M€ by NEC in Stuttgart in the coming four years.

Dr. Christoph Gümbel head of simulation and computation at Porsche Research brought greetings from Porsche AG which is one of the main users of the systems at HLRS. Dr. Gümbel emphasized the importance of high speed computers for industry and expressed his hope that the very positive collaboration with HLRS will be continued and extended in the future. In a press release the CEO of Porsche AG Dr. Wendelin Wiedeking was quoted as "Commerce and science in Germany have a shared interest in powerful supercomputers, which are becoming more and more important for research and development in the face of international competition". According to Wiedeking, the many years of commitment being provided by the automobile manufacturer would contribute not only to improved levels of efficiency in development work at Porsche, but would also ultimately strengthen Germany's standing in the world of science.

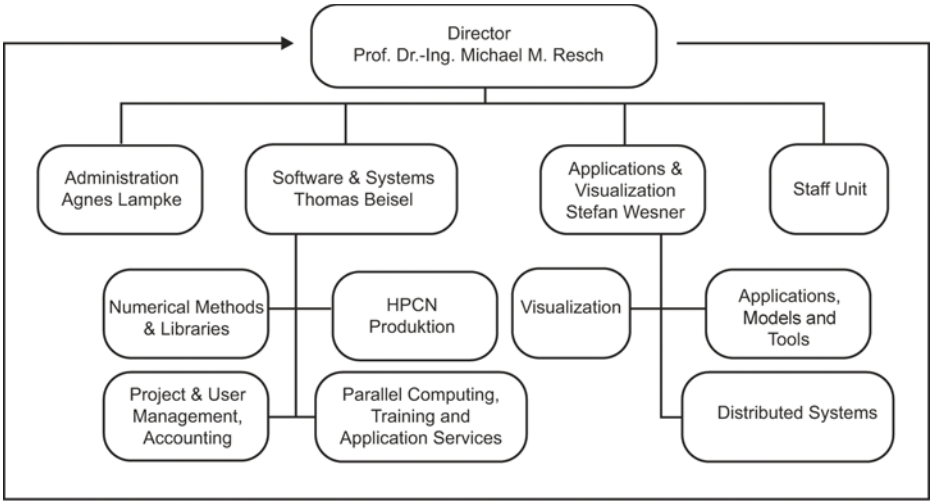
On July 22nd a scientific colloquium was held showing the variety of applications users of the HLRS are working on. The day was opened by a key note speech of Dr. Ryutaro Himeno head of the computer and information division of the Japanese Center for Physical and Chemical Research (RIKEN). Dr. Himeno - who is collaborating with HLRS since several years – first gave an overview of the history of simulation. Pointing out the achievements of the last two decades in supercomputing he emphasized that the community should prepare for similar achievements in technology for the next years to come. As an example Dr. Himeno presented an overview of the Japanese Next Generation Supercomputing project for the development of a Petaflop computing system. HLRS and RIKEN will collaborate in this project focusing on application and system design issues.

In the following a number of brilliant presentations gave a glimpse of what will be possible in the future with the new NEC SX-8/576M72 system. Prof. Wolfgang Wall chair for Computational Mechanics of the Technical University of Munich presented some projects in multiphysics applications. It became obvious that this field will become increasingly important for engineering and will require a tremendous level of performance. Prof. Cord Rossow director of the Institute for Design Aerodynamics of the German Aerospace Center (DLR) gave an overview of supercomputing in aerospatial research. Dr. Matthias Meinke from the Institute of Aerodynamics of the RWTH Aachen gave a comprehensive overview of new challenges in aerodynamics simulation. Both Prof. Rossow and Dr. Meinke made clear that supercomputers will remain a key tool for research and development in aerospatial engineering for decades to come.

Prof. Hanns Ruder from the sections Theoretical Astrophysics and Computational Physics at the Institute for Astronomy and Astrophysics (IAAT) of the Eberhard-Karls-Universität Tübingen showed the potential of supercomputers in visualization. His presentation of the effects of traveling at a speed close to the speed of light was very impressive for the audience. A similar approach of using visualization coupled to supercomputer simulations was presented by Prof. Eberhard Göde from the Institute for Fluid Mechanics and Hydraulic Machinery of the University of Stuttgart.

3 Organization

3.1 Structure



3.2 Staff

3.2.1 General Information

The year 2005 has seen no change in staff numbers compared to the previous years. This is mainly due to an increase in external funding through projects while the number of permanent staff decreased substantially. The head count on January 1st 2006 was as given:

Permanent staff	27
Third party funded staff	35
Research Ass. (Students)	25
Total	87

HLRS staff including students now totals 87 of which 2 are currently on parental leave. A breakdown of gender shows that percentage of female scientists has become relatively high. A general problem that is also visible at HLRS is that female PhD students tend to go on maternal leave and then break off their scientific career.

Scientific		Non-Scientific		Total	
42		20		62	
Male [#/%]	Female [#/%]	Male [#/%]	Female [#/%]	Male [#/%]	Female [#/%]
32 / 76%	10 / 24%	10 / 50%	10 / 50%	42 / 67%	20 / 33 %

3.2.2 Key Staff Changes

Dr. Matthias Müller, deputy director of the HLRS has left the center to become the deputy director of the Center of Information Services and High Performance Computing (ZIH) of the Technical University of Dresden. Dr. Matthias Müller joined HLRS in 1999 and became head of the working group "Technical & Scientific Computing" in 2000. He became deputy director "Applications & Visualization" of HLRS in 2003. Dr. Matthias Müller left HLRS in August 2005 to take over his responsibilities at TU Dresden.

Agnes Lampke was appointed deputy director administration of HLRS in September 2005. She started a training in administration at the Community of Helgoland in 1990. From 1996 till 2001 she was a specialist for personnel and budgetary concerns at the Kiel Institute for World Economics. In 2001 she came to Stuttgart for Deputy Administration Manager at the Center of Technology Assessment in Baden-Württemberg, specialist in the field of finances. Since 2004 she is Administration Manager at the High Performance Computer Center of the University of Stuttgart (HLRS).

Stefan Wesner was appointed deputy director "Applications & Visualization" of HLRS in September 2005. Stefan Wesner holds a degree in Electrical Engineering from the University of Saarbrücken. He joined the HLRS in 2000 as head of the working group "Software Technology" since 2003. Stefan Wesner took over responsibility for "Applications & Visualization" in September 2005 from Dr. Matthias Müller.

Dr. Edgar Gabriel, head of the HLRS cluster group has left HLRS to accept an offer from the University of Houston as an Assistant Professor. Dr. Edgar Gabriel joined the HLRS in 1997 as a research assistant. He became a scientific employee of HLRS in 1999 and became head of the working group “Clusters and Distributed Units” in 2001. Dr. Edgar Gabriel joined ICT at the University of Tennessee in 2003 before returning to HLRS in September 2004. Dr. Edgar Gabriel left HLRS in August 2005 to take over a position as an Assistant Professor at the Department of Computer Science of the University of Houston.

Thomas Bönisch was appointed head of the working group “Projects & User Management, Accounting” in September 2005. Thomas Bönisch holds a degree in Computer Science from the University of Stuttgart. He joined HLRS in 1992 as a research assistant. 1996 he became a scientific employee of HLRS.

Rainer Keller was appointed head of the working group “Applications, Models and Tools” in September 2005. Rainer Keller holds a degree in Computer Science from the University of Stuttgart. He joined HLRS in 1997 as a research assistant and became a scientific employee in October 2001. Since then he has worked in the field of Grid computing and has been a driving force in a number of international collaborations. Rainer Keller also participates in the Open MPI initiative and represents HLRS there.

Dr. Rolf Rabenseifner was appointed head of the working group “Training and Application Services” in September 2005. Rolf Rabenseifner holds a degree in Mathematics from the University of Stuttgart and a doctoral degree in Computer Science from the University of Stuttgart. He joined HLRS in 1996 and was head of parallel computing since 2000.

3.2.3 Guest Scientists

January 16th – February 28th 2005, Mrs. Agnieszka Debudaj
Politechnika Slaska, Poland. HPC-Europa guest working on simulated annealing application using clusters of SMPs with mixed MPI/OpenMP.

March 10th – March 24th 2005, Dr. Tomasz Olas
Czestochowa University of Technology, Poland. HPC-Europa guest evaluating and using PACX-MPI for Polish Computational Grid.

June 1st – July 7th 2005, Dr. Federico Boschetti
Dipartimento di Scienze fiologiche e storiche, Trento University, Italy. HPC-Europa guest working at HLRS in collaboration with IMS on extending TigerSearch for distributed text-annotation.

June 1st – August 31st 2005, Mr. Luis Miquel Sanchez Garcia
Carlos III University, Madrid, Spain. Evaluating the performance of the parallel filesystem on clusters.

June 6th – July 29th 2005, Mr. Hatem Ltaief
Researcher at TCLL (Texas Learning and Computation Center) at the University of Houston, Texas, USA. Mr. Ltaief works in the fields of MetaComputing projects on different architectures, fault tolerant algorithms and applications to heat conduction and air quality problems.

October 1st 2002 – September 30th 2005, Dr. Nina Shokina
Institute of Computational Technologies, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia. Dr. Shokina works in the field of algorithms in computational fluid dynamics.

June 1st – July 31st 2005, Prof. Barbara Chapman
Department of Computer Science, University of Houston, Texas, USA. Prof. Chapman works in the field of compilers for high performance computers and in the field of Grid computing.

January 25th – March 25th 2005, Prof. Alexander Rychkov
Institute of Computational Technologies of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia. Project: Mathematical modelling of gas-dynamic processes in solid-propellant airbag-gas generators.

4 Systems

This section describes changes in the configuration of systems that are available to the users of the HLRS. HLRS installed a new generation NEC Supercomputer in the first half of 2005. The system passed acceptance in July and August 2005 and went into production in September. Another new system was installed at the end of 2005. The Cray XD1 will mainly be used by industry for simulation in car development.

4.1 NEC SX-8 576 M72

This is the latest generation of NEC's Vector System. HLRS builds a supercomputer by clustering NEC SX-8 nodes using NEC's high performance crossbar interconnect. System installation started in December 2004 and was finished in June 2005. Production started with 36 nodes on March 23, 2005 while the full system was available for general usage on September 1st 2005. The specification of the system is:

CPU	NEC SX-8 2GHz
Number of CPUs	8 per node total of 576
Peak Performance	12,7 TFLOPS
Memory	9.2 TB
Interconnect	NEC IXS 16 GB/s bi-directional
Disk Space	160 TB

During acceptance a number of tests were performed, results of which are presented briefly here:

Type of Benchmark	**Required**	**Achieved Value**
Memory Bandwidth/Node	320 GB/s	360 GB/s
MPI Latency	8 µs	4,6 µs
MPI Bandwidth	12 GB/s	14,2 GB/s
Bisectional Bandwidth	460 GB/s	1120 GB/s
I/O Bandwidth	7 GB/s	7,96 GB/s

The application performance expectations were high with a maximum level of performance to be in the range of 4 TFLOP/s. The final system configuration exceeded all expectations. Some performance numbers are given here. For further information see http://www.teraflop-workbench.de/

Benchmark	**1 Node Performance**		**Full Systems Performance**	
	Required	Achieved	Required	Achieved
Linpack			8,76 TF/s	8,923 TF/s
FENFLOSS (CFD)	45 GF/s	45,5 GF/s		
URANUS (Aerospace)	46 GF/s	49,2 GF/s		
N3D (CFD)	50 GF/s	52,6 GF/s		
Parapyr (Combustion)			4 TF/s	4,46 TF/s
BEST (Lattice-Boltzmann)			4 TF/s	5,77 TF/s

Stability tests for the system were conducted during August. The SX-8 turned out to be extremely stable with a total availability of the system at 99,91% over a 30 days period.

4.2 NEC SX-6 32

This is the follow on generation of the SX-5 system and the predecessor of the SX-8 system. It was used for the transitional period before the installation of the SX-8 and will be available for preparatory work and code development for a while.

CPU	NEC SX-6 565 MHz
Number of CPUs	8 per node total of 32
Peak Performance	256 GFLOPS
Memory	512 GB
Interconnect	NEC IXS (8 GB/s bidirectional)
Disk Space	1,6 TB

4.3 Cray Opteron Cluster

To reduce operational costs and increase performance and memory size for users of the Cray T3e MPP System the University of Stuttgart replaced it by an AMD Opteron based cluster. The cluster is operational since Q2 2004.

CPU	AMD Opteron 2.2 GHz
Number of CPUs	256
Peak Performance	1 TFLOPS
Memory	512 GB
Interconnect	Myrinet
Disk Space	512 GB

4.4 Intel EM64T Cluster

Together with its partners NEC and Intel HLRS has set up a cluster of Intel Xeon 64 Bit – processors. The specifications of the system are:

CPU	Intel Xeon EM64T 3.2 GHz
Number of CPUs	404
Peak Performance	2.6 TFLOPS
Memory	240 GB
Interconnect	Infiniband
Disk Space	1 TB

4.5 Cray XD1

The Cray XD1 is a cluster-like system that is based on a proprietary interconnect that increases the speed of simulation for certain specific applications. HLRS has acquired such a system for use by researchers but mainly for industrial usage. The specifications of the system are:

CPU	AMD Opteron 2.8 GHz
Number of CPUs	48
Peak Performance	0,27 TFLOPS
Memory	96 GB
Interconnect	Proprietary
Disk Space	1,8 TB

5 User Support

Comprehensive user support in problem solving in the area of high performance computer simulations for science and engineering is performed in a wide range of application fields.

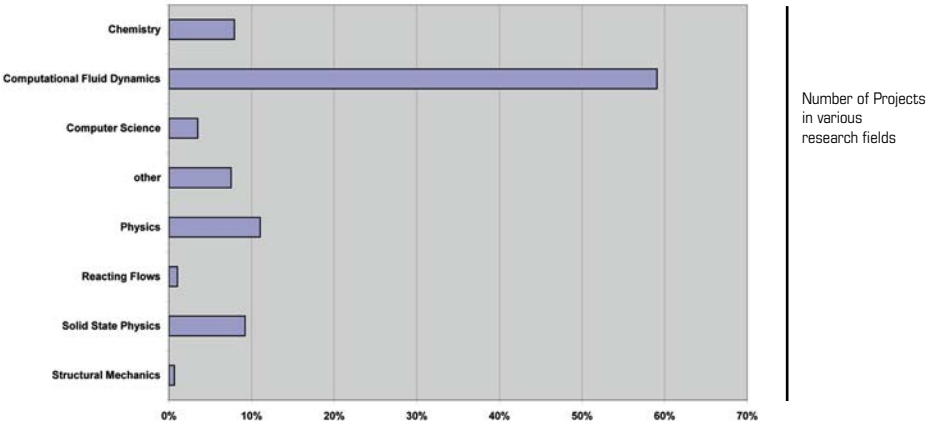
Above all, this includes content and research specific consulting as well as selection, licensing, installation and maintenance of appropriate application software packages on supercomputer platforms. Optimal usage of supercomputer resources and use of vectorized and/or parallelized program versions is thereby essential.

Skilled scientific staff substantially contributes to achieve relevant results and to the efficient usage of computer equipment by consulting, supporting and co-operating in a lot of research projects, especially in the areas of Computational Chemistry, Computational Fluid Dynamics, Computational Physics and Structure Mechanics.

5.1 User Projects

In total 59 projects were active on the national supercomputer systems of HLRS in 2005. Of these 49 were running projects and 10 new projects. The number of projects has started to increase with a rate of about 2-4 new projects with every month the SX-8 was in operation.

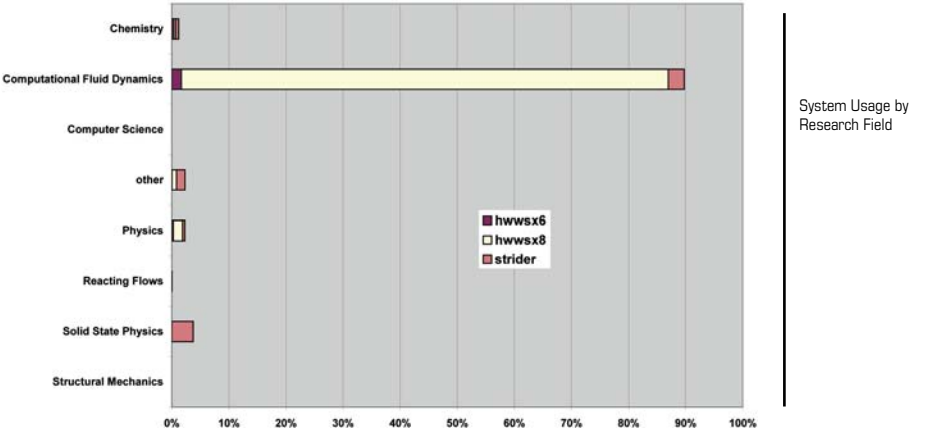
5.1.1 Distribution by Fields



The distribution of application fields in number of projects shows both the traditional strengths of HLRS and the type of architecture available in Stuttgart. The field of Computational Fluid Dynamics summarizes all activities that relate to flows. This includes climate research as well as blood flow simulation and traditional engineering CFD as is used in car and aerospace industries. These applications benefit from the vector supercomputer architectures. The second largest application field is physics together with solid state physics. These applications are typically found on the cluster systems of HLRS. The very strong dominance of CFD in the year 2005 is due to the lack of a competitive system for other fields in 2005. As part of the collaboration of NEC and HLRS increased user support for other fields in tuning codes for vector based systems is provided.

5.2 Usage of the Systems

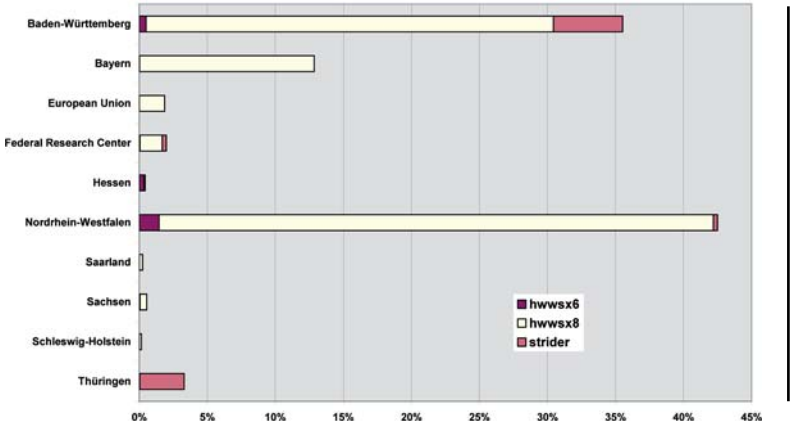
5.2.1 Distribution by Fields



The strong role of CFD is emphasized again when looking at system usage. Almost 90% go to projects in this field. It is interesting to note that CFD is the strongest field both on vector based systems and on micro-processor based systems. The second strongest field – mainly using the Opteron cluster (Strider) - is solid state physics. The reader has to keep in mind, however, that the SX-8 has a by far higher level of performance than the

Opteron cluster. Hence the percentage of CPU time used on the SX-8 is about 80% of the total CPU time provided.

5.2.2 System Usage by State



System Usage by State

System usage broken down by states of Germany reveals that the HLRS is established as a true national centre. HLRS has kept its nation wide user base which is reflected by the fact that still about 65% of all users are not from the state of Baden-Württemberg. The increased fraction of usage by European projects indicates the international role of HLRS.

5.3 Workshops

Date		Organizer	Location	Topic
Jan	17-19 2005	NIC	Jülich	Parallel Programming
Feb	09-11 2005	ZIH	Dresden	Parallel Programming
Feb	21-25 2005	HLRS	Stuttgart	Iterative Linear Solver and Parallelization
Apr	06-07 2005	HLRS	Stuttgart	NEC SX-8 Usage and Programming
Apr	04-08 2005	Fak. Math. & Inf.	Kassel	Introduction to Computational Fluid Dynamics
Jun Jul	27-08 2005	ICT, HLRS	Novosibirsk, Russia	2nd Russian- German Advanced Research Workshop on Computational Science and High Performance Computing
Aug	10-12 2005	CSCS	Manno, Switzerland	Parallel Programming
Sep	12-14 2005		Stuttgart	Parallel Programming with MPI, OpenMP and PetSc for Beginners
Sep	15-16 2005	HLRS	Stuttgart	Advanced Topics in Parallel Programming
Sep	26-30 2005	Fak. Math. & Inf.	Kassel	Iterative Linear Solver and Parallelization
Oct	10-14 2005	HLRS	Stuttgart	Introduction to Computational Fluid Dynamics
Nov	28-30 2005	NIC	Jülich	Parallel Programming

In these workshops 2005, about 300 researchers, PhD students and students mainly from many research labs and universities in Germany, but also from industry have been taught in parallel programming on HPC systems. In all of these workshops, hands-on sessions allow participants to immediately test and understand basic and advanced constructs of parallelization with the Message Passing Interface (MPI) and the shared memory directives of OpenMP, of iterative solvers or Computational Fluid Dynamics.

Short Descriptions of Workshops

Jan. 17-19, Feb. 09-11, Aug. 10-12, Nov. 28-30 at ZIH, NIC, and CSCS: The focus is on programming models MPI, OpenMP, and PETSc. Hands-on sessions (in C and FORTRAN) will allow users to immediately test and understand the basic constructs of the Message Passing Interface (MPI) and the shared memory directives of OpenMP. The workshop was organized by ZIH (Dresden), NIC/ZAM (Jülich), and CSCS (Manno) in collaboration with HLRS. Course language is German at ZIH and NIC, and English at CSCS.

Feb. 21-25 at HLRS and Sep. 26-30 in Kassel: The focus is on iterative and parallel solvers, the parallel programming models MPI and OpenMP, and the parallel middleware PETSc. Thereby, different modern Krylov Subspace Methods (CG, GMRES, BiCGSTAB …) as well as highly efficient preconditioning techniques are presented in the context of real life applications. Hands-on sessions will allow users to immediately test and understand the basic constructs of iterative solvers, the Message Passing Interface (MPI) and the shared memory directives of OpenMP. The workshop was organized by HLRS, IAG, and University of Kassel.

Apr. 06-07 at HLRS: The focus is on vectorization and parallelization (1st day), and on parallel file-systems and parallel I/O with MPI-2 on NEC SX-8 (2nd day) on the NEC SX-8 system.

Apr. 04-08 in Kassel and Oct. 10-14 at HLRS: Numerical methods to solve the equations of Fluid Dynamics are presented. The main focus is on explicit Finite Volume schemes for the compressible Euler equations. Hands-on sessions will manifest the content of the lectures. Participants will learn to implement the algorithms, but also to apply given (black-box, commercial) software and to interpret the solutions correctly. Methods and problems of parallelization are discussed. This course is organized by HLRS, IAG, and University of Kassel, and is based on a computational practical awarded with the “Landeslehrpreis Baden-Württemberg 2003” (held at University of Stuttgart, under auspices of the BMBF project NUSS, contract 08NM227).

Sep. 12 - 16 at HLRS: The focus was on programming models MPI and OpenMP, domain decomposition, parallelization with PETSc, and optimization. Hands-on sessions are included. Course language is English. The course has two parts, the first three days are a beginners' course, the last two days are dedicated to advanced topics in parallel programming.

5.3.1 Russian-German Summer School

The second school was jointly organized by the Institute for Computational Technologies (ICT), Russian Academy of Sciences, Siberian Branch and HLRS. This years lectures covered topics like parallel programming paradigms, MPI, OpenMP, parallel debugging, tools and also single processor optimization. Russian lecturers gave an overview about Russian computer resources and Russian investigations in the field of distributed systems and parallel computations. Several practical sessions on the cluster of ICT allowed the participants to deepen their new knowledge. The attendees came from all scientific centers of the Siberian Branch of Russian Academy of Sciences as well as from Kazakh Universities.

6 Teaching

The director of the HLRS is at the same time holding a chair for high performance computing at the University of Stuttgart. In that capacity he is responsible for teaching undergraduate students in Computer Science for the fields of Mechanical Engineering, Technology Management, and Automotive Engineering. He is also responsible for teaching computational Science and Engineering for graduate students.

6.1 Lectures

A number of other staff from HLRS has given lectures at the University of Stuttgart and at the University of Applied Sciences at Stuttgart. A focus is on simulation and high performance computing.

Lecturer	Title of Lecture	Semester	University
Michael Resch	Introduction to Computer Science (II) in Mechanical Engineering	SS 05	Univ. of Stuttgart
Michael Resch	Introduction to Computer Science (I) in Mechanical Engineering	WS 05/06	Univ. of Stuttgart
Michael Resch	Introduction to Computer Science (II) in Automotive Engineering	SS 05	Univ. of Stuttgart
Michael Resch	Introduction to Computer Science (I) in Automotive Engineering	WS 05/06	Univ. of Stuttgart
Michael Resch	Introduction to Computer Science (II) in Technology Management	SS 05	Univ. of Stuttgart
Michael Resch	Introduction to Computer Science (I) in Technology Management	WS 05/06	Univ. of Stuttgart
Michael Resch, Peter Streiner	Seminar on Computational Science and Engineering	WS 05/06	Univ. of Stuttgart
Michael Resch	Simulation on Supercomputers	SS 05	Univ. of Stuttgart
Peter Haas	Microprocessors	WS 05/06	Univ. of Stuttgart

Lecturer	Title of Lecture	Semester	University
Matthias Müller	C++ for Scientific Computing	SS 05	Univ. of Stuttgart
Claus-Dieter Munz (IAG), Sabine Roller	Computer Practical on Numerical Fluid Mechanics	SS 05	Univ. of Stuttgart
Sabine Roller, Mark Ferch (IAG)	Computer Practical on Numerical Gasdynamics	WS 05/06	Univ. of Stuttgart
Stefan Wesner, Robert Piotter, Michael Resch	Software Development for Scientific and Technical Applications	WS 05/06	Univ. of Stuttgart
Uwe Wössner	Visualization of Technical and Scientific Data	WS 05/06	Univ. of Stuttgart
Uwe Küster	Numerical Methods for Supercomputers	WS 05/06	Univ. of Stuttgart

6.2 100-online and self study

Parallel Programming Workshop Online: Recording of the courses at HLRS (see Workshops) with Lecturnity has been continued. The recording is available online in two formats (Lecturnity and RealMedia), see http://www.hlrs.de/organization/par/par_prog_ws/. A CD-version is also available.

6.3 PhD Theses

Dipl.-Inf. Panagiotis Adamidis, Efficient methods for coupled field problems in casting industries (in German), Stuttgart, Germany, 2005. The thesis investigates numerical algorithms and their parallelization for casting processes in industry. Such industrial applications require the coupling of processes like flow and cooling. The coupling creates new problems that have to be considered by any numerical algorithm. The thesis was partially developed in the frame of the European Project DECAST. A number of real world examples were chosen to prove the feasibility of the algorithms proposed.

6.4 Master Theses

In total 16 master theses were conducted and supervised by HLRS staff. In this HLRS was supported by the Institute of High Performance Computing of the University of Stuttgart.

1. Sheng, Feng; Entwicklung eines Programms zur Aufarbeitung von Tracing-Daten für eine vergleichende Leistungsanalyse mittels EARL und HDF5
2. Schützle, Thomas; Design and implementation of a GeneSys based web-service interface for the OpenPBS batch system
3. Bürkle, Friedemann; Entwicklung eines Funk-3D-Eingabe-Gerätes für VR-Umgebungen
4. Ariöz, Muhammet; Konzeption und Implementierung einer Visualisierungssoftware zur zeitbasierten Analyse von Produktionsprozessen mit der objektorientierten Programmiersprache Java
5. Vukusic, Ivanka; Differenzformel für den Laplace-Operator in beliebigen Nachbarschaften
6. Schröder, Maxim; Vergleich von lokaler und globaler Mittelung im physikalischen Mehrgitterverfahren zur Berechnung von Low-Mach Number Aeroakustik auf versetzten Gittern
7. Sentürk, Harun; Entwurf einer Dateneingabe ohne Tastatur für ein Virtual Reality System
8. Walter, Christian; Entwicklung, Implementierung einer Programmkette zur Lebensdauerabschätzung aufgrund von FE-Berechnungen
9. Liebing, Markus; Untersuchung zur Beschleunigung der Kommunikation der Metacomputing-Bibliothek PACX-MPI
10. Yassine, Maardji; Design und Implementierung eines graphischen Workflow Editors für das SAPHIR System (Secure Access Portal for HPC Internet Resources)
11. Schwindt, Matthias; Java PDA GUI für eine interaktive eLearning-Anwendung
12. Schröder, Maxim; Sequenzen von Eigenwertproblemen
13. Frenzel, Lars; Konzeption und Entwicklung eines objektorientierten Particle Tracers
14. Ben Hnia, Mehrez; Analyse von Verzweigungspunkten bei parameterabhängigen Eigenwertproblemen
15. Torka, Eva; Finite-Element-Analyse eines proximalen Femurnagel-Knochen-Verbundes am Fallbeispiel PFN-A
16. Klimach, Harald; Blockstrukturierte Implementierung des Low-Mach Number Codes Mpv2d

7 Research

7.1 Projects

This section covers in more detail the HLRS research projects that were running or newly started in 2005. In total 20 externally funded projects were conducted. A complete list of currently running projects includes:

Project	Funded by	Duration	Web page
GeoHPC	Landesstiftung Baden-Württemberg	01.09.04 - 31.08.06	http://www.uni-tuebingen.de/zag/geohydrology/HPC
Lunar-probe	Landesstiftung Baden-Württemberg	01.10.04 - 30.09.06	http://www.landesstiftung-bw.de/projekte/wissenschaft.php?id=187
Dissipative Particle Dynamics (DPD)	Landesstiftung Baden-Württemberg	01.10.04 - 30.09.06	http://www.landesstiftung-bw.de/projekte/wissenschaft.php?id=187
Dissipative Particle Dynamics (DPD)	Landesstiftung Baden-Württemberg	01.10.04 - 30.09.06	http://www.landesstiftung-bw.de/projekte/wissenschaft.php?id=187
SFB374 Rapid Prototyping	DFG	01.09.94 - 31.08.06	http://www.sfb374.uni-stuttgart.de
InGrid	BMBF	01.09.05 - 30.08.08	http://www.ingrid-info.de
DAAD Exchange Program	DAAD		
HPC-Europa	European Commission	01.01.04 - 31.12.07	http://www.hpc-europa.org
DEISA	European Commission		
CoreGRID	European Commission	01.09.04 - 31.08.08	http://www.coregrid.net
CROSSGRID	European Commission	01.03.02 - 30.04.05	http://www.crossgrid.org
GridCoord	European Commission	01.07.04 - 30.06.06	http://www.gridcoord.org
Akogrimo	European Commission	01.07.04 - 30.06.07	http://www.mobilegrids.org
ELeGI	European Commission	01.02.04 - 31.01.08	http://www.elegi.org
NextGRID	European Commission	01.09.04 - 31.08.07	http://www.nextgrid.org
TrustCoM	European Commission	01.02.04 - 31.01.07	http://www.eu-trustcom.com

NATO Co-operation	NATO Science Program	01.01.05 - 31.12. 05	http://www.nato.int/science
Intel Co-operation	Intel & HLRS	14.01.05 - 31.12.06	
Microsoft HPC Institute	Microsoft & HLRS	01.05.05	
Teraflop Workbench	NEC & HLRS	01.03.04 - 28.02.09	http://www.teraflop-workbench.de

7.1.1 National

7.1.1.1 GeoHPC

Abstract - The finite-element program GeoSys/RockFlow is used for manifold applications in Geo-Sciences. In this project, the simulation program is adopted to the challenges in high performance computing. Transient, nonlinear, coupled multi-physics applications with several millions of unknowns will be solved on massively parallel and vectorizing systems. Test applications will be the geothermic project in Bad Urach and the test-case South in Stuttgart.

Partners - Center for Applied GeoScience, University of Tübingen, HLRS

7.1.1.2 Lunar-probe

Abstract - The aim of this project is the simulation and design of an instationary pulsed plasma engine as main engine for a scientific micro satellite for lunar exploration. The low particle density within the engines requires a kinetic description for a rarified plasma. The simulation contains the calculation of the electromagnetic fields, the localization and movement of charged and neutral particles within these fields and the interaction of the particles due to collisions and chemical reactions. The algorithm is a so-called Particle-In-Cell (PIC)-scheme. Here, the calculation of the electromagnetic fields uses a Finite-Volume (FV)-scheme to solve Maxwell's equations, coupled with the solution of the Vlasov equation for the charged macro particles. For the collision terms, a Direct Simulation Monte-Carlo (DSMC) algorithm has to be applied. The requirements of the

three parts of the code are very distinguished, therefore hybrid parallelization techniques are considered, maybe leading to a realization on hybrid architectures.

Partners - Institut für Raumfahrtsysteme Universität Stuttgart, Institut für Aero- und Gasdynamik Universität Stuttgart, Institut für Hochleistungsimpuls- und Mikrowellentechnik Forschungszentrum Karlsruhe, HLRS

7.1.1.3 Dissipative-Particle-Code

Abstract - Dissipative-Particle-Dynamics is capable for simulation of production relevant mechanisms like filling, coating und sintering even for complicated technical geometries. This project is due to the development and parallelization of such a package.

Partners - Fraunhofer-Institut für Werkstoffmechanik (IWM), Institut für Mikrosystemtechnik, Albert-Ludwigs-Universität Freiburg (IMTEC), HLRS.

7.1.1.4 SFB374 Rapid Prototypinge

Abstract - The SFB374 Development and Testing of Innovative Products - Rapid Prototyping aims at enhancing and shortening development cycles for new products. It integrates several aspects of product development, such as economical, engineering and collaborative considerations. The HLRS contributes to the project with its competence in the area of computational simulation and visualization. Here, the research activities are centered around Augmented Reality for combining real prototypes of future products with simulation results and parallel rendering of large data sets that become more and more commonplace in daily engineering work.

7.1.1.5 InGrid

InGrid is one of six community projects in the German d-grid initiative, funded by the Ministry for Education and Research (Bundesministerium für Bildung und Forschung). InGrid will enable engineering projects for Grid-based application and efficient use of common compute and software resources.

The community project InGrid provides a Grid environment for scientific engineering applications. The flexible use of Grid technologies will combine the competences in modeling, simulation and optimization and allow for the common, efficient use of distributed resources. The development of a Grid-based "computational engineering community" demonstrates technologically advanced applications of engineering work in research as well as in operational innovation management.

InGrid is based on five prototype applications in the fields of coupled multiscale problems, coupled multidisciplinary simulations and distributed simulation-based optimization. Adaptive and scalable process models and runtime environments are to be developed. The aim is to give the user simulation-based tools on different levels of complexity.

Partners - HLRS (Project Leader), Institute of Fluid Mechanics and Hydraulic Machinery (IHS) University of Stuttgart, Institute of Scientific Computing and Algorithms (SCAI) Fraunhofer-Gesellschaft, T-Systems Solutions for Research (SfR) GmbH, Institute of Business Information Technology University of Siegen, Department of Mathematics and Computer Science Philipps-University of Marburg, Wasy Gesellschaft für wasserwirtschaftliche Planung und Systemforschung, Access e.V.

7.1.1.6 DAAD Exchange Programme

In order to strengthen the collaboration of HLRS and the University of Tennessee, Knoxville, in the area of MPI-development, an Collaborative OpenMPI-Initiative has been started with the help of the German Academic Exchange Service (DAAD).

7.1.2 International (European and Others)

7.1.2.1 HPC-Europa

Abstract - The HPC-Europa project is an EU-funded project within the 6th Framework Program (FP6) with the focus on providing HPC services to the European research community in an innovative and coherent manner. HPC-Europa consists of several interrelated subprojects, at the core of which lies the transnational access visitor program, accompanied by several networking and research activities.

The consortium of HPC-Europa consists of eleven leading centers working on the three parts of the project: Transnational Access, Networking Activities and Joint Research Activities.

While the first and biggest part is the visitor program, the other two parts go hand in hand with this activity by developing new solutions for the AccessGrid video-conferencing toolset, a seamless integration of performance measurement tools into the development chain on up-to-date HPC machines and single-point of access to HPC-facilities.

Partners - CINECA, EPCC, CEPBA-CESCA, HLRS, IDRIS, SARA, PSNC, PARALLAB, CASPUR, TCD, NTUA

7.1.2.2 DEISA

Abstract - DEISA is a consortium of leading national supercomputing centres that currently deploys and operates a persistent, production quality, distributed supercomputing environment with continental scope. The purpose of this FP6 funded research infrastructure is to enable scientific discovery across a broad spectrum of science and technology, by enhancing and reinforcing European capabilities in the area of high performance computing. This becomes possible through a deep integration of existing national high-end platforms, tightly coupled by a dedicated network and supported by innovative system and grid software.

Partners - IDRIS, FZJ, RZG, CINECA, EPCC, CSC, SARA, ECMWF, LRZ, BSC, HLRS

7.1.2.3 CoreGRID

Abstract - The CoreGRID Network of Excellence (NoE) aims at strengthening and advancing scientific and technological excellence in the area of Grid and Peer-to-Peer technologies. To achieve this objective, the Network brings together a critical mass of well-established researchers (119 permanent researchers and 165 PhD students) from 42 institutions who have constructed an ambitious joint programme of activities. This joint programme of activity is structured around six complementary research areas that have been selected on the basis of their strategic importance, their research challenges and the recognized European expertise to develop next generation Grid middleware, namely:

> Knowledge & Data Management;
> Programming Models;
> System Architecture;
> Grid Information and Monitoring Services;
> Resource Management and Scheduling;
> Problem Solving Environments; Tools and Grid Systems.

HLRS mainly contribute with its experience in the area of Problem Solving Environments; Tools and Grid Systems and will especially participate in design and implementation of an application Meta-data repository as well as the integration and further development of a Grid Application Management Tool.

Partners - The project consists of 42 partners from 18 countries (17 from Europe): ERCIM, CETIC, IPP-BAS, CNR-ISTI, CNRS, TUD, EPFL, FhG, FZJ, HLRS, ICS-FORTH, IC, INFN, INRIA, KTH, MU, PSNC, RAL - CCLRC, SICS, SZTAKI, QUB, WWU Muenster, UNICAL, UCAM-DAMTP, UWC, UCHILE, UCO, UCY, UNI DO, UNILE, UCL, UoM, UNCL, UNI PASSAU, UNIPI, HES-SO, UoW, UPC, VUA, VTT, ZIB, CYFRONET

7.1.2.4 CROSSGRID

Abstract - CROSSGRID is a European R&D project, which aims to develop, implement and exploit new Grid components for interactive compute and data intensive applications. Examples are simulation and visualization

for surgical procedures, flooding crisis, distributed data analysis in high-energy physics, or air pollution combined with weather forecasting. The current CROSSGRID testbed includes resources from 18 sites across 9 European countries.

The contribution of HLRS is to develop the MPI analysis and checking tool MARMOT, a portable tool to verify automatically at runtime if an MPI application conforms to the MPI standard. The tool contains also a mechanism to detect deadlocks. MARMOT supports the complete MPI-1.2 standard and has been used successfully with benchmarks and several applications on different platforms.

Partners - The consortium consists of 21 partners from 11 European countries, CYFRONET in Poland acting as coordinator. The technical partners are HLRS, ICM, INP, INS, UvA, II SAS, University of Linz, FZK, TUM, PSNC, UCY, Datamat, TCD, CSIC, UAB, U.S.C., Demo, A.U.Th., LIP, and Algo

7.1.2.5 GRIDSTART

Abstract - The objective of the project is to maximize the impact of EU-funded Grid projects and related other activities through clustering. GRIDSTART is an initiative sponsored by the European Commission with the specific objective of consolidating technical advances in Europe, encouraging interaction amongst similar activities both in Europe and the rest of the world and stimulating the early take-up by industry and research of Grid-enabled applications. The initiative brings together technologists, scientists and industry in multi-disciplinary approach to developing the Grid infrastructure. The clear goal is to develop sustainable, effective and universal solutions addressing the needs of science, industry and the public. This will be primarily done by driving forward Grid developments by identifying and amplifying synergies between application areas and by encouraging interaction amongst similar activities in Europe.

Partners - The list of partners consists of the EPCC (project coordinator), HLRS, CERN, CYFRONET, ESO, FZJ, University of Southampton, Poznan SNC, and University College London

7.1.2.6 GridCoord

Abstract - The GridCoord project aims at strengthening the co-operations amongst the European funding authorities and Grid projects in order to improve the coordination of the future activities in the field of Grid computing. Furthermore it plans to develop a roadmap for future Grid activities within the European Union and its associated states.
To reach its goals, GridCoord is organizing a series of workshops, each focusing on a specific interest and/or research group. The HLRS is organizing the GridCoord Industrial Workshop, a key event in this series, focusing on the requirements, plans and current trends of European industry. This includes software- and hardware vendors, service providers and end-users of various industrial fields.

Partners - The project consists of 13 partners: DIST, UP, HLRS, QUB, EPSRC, INRIA, UNSA, ZIB, UvA, MTA, SZTAKI, UPM, PSNC, OMII

7.1.2.7 NextGRID

Abstract - The NextGRID project is an integrated project in the sixth Framework Programme of the European Commission under the strategic objective of "Grids for Complex Problem Solving" with an overall budget of 15M€. It aims for providing a framework covering all needs in the evolving field of Grid applications. The goal of this European project is finding solutions allowing easy installation and maintenance, development and deployment as well as user orchestration in the resulting Grid application. The facility to realize scalable and economically viable applications leveraging the next generation Grid framework will prepare the way for broad usage of Grid technologies for solving real world problems, thus leading to the emergence of the next generation Grid. In order to realize the next generation Grid current Grid architectures will be extended in three phases:

1. Meeting the needs of business users
2. Enabling participation by the public
3. Consolidating and standardizing.

The development of the next generation Grid will result in a collection of new architectural designs, key middleware components, application sup-

port mechanisms, know-how and standards that will underpin the next generation Grid.
HLRS will contribute in particular to the realization of the Service Level Agreement subsystem, is leading the task on Virtual Organizations and is contributing to the definition and the Next Generation Grid architecture.

Partners - UEDIN, IT Innovation, Intel, BT, DATAMAT, FLE, FZJ, GRIDSYSTEMS, USTUTT-HLRS, KTH, Microsoft, NEC, ICCS/NTUA, QUB, SAP, TSI, UvA, CNR-ISTI, First Derivatives, KINO, TUD, HP

7.1.2.8 Akogrimo

Abstract - The Akogrimo (Access to knowledge through the Grid in a mobile world) project is an integrated project in the sixth Framework Program of the European Commission under the strategic objective of "Grids for Complex Problem Solving" with an overall budget of 11M€. The aim of the Akogrimo project is to architect and prototype a blueprint of a Next Generation Grids with exploits and closely co-operates with evolving Mobile Internet infrastructure based on Ipv6. Accordingly, Akogrimo will bring together the market orientation and pervasiveness of mobile communication technology in everyday life with the promise of a dynamic concerted use of resources and services through a Grid infrastructure. The main project objectives are:

1. From a technical point of view, Akogrimo will especially leverage mobility, QoS, AAA and security functionalities provided by corresponding network-related middleware systems of such infrastructures.
2. From a user's point of view, Akogrimo will provide the technologies and concepts to establish a 'virtual home', with nomadic and mobile environments for solving complex problems across network technology and provider domains.
3. From the provider's point of view, an Akogrimo world will provide new business models and opportunities eventually making commercially viable Next Generation Grids a reality.
4. From a service provider viewpoint the integration with modern networks will take off the burden of many elements preventing the wide take up Grids such as user and accounting services.

HLRS is the technical coordinator of the overall project and is leading several large activities such as Architecture and Grid Infrastructure Services Layer. This project is performed in collaboration with Rechenzentrum Universität Stuttgart (RUS) being responsible for the network oriented aspects.

Partners - TID, USTUTT, UPM, ATOS, CRMPA, BOC, IT-Aveiro, UniZH, CCRLC, TN, ICCS/NTUA, DM, UHOH

7.1.2.9 TrustCoM

Abstract - The TrustCoM project is an integrated project funded by the European Commission in the sixth Framework Program. The objective of TrustCoM (Trust and Contract Management) is to develop a framework which enables trustworthy business processing in dynamic Virtual Organizations (VOs). Virtual Organizations are formed by various participants (companies, institutions, individuals, etc.) to supply services or produce goods co-operatively. The TrustCoM framework shall facilitate to securely share some resources (data, software, hardware) across organization boundaries, and to isolate others. It will support the entire lifecycle of VOs, i.e. identification, formation, operation, and termination.

The framework leverages and extends the emerging convergence of open-standards such as web services and Grid technologies and protocols for inter-enterprise interactions. TrustCoM will deliver specifications and a reference implementation of the infrastructure. Validation will take place within industrial strength test-beds in the areas of collaborative design engineering and dynamic processes for on-demand aggregation of electronic services.

HLRS role in this project is twofold. First HLRS is leading the architecture activity and is realizing services related to the Virtual Organization infrastructure and Service Level Agreements. Secondly HLRS is participating in the realization and demonstration activities of an innovative collaborative engineering scenario in collaboration with several industrial partners including British Aerospace, AtosORIGIN and SAP.

Partners - ATOS, CCLRC, BAE, BT, HLRS, SAP, SICS, EMIC, ETH, IC, KCL, NRCCL, SINTEF, UoM, IBM, UoK

7.1.2.10 E-LeGI

Abstract - The European Learning Grid Infrastructure (ELeGI) project is an integrated project in the sixth Framework Programme of the European Commission under the strategic objective of "Advanced ELearning Systems" and has the ambitious goal to develop software technologies for effective human learning. With the ELeGI project we will promote and support a learning paradigm shift. A new paradigm focused on knowledge construction using experiential based and collaborative learning approaches in a contextualized, personalized and ubiquitous way will replace the current information transfer paradigm focused on content and on the key authoritative figure of the teacher who provides information. The ELeGI project has three main goals:

Goal 1: To define new models of human learning enabling ubiquitous and collaborative learning, merging experimential, personalized and contextualized approaches.

Goal 2: To define and implement an advanced service-oriented Grid based software architecture for learning. This will allow us to access and integrate different technologies, resources and contents that are needed in order to realize the new paradigm. This objective will be driven by the pedagogical needs and by the requirements provided by the test-beds (SEES) and informed by the experience gained through implementing the demonstrators.

Goal 3: To validate and evaluate the software architecture and the didactical approaches through the use of SEES and demonstrators. The project will build extensively on advanced work already done, creating new learning environments rather than creating new learning resources per se.

HLRS is leading the activity exploring existing Grid technologies for this new application domain and is contributing to the architecture activity designing the overall system.

Partners - RESIT, AtosOrigin, CCLRC, CEMSAC, CNRS, CRMPA, CRSA, CS SI, Microsoft EMIC, FAU Erlangen, FUNDP, HOU, KFU-Graz, UM2-Montpellier, University of Dundee, University of Southampton, UPPA, University of St. Andrews, HLRS

7.1.2.11 NATO Project

The NATO-funded project entitled “Improving the Reliability of Computer Simulations to predict environmental risks” is a co-operation of the University of Houston, the University of Erlangen, the University of Stuttgart and the Institute of Numerical Mathematics, Russia with Prof. Marc Garbey, University of Houston being the project leader. It focuses on the collaboration of the partners with regard to fault-tolerance of critical applications.

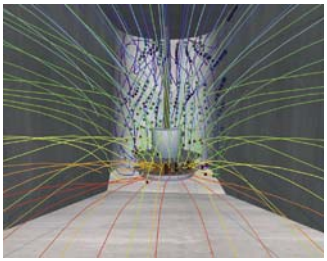
7.1.3 Industry

7.1.3.1 Intel Co-operation

Abstract - HLRS and Intel are partners to develop initiatives and enhance solutions around the next generation enterprise server and High Performance Computing (HPC) building blocks in hardware and software. In the framework of this project HLRS get access to new and early Intel pre-release hardware technologies. Through the participation in HPC relevant Intel software tools alpha & beta evaluation HLRS plays an important role in the development of Intel tools. The two partners also work together in the performance analysis and tuning of parallel applications running on the EM64T Xeon cluster with Infiniband interconnect. This enables more applications to benefit from the high bandwidth and low latency offered by this platform.

Partners - Intel GmbH, HLRS

7.1.3.2 Microsoft HPC Institute



Abstract - HLRS and Microsoft are working together in the Microsoft HPC Innovation Center program. Microsoft recently launched a new Windows version called Windows Server 2003, Compute Cluster Edition, which is specifically used for high performance computing clusters. The goal of this co-operation is to evaluate this platform as an alternative for

HPC clusters. To show its potential and possibilities, HLRS implemented interactive simulations running under Windows Server 2003 Compute Cluster Edition.

A sample application is the virtual water turbine test-bed, which helps turbine designers by simplifying and optimizing the water turbine design process to achieve an improved efficiency with less effort.

Partners - Microsoft, HLRS

7.1.3.3 Teraflop Workbench

Abstract - The Teraflop Workbench will enable sustained teraflop performance for a wide range of scientific and industrial applications. It is a co-operation project between HLRS and the Japanese vendor of high performance computing platforms NEC. Its goal is to demonstrate the efficiency of the NEC SX vector systems and that this architecture can deliver teraflop/s application performance for a broad range of research and ISV codes. To improve the application performance NEC and HLRS work together in selected projects with scientific and industrial developers and end users. The applications itself come from areas like Computational Fluid Dynamics, Bioinformatics, Structural Mechanics, Chemistry, Physics, Combustion, Medical Applications and Nanotechnology.

In addition to the efficiency of the simulation itself, the Teraflop Workbench will also work towards an integrated workflow environment from pre-processing to visualization for the scientific applications.

Motivation - For the new installation of a federal high performance computer the HLRS chose a parallel vector system of NEC: a SX-8. This architecture turned out to be the best offer with respect to the total cost of ownership. With this system, the HLRS continued its long tradition in operating vector systems at the federal computing centre. Of course, this continuity has the advantage that the present users of the HLRS's systems can carry on with their work without much effort in porting their codes to the new system and moreover, they will immediately profit from the increased performance of the latest hardware. This provides the possibility to concentrate immediately on improvements of the application software in

respect to new features of the hardware. Only to mention one point: with the increasing number of shared-memory nodes, the users are now challenged with the problem of scalability more than ever before, when trying to utilize the whole system for their research activities.

Another aspect we want to take care of becomes clear if one looks at the spectrum of installed HPC-systems worldwide: Vector systems definitely are minority despite their unquestionable capability for scientific applications. Consequently the users do not develop their software for vector systems anymore. Thus one has not only to set oneself the goal of maintaining and improve existing software but also to bring in new users to the vector system. Keeping this in mind, NEC and HLRS decided to focus on the software related aspects of the installation by establishing a joint co-operation for the runtime of the NEC SX-8.To give a concrete overview of this co-operation, a brief description of the currently running projects follows.

Projects and Results

Due to the historically developed spectrum of the users at HLRS, the focus area of most of the projects is fluid mechanics. Hence not astonishing, two project codes deal with the simulation of turbulent flows. In both cases the scalability of the codes has been further improved.

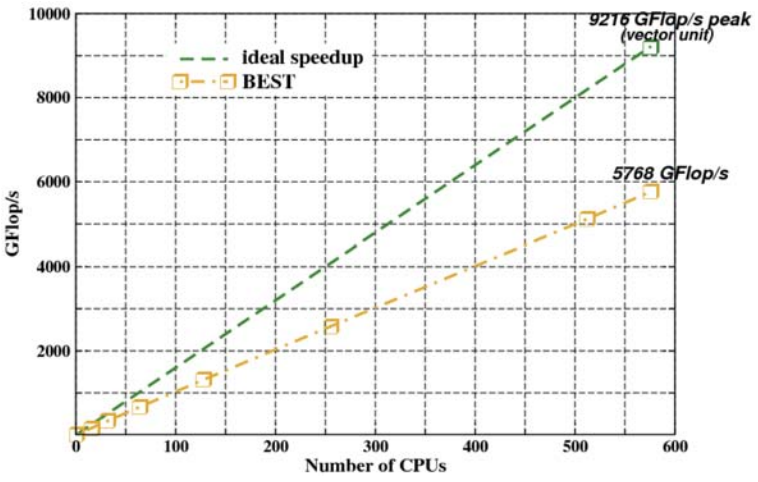


Figure 1: Performance of the fluid mechanic application BEST on the NEC SX-8

The spectral/finite-difference code N3D of the Institute of Aero- and Gas Dynamics (IAG), Universität Stuttgart is now achieving 2.5 TFlop/s on 64 nodes (512 CPUs). The second code tackling similar problems is the lattice Boltzmann solver BEST of the Chair of Fluid Dynamics (LSTM), Universität Erlangen-Nürnberg. The recent performance of this application is shown in Figure 1 revealing that this code runs at more than 5.7 TFlop/s on the whole system.

Another fluid mechanics code is FENFLOSS of the Institute of Fluid Mechanics and Hydraulic Machinery (IHS), Universität Stuttgart. It uses the finite element method to simulate turbo machines. In FENFLOSS it was possible to improve the single processor performance significantly by modifying the internal data structures. The scalability was improved by implementing a shared memory parallelization. The code now achieves a sustained performance of more than 2.5 TFlop/s on 64 nodes.

The Institute of Theoretical and Applied Physics (ITAP), Universität Stuttgart is using amongst others classical molecular dynamic codes for their research. In this application it is inevitable to reduce the effort in accumulating the interaction. This is already an n2-problem in the easiest case of a two particle interaction. Therefore the pairs of the interaction are normally restricted. This requires an indirect memory addressing. It becomes evident during the efforts in optimizing this operation that the capability of the SX-8 in handling indirect memory addressing should be further improved for the next generation. At the moment one vector processor is only twice as fast as a typical cache based CPUs. To classify this, it should be stated that the same factor for the BEST application is at least eight. Not surprisingly the researchers at ITAP prefer large PC-clusters.

The efficiency of the SX-8 could also be demonstrated for two standard ab-initio molecular dynamic codes VASP and CPMD. Here, the optimization was limited to compiler level tuning. A typical 16 nodes (128 CPU) VASP run achieves an efficiency of more than 50%, accounting to over 1 TFlop/s. The results for CPMD looks even better: 16 nodes deliver a performance of 1.43 TFlop/s or an efficiency of 70%. The matrix-matrix multiplication, most time consuming operation, runs with 14 GFlop/s (of 16 Gflop/s vector peak) on one CPU.

A further important project deals with the development of an efficient, parallel library for solving sparse linear systems. The efforts focus on the performance of the algorithms on the vector hardware as well as on efficient convergence behaviour of the solver itself. Sparse matrix vector product is one of the key operations in an iterative solver. The performance of this operation was 800 MFlop/s using third party software and over 6.5 GFlop/s (about 40% vector peak) in the case of the SX tuned solver.

Workshops - The Teraflop Workbench goes along with yearly workshops. With more than 50 participants from Europe, Asia and the US, the second workshop in March 2005 brought together scientists, application developers, HPC experts and hardware designers to discuss the present and future of supercomputing. Speakers like J.T. Carter (LBNL) and Yoshiyuki Miyamoto (NEC Research) talked about performance and applications on vector systems, experts like Jack Dongarra (ICL, University of Tennessee) and Ryutaro Himeno (Riken, Japan) discussed future architectures in supercomputing. Computational scientists of different fields presented their current work and first results obtained on the new SX-8 system. The discussion during the workshop will be documented as conference proceedings.

Conclusion and Outlook - Most of the current projects of the Teraflop Workbench were able to demonstrate a sustained performance of several TFlop/s on the HLRS NEC SX-8. On the other hand the initiative was able to show important directions for future architectural improvements which can and indeed are directly communicated to the hardware engineers.

In addition to the vector-parallel SX-8 system an SMP front end system and a NEC Linux cluster were installed. The Linux cluster and the SMP system form together with the SX vector system an environment that allows to perform the complete pre-processing – simulation – post-processing – visualization workflow in an integrated and efficient way. The support of the users in using this environment will also be a task for the Teraflop Workbench in the future.

The presented initiative is open to new participants. An application has to demonstrate scientific merit as well as suitability and demand for teraflop performance in order to qualify for the Teraflop Workbench.

Partners - NEC GmbH, HLRS

7.2 Scientific Co-operations

This section gives a list of existing co-operations with partners in Germany, Europe and worldwide.

7.2.1 Co-operations continued in 2005

> Japan Atomic Energy Research Institute (JAERI), Tokyo, Japan
> National Center for High performance Computing (NCHC), Hsinchu, Taiwan
> Pittsburgh Supercomputing Center (PSC), Pittsburgh, PA, USA
> Sandia National Laboratories (SNL), Albuquerque, NM, USA
> University of Houston, TX, USA
> Indiana University, USA
> Institute for Computational Technologies, Russian Academy of Sciences, Novosibirsk, Russia
> Supercomputing Center Korea Institute of Science and Information (KISTI), Seoul, Korea
> OpenMPI Consortium: Los Alamos National Laboratories, Indiana University, the University of Tennessee, USA

7.3 Scientific Workshops

Date	Organizer	Location	Topic
Mar 07-09 2005	HLRS	Stuttgart	8th HLRS Metacomputing Workshop and GridCoord Workshop
Mar 14-16 2005	HLRS, ICT	Stuttgart	2nd Russian- German Advanced Research Workshop on Computational Science and High Performance Computing
Mar 17-18 2005	HLRS	Stuttgart	2nd Teraflop Workbench Workshop

Apr	04-05 2005	HLRS, hww	Stuttgart	4th hww Workshop on Scalable Global Parallel File Systems
Sep Oct	25 - 01 2005	HLRS, Al-Farabi Kazakh Nat. University	Almaty, Kazakhstan	1st Kazakh-German Advanced Research Workshop on Computational Science and High Performance Computing
Oct	13-14 2005	HLRS	Stuttgart	High Performance Computing in Science and Engineering – The 8th Results and Review Workshop of the HPC Center Stuttgart (HLRS)
Nov	10 2005	HLRS, NEC	Tokyo	3rd Teraflop Workbench Workshop

7.3.1 GridCoord Industrial Workshop & 8th HLRS Metacomputing and Grid Workshop

March 7th - 9th, 2005, Stuttgart, Germany

On this two-and a half day joint workshop, experts from industry and research presented the newest developments in Grid and Metacomputing. Attendees from research were mainly from the European projects, namely DEISA, GridCoord, CoreGrid, Akogrimo, NextGrid and SimDat, but also interested persons joined from the US, as well as participants from Asian countries, like Japan and South Korea. Overall 31 talks were given (accessible from our web-server); from the European Commission a very concise overview on the current status of European Grid projects was given.

7.3.2 2nd Russian-German Advanced Research Workshop on Computational Science and HPC

March 14th - 16th, 2005, Stuttgart, Germany

The 2nd Russian German Research Workshop on Computational Science and High Performance Computing took place in Stuttgart from 14th to 16th of March. As the 1st workshop in Akademgorodok it was arranged by Prof. Yurii Shokin (member of the presidium of the Russian Academy of Sciences http://www.ras.ru/ and director of the Institute of Computati-

onal Technologies of the Siberian Branch of the Russian Academy of Sciences http://www.ict.nsc.ru) and Prof. Michael Resch (Director of the High Performance Computing Center Stuttgart http://www.hlrs.de and chair for high performance computing at the University of Stuttgart http://www.uni-stuttgart.de).Thirty Russian, Kazakh and German scientists discussed a broad range of topics spanning from theoretical to application problems and covering multiple disciplines like the Discretization of the Navier-Stokes Equations, Analysis of Vortices, Relativistic Systems, Turbulent Flows, Computational Aero Acoustics, Airbag Simulation, Molecular and Dissipative Particle Methods, Meteorological Flood Forecast, Web based Frameworks, Software Engineering for Numerical Methods, Water Turbine Simulation, Image Registration in Medical Applications, Visualization, Hardware Properties and Performance Analysis.

Long term target of the collaboration between the Russian Academy of Sciences and the HLRS is the fruitful interaction of the two scientific cultures. More information on the workshop and the collaboration can be found at http://www.grc-hpc.de/. The workshop was sponsored by the German Research Foundation (DFG).

7.3.3 2nd HLRS-NEC Teraflop Workbench Workshop

March 17th - 18th, 2005, Stuttgart, Germany

The Teraflop Workbench Workshop is part of the Teraflop Workbench cooperation between NEC and HLRS. With more than 50 participants from Europe, Asia and the US, it brought together scientists, application developers, HPC experts and hardware designers to discuss the present and future of supercomputing. Speakers like J.T. Carter (LBNL) and Yoshiyuki Miyamoto (NEC Research) talked about performance and applications on vector systems, experts like Jack Dongarra (ICL, University of Tennessee) and Ryutaro Himeno (Riken, Japan) discussed future architectures in supercomputing. Computational scientists of different fields presented their current work and first results obtained using the new SX-8 system.

7.3.4 4th hww/HLRS Workshop on Scalable Global Parallel File Systems and HNF Europe 2005 Spring Meeting

April 04th - 05th, 2005, Stuttgart, Germany

One focus in this year's workshop with nearly 90 participants were cluster file systems. The key note speech was given by Dr. Peter Braam, founder and CEO of Cluster File Systems INC. and also the mind and spirit behind Lustre. In other presentations, also SAN file systems and Grid file systems were introduced and discussed. On the second day, topics from the field of HSM as well as storage networking technologies were addressed. In addition, the OpenIB Users Group Europe was established. The formation session covered several Infiniband issues from physical layer and kernel problems to storage and message passing.

7.3.5 HPC-Europa Transnational Access Meeting (TAM'05)

September 21st - 24th, 2005, Stuttgart, Germany

In conjunction with the selection of new HPC-Europa guests, the second Transnational Access Meeting of HPC-Europa guests of all centers was held at HLRS in Stuttgart. The Workshop was highly successful for our scientific participants as well as for representatives of the European Commission. Within this 2½ day workshop, we had 91 participants (SUSP-members, HPC-Europa project personnel and HPC-Europa guests). The workshop started off with the Invited Talks on "The Development of Simulation in Computational Engineering" from Prof. Dr.-Ing. Göde, University Stuttgart, Prof. Dr. Kolditz, University of Tübingen, Dr. Badcock, University of Glasgow and Prof. Dr. Wittum, University of Heidelberg. Then HPC-Europa guests presented their research done at their respective hosts. The Workshop was organized with two parallel sessions with topics on CFD, Computational Chemistry, Computer Science, Mathematics, BioInformatics and Life-Science and Computational Physics. Overall 31 talks were held and ten poster presentations given by HPC-Europa guests.

7.4 Conference Shows

7.4.1 International Supercomputer Conference 2005

June 21st - 24th, 2005, Heidelberg, Germany

As every year HLRS was presenting its research activities at the ISC in Heidelberg. Together with the three other large German centers (NIC, LRZ and HLRN) HLRS had a booth at which poster and video presentations were shown. HLRS was also present at the Microsoft booth showing its results of the collaboration with Microsoft in the field of high performance computing.

7.4.2 Microsoft Company Meeting 2005

September 23rd, 2005, Seattle, WA, USA

At this year's Microsoft Annual Meeting on September 23rd, 2005 the High Performance Computing Center of the University of Stuttgart (HLRS) has been invited to present the results of its co-operation in the area of modeling and simulation with the Windows Server High Performance Computing team. 20.000 employees and guests in Safeco Field in Seattle celebrating the 30th anniversary of the company enjoyed the live demonstration of HLRS applications running on a cluster powered by Windows Server 2003 Compute Cluster Solution. Uwe Wössner and Martin Becker from HLRS presented an interactive simulation of a hydroelectric power plant. This has been developed in collaboration with the Institute of Fluid Mechanics and Hydraulic Machinery of the University of Stuttgart. The goal of this co-operation is the simplification and optimization of the design process of water turbines as well as their improved efficiency. Additionally a blood flow simulation of an aneurysm showing modern simulation techniques and me-

thods in high performance computing and how they could contribute to the treatment of such bulges in blood vessels has been demonstrated.

The director of HLRS Prof. Resch called this event a large success for the efforts to strengthen the role of industrial users and their integration into the supercomputing domain. Only through co-operation like this with companies such as Microsoft the research results can be applied to real world problems and enable their application outside the purely academic context. Kyril Faenov, Director of High Performance Computing within the Windows Server group of Microsoft: "It was a great way to share our joint vision and results of collaboration in front of a global audience of Microsoft employees."

7.4.3 iGrid 2005

September 26th - 29th, San Diego, CA, USA

The HLRS presented collaborative interactive simulation analysis of ongoing simulations.

7.4.4 Supercomputing Conference 2005

November 12th - 18th, 2005, Seattle, WA, USA

As last year, HLRS presented it's on-going projects and research on its booth at the Supercomputing Conference, which was held in Seattle. With around 9.000 participants SC was bigger than ever. At the HLRS booth presentation was given on HLRS projects such as Teraflop Workbench, as well as European and German projects like CoreGrid, GridCord, Akogrimo and HPC-Europa. This year, the visualization group was able to install an eye-catcher: A Mercedes SLK showing Augmented Reality Visualization on "the real thing". Presentations on Visualization were given at the HP Booth, the collaboration with Microsoft presented at the respective booth, metacomputing activities presented at the KISTI booth as well as the Teraflop Workbench introduced at the NEC booth.

7.5 Publications

7.5.1 Books

HW. E. Nagel, W. Jäger, M. Resch, High Performance Computing in Science and Engineering 05, Springer, Berlin, Heidelberg, New York, 2005.

This book presents the state-of-the-art in modelling and simulation on supercomputers. Leading German researchers present results achieved on systems of the High Performance Computing Center Stuttgart (HLRS) for the year 2005. The reports cover all fields of computational science and engineering ranging from CFD via computational physics and chemistry to computer science. Special emphasis is given to industrially relevant applications. Presenting results for both vector-systems and micro-processor based systems the book allows to compare performance levels and usability of various architectures. In the light of recent discussions about systems like BlueGene versus the Earth-Simulator this book may serve as a guide book for further discussion. The book covers the main methods in high performance computing. Its outstanding results in achieving highest performance for production codes are of particular interest for both the scientist and the engineer. The book comes with a wealth of coloured illustrations and tables of results.

E. Krause, Y. Shokin, M. Resch, N. Shokina (Eds.), Computational Science and High Performance Computing, Notes on Numerical Fluid Mechanics and Multidisciplinary Design - Volume 88, Springer, Berlin, Heidelberg, New York, 2005.

This volume contains contributions to the Russian-German Advanced Research Workshop on Computational Science and High Performance Computing as presented in September 2003 at Novosibirsk (Academgorodok), Russia. The workshop was organized jointly by the German High Performance Computing Center Stuttgart (HLRS) and the Russian Institute for Computational Technologies (ICT SB RAS). The contributions range from computer science, mathematics and high performance computing to applications in mechanical and aerospace engineering. They bring together a wealth of theoretical work and simulation experience and thus show the potential of bringing

together theoretical mathematical modeling with the usage of powerful high performance computing systems, and present the state of the art of computational technologies.

7.5.2 Journal Papers

1. Peggy Lindner, Edgar Gabriel, Michael Resch, GCM: A Grid configuration manager for heterogeneous Grid environments, International Journal of Grid and Utility Computing, Vol. 1, No. 1, pp. 4 - 12, 2005
2. Michael M. Resch, Remarks on supercomputing in Germany, PIK Praxis der Informationsverarbeitung und Kommunikation, 28 (2005), 238-242
3. Michael Resch, Matthias Müller (Eds.), The Grid, Special Issue of it - Information Technology, 47 (2005), 6
4. Sabine Roller, Thomas Schwartzkopff, Roland Fortenbach, Michael Dumbser, Claus-Dieter Munz: Calculation of low mach number acoustics: A comparison of MPV, EIF and linearized Euler equations, M2AN, Vol. 39, No. 3 (2005), pp. 561-576
5. Sabine Roller, Roland Fortenbach, Thomas Schwartzkopff, Claus-Dieter Munz: The numerical modeling of acoustic wave propagation using the multiple pressure variables approach, accepted by Computing & Visualization in Science
6. Stefan Wesner, Towards a mobile Grid architecture, Special Issue of it - Information Technology, 47 (2005), 6
7. Rajeev Thakur, Rolf Rabenseifner, and William Gropp, Optimization of collective communication operations in MPICH, to be published in the International Journal of High Performance Computing Applications, Sage Science Press, Vol. 19, No. 1, pp. 49-66, 2005

7.5.3 Other Refereed Papers

1. T. Dimitrakos, G. Laria, I. Djordjevic, N. Romano; F. D'Andria; V. Trpkovski, P. Kearney, M. Gaeta, P. Ritrovato, L. Schubert, B. Serhan, L. Titkov and S. Wesner, Towards a Grid Platform enabling Dynamic Virtual Organisations for Business Applications, in Lecture Notes in Computer Science, Volume 3477, Springer, 2005, pp. 406 - 410.
2. A.E. Arenas, I. Djordjevic, T. Dimitrakos, L. Titkov, J. Claessens, C. Geuer-Pollmann, E. Lupu, N. Tuptuk, S. Wesner, L. Schubert, Trust and Security in Virtual Organisations, in Collaborative Networks and Their Breeding Environments (PRO-VE 05).
3. C. Loos, S. Wesner and J.M. Jähnert, Specific Challenges of Mobile Dynamic Virtual Organizations, in Paul Cunningham & Miriam Cunningham (Eds.), Innovation and the Knowledge Economy: Issues, Applications, Case Studies, IOS Press Amsterdam, 2005, pp. 1209 - 1216.
4. L. Schubert, S. Wesner, T. Dimitrakos, Secure and Dynamic Virtual Organizations for Business, in Paul Cunningham & Miriam Cunningham, ed., Innovation and the Knowledge Economy: Issues, Applications, Case Studies, IOS Press Amsterdam, 2005, pp. 1201 - 1208.
5. M. Auweter-Kurtz, M. Fertig, D. Petkov, T. Stindl, M. Quandt, C.-D. Munz, P. Adamidis, M. Resch, S. Roller, D. D'Andrea, R. Schneider, Development of a hybrid PIC/DSMC Code, The 29th International Electric Propulsion Conference, Princeton University, USA, October 31 - November 04, 2005.
6. P. Haas, M. Resch, High Performance Computing in Science and Engineering, 17th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD 2005), Rio de Janeiro, Brasil, October 24 - 27, 2005.
7. N. Currle-Linde, U. Küster, B. Risio, M. Resch, Science Experimental Grid Laboratory (SEGL) Dynamical Parameter Study in Distributed Systems, ParCo 2005, Malaga, Spain, 13 - 16 September, 2005.
8. F. Infed, M. Fertig, F. Olawsky, P. Adamidis, M. Auweter-Kurtz, M. Resch, E. W. Messerschmid, Numerical Simulation of High-Enthalpy Nonequilibrium Air Flows, in Dieter Jacob, Gottfried Sachs, and Siegfried Wagner (Eds.), Basic Research and Technologies for Two-Stage-to Orbit Vehicles, pp. 147 - 164, Wiley-VCH Verlag, Weinheim, 2005.
9. M. Neumann, S.R. Tiyyagura, W.A. Wall, E. Ramm, Efficiency Aspects for Advanced Fluid Finite Element Formulations. 13th Conference on Finite Elements for Flow Problems, Swansea, Wales, April 04 - 06, 2005.

10. R. Rabenseifner, S.R. Tiyyagura, M. S. Müller, Network Bandwidth Measurements and Ratio Analysis with the HPC Challenge Benchmark Suite (HPCC), in Recent Advances in Parallel Virtual Machine and Message Passing Interface, B. Di Martino, D. Kranzlmüller, and J. Dongarra (Eds.), Proceedings of the 12th European PVM/MPI Users' Group Meeting, LNCS 3666, pp. 368 - 378, Springer, EuroPVM/MPI 2005, Sorrento, Italy, September 18 - 21, 2005.
11. B. Krammer, M. Müller, and M. Resch. Runtime Checking of MPI Applications with MARMOT, Mini-Symposium Tools Support for Parallel Programming, ParCo 2005, Malaga, Spain, September 12 - 16, 2005.
12. A. Debudaj-Grabysz, R. Rabenseifner, Nesting OpenMP in MPI to Implement a Hybrid Communication Method of Parallel Simulated Annealing on a Cluster of SMP Nodes, in Recent Advances in Parallel Virtual Machine and Message Passing Interface, Dieter Kranzlmüller, Beniamino Di Martino, and Jack Dongarra (Eds.), Proceedings of the 12th European PVM/MPI Users' Group Meeting, EuroPVM/MPI 2005, September 18 - 21, Sorrento, Italy, LNCS Springer, 2005, pp. 18 - 27.
13. R. Rabenseifner, S. R. Tiyyagurra, M. Müller: Network Bandwidth Measurements and Ratio Analysis with the HPC Challenge Benchmark Suite (HPCC), in Recent Advances in Parallel Virtual Machine and Message Passing Interface, Dieter Kranzlmüller, Beniamino Di Martino, and Jack Dongarra (Eds.), Proceedings of the 12th European PVM/MPI Users' Group Meeting, Euro PVM/MPI 2005, September 18 - 21, Sorrento, Italy, LNCS Springer, 2005, pp. 368 - 378.
14. D. Kemmler, O. Kolditz, P. Adamidis, R. Rabenseifner: Application of High Performance Computing Techniques (Parallel Processing) to the Modelling of Complex coupled Geo-Processes using a Finite Element Approach (GeoSys/RockFlow), in Proceedings of International Conference on Environmental Science and Technology (IC EST 2005), January 23 - 26, 2005, New Orleans, USA.
15. D. Kemmler, P. Adamidis, W. Wang, S. Bauer, O. Kolditz: Solving coupled Geoscience Problems on High Performance Computing Platforms, Proceedings of ICCS 2005, Emory University Atlanta, USA, May 22 - 25, 2005, V.S. Sunderam et al. (Eds.): ICCS 2005, LNCS 3515, pp. 1064 - 1071, 2005, Springer-Verlag Berlin, Heidelberg, 2005.
16. M. Bolten, N. Papenberg, B. Fischer, P. Adamidis, R. Rabenseifner, H. Berger: Parallelisierung eines nichtlinearen Registrierungsalgorithmus zur Verarbeitung sehr großer Volumen-Daten, in Proceedings, H.-P Meinzer, H. Handels, A. Horsch, T. Tolxdoff (Eds.), Bildverarbeitung für die Medizin 2005, Workshop, Heidelberg, March 13 - 15, Springer, 2005.

7.5.4 Other Papers

1. S. Wesner, L. Schubert. & T. Dimitrakos, Dynamic virtual organisations in engineering, 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, March 14 - 16, 2005.
2. T. Kielmann, G. Wrzesinska, N. Currle-Linde, and M. Resch, Redesigning the SEGL problem solving environment: A case study of using mediator components, Workshop "Integrated Research in Grid Computing", Pisa, Italy, November 28 - 30, 2005.
3. M. Resch, The chain of abstraction in high performance computing and simulation, 1st German Kazakh Workshop, Almaty, Kazakhstan, September 26 - 30, 2005.
4. M. Resch, M. Müller, P. Lammers, H. Berger, J. Stadler, The SX-8: A European flagship for supercomputing, KONWIHR, Quartl, Mitteilungsblatt des Kompetenznetzwerks für technisch-wissenschaftliches Hoch- und Höchstleistungsrechnen, 1/2005, 39. Ausgabe, 2005.
5. N. Currle-Linde, P. Adamidis, M. Resch, A tool for complex parameter studies in grid environments: SGML-Lab, The 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, Stuttgart, Germany, March 14 - 16, 2005.
6. M. Resch, The SX-8: A European flagship for supercomputing, InSiDE, Vol. 3, No. 1, Spring 2005.
7. A.D. Rychkov, N. Shokina, T. Bönisch, M. Resch, U. Küster, Parallel numerical modelling of gas-dynamic processes in airbag combustion chamber using different computing platforms", 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, March 14 - 16, 2005.
8. T. Bönisch, G.S. Khakimzyanow, N. Shokina, On effectiveness of parallelization of a 3D fluid flow simulation code using software engineering principles, 1st Kazakh-German Advanced Research Workshop on Computational Science and High Performance Computing, Almaty, September 26 - 30, 2005.
9. T. Bönisch and N. Shokina, Parallelization of a 3D fluid flow simulation code using software engineering principles, in Yu.I. Shokin, O.I. Potaturkin (Eds.), ACIT – Software Engineering 2005, ACTA Press, 2005.
10. R. Keller, M. Liebing, Using PACX-MPI in metacomputing applications, 18th Symposium Simulationstechnique, Erlangen, September 12 - 15, 2005.
11. F. Gähler, K. Benkert, Atomistic simulations on scalar and vector computers, 2nd Teraflop Workshop, Stuttgart, April 17 - 18, 2005.

12. M. Neumann, S. R. Tiyyagura, W.A. Wall, E. Ramm, Robustness and efficiency aspects for computational fluid structure interaction. 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, Stuttgart, Germany, March 14 - 16, 2005.
13. M. Neumann, U. Küttler, S. R. Tiyyagura, W.A. Wall, E. Ramm, Computational efficiency of parallel unstructured finite element simulations, 2nd Teraflop Workshop, HLRS, Stuttgart, Germany, March 17 - 18, 2005.
14. R. Rabenseifner, Balance of HPC systems based on HPCC benchmark results, in Proceedings of the Cray Users Group Conference 2005 (CUG 2005) May 16 - 19, Albuquerque, NM, USA, 2005.
15. M. Becker and U. Wössner, Tangible interfaces for interactive flow simulation, 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, March 14 - 16, 2005.

7.5.5 Talks

1. Thomas Bönisch, HLRS – Deutschlands leistungsfähigster Rechner in der Praxis, ZKI AK Supercomputing Herbsttreffen, Karlsruhe, Germany, September 22 - 23, 2005.
2. Thomas Bönisch, Die Teraflop Workbench, Invited Talk. ZAIK/RRZK Colloquium, Universität zu Köln, Cologne, Germany, November 09, 2005.
3. Thomas Bönisch, Höchstleistungsrechnen in Deutschland, Invited Talk. Arbeitstagung der IT-Manager der Fraunhofer–Gesellschaft, Kassel, November 22, 2005.
4. Natalia Currle-Linde, Michael Resch, GridCoord and the role of standardization in grids, First ETSI GRID Standardization Meeting, Sophia-Antipolis, France, September 30, 2005.
5. Rainer Keller, Workshop on Grids in Astronomy, Developments in the Meta-Computing Library PACX-MPI, Strasbourg, France, June 07, 2005.
6. Rolf Rabenseifner, Die MPI-2 Erweiterungen, Chancen und Probleme (The MPI-2 extensions - chances and problems), Institute for Computerapplications in Civil Engineering (CAB), Technical University at Braunschweig, Germany, November 23, 2005.
7. Rolf Rabenseifner, MPI – a surgery in the framework of the HPC Europa project, Talk by AccessGrid Video Conference between EPCC Edinburgh, SARA, Amsterdam, CINECA, Bologna, HLRS, Stuttgart, Germany, April 20, 2005.
8. Michael M. Resch, Die Welt von morgen im Supercomputer von heute, Stuttgart zu Gast in der Universität, Stuttgart, Germany, December 04, 2005.

9. Michael M. Resch, Grid computing in Europe and beyond, First Austrian Grid Symposium, Invited Keynote, Schloß Hagenberg, Austria, December 01, 2005.
10. Michael M. Resch, Simulation on supercomputers - a key technology for Europe?, Bochum-Ruhr-Universität, Bochum, Germany, November 23, 2005.
11. Michael M. Resch, Uwe Küster, General Issues related to Supercomputing, Teraflop Workshop, Tokyo, Japan, November 10, 2005.
12. Michael M. Resch, Applying HPC to create industrial leadership, IDC HPC User Forum, Oak Ridge, USA, September 26 - 28, 2005.
13. Michael M. Resch, Supercomputing in science and industry - The High Performance Computing Center Stuttgart, Summer School of Advanced Computing, Castel Gandolfo, Italy, August 29 - September 09, 2005.
14. Michael M. Resch, Supercomputing und die industrielle Anwendung der Grid-Technologien, doIT online Veranstaltung „Next Generation Computing - ein Ausblick in die Zukunft", Medienzentrum Baden-Württemberg, Stuttgart, Germany, July 07, 2005.
15. Michael M. Resch, Advanced Supercomputing Concepts in Science and Engineering, International Supercomputer Conference 2005, Heidelberg, Germany, June 22, 2005.
16. Michael M. Resch, Synergy at Work – das Höchstleistungsrechenzentrum Stuttgart (HLRS), 6. Forschungsseminar Wissenschaftliches Rechnen an der Universität Ulm, Ulm, Germany, June 08, 2005.
17. Michael Resch, Grid Research in Europe - GridCoord Survey, European Grid Technology Days, Brussels, Belgium, May 31, 2005.
18. Michael M. Resch, Supercomputing in the 21st century - Learning from industry?, Invited Keynote, NEC User Group Meeting, Exeter, UK, May 25, 2005.
19. Michael M. Resch, E-Science in a Teraflop Workbench concept, University of Houston, USA, May 06, 2005.
20. Michael M. Resch, Old problems - New ideas: HLRS and the future of supercomputing, Pittsburgh Supercomputing Center, Pittsburgh, USA, May 04, 2005.
21. Michael M. Resch, NEC SX-8 and Intel EMT 64, T-Systems DLR High Performance Computing and Networking Workshop, Braunschweig, Germany, April 11 - 12, 2005.
22. Michael M. Resch, Industrial and scientific frameworks for computational science and engineering, 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, Stuttgart, Germany, March 14 - 16, 2005.
23. Michael M. Resch, GridCoord, GridCoord Industrial Workshop, Stuttgart, Germany, March 07 - 09, 2005.

24. Michael M. Resch, The future of e-science, Friedrich-Alexander-Universität Erlangen, Germany, February 17, 2005.
25. Sabine Roller, InGrid, Innovative Grid-Entwicklungen für ingenieurwissenschaftliche Anwendungen. D-Grid Kick-Off Meeting, Kassel, Germany, September 08, 2005.
26. Sabine Roller, Martin Quandt, Torsten Stindl, Dejan Petkow, Pulsed plusma thruster for a lunar satellite, Presentation on CEMRACS Summer School, Marseille, France, August 23, 2005.
27. Uwe Wössner, Joachim Kieferle, Real-time visualization and participation, 6th International Conference for Information Technologies in Landscape Architecture, Dessau, Germany, May 26, 2005.
28. Uwe Wössner, Joachim Kieferle, Betting on the future of architecture: Risks, rewards, and opportunities of technology, AIA-TAP 2005 Conference, Las Vegas, USA, May 17 - 18, 2005.
29. Uwe Wössner, 2nd COVISE User Meeting, Fellbach, Germany, November 25, 2005.
30. Uwe Wössner, Joachim Kieferle, Real-time building wind analysis using super computing, AIA New York Chapter, New York, USA, December 13, 2005.
31. Uwe Wössner, Joachim Kieferle, Improving the architectural design process using interactive simulations, GSD, Harvard, Boston, USA, December 12, 2005.

7.5.6 Professional Activities

Edgar Gabriel

> Member of the program committee of the 10th International Workshop on High-Level Parallel Programming Models and Supportive Environments, to be held in conjunction with the IPDPS 2005, Denver, Colorado, USA, April 04 - 08, 2005
> Member of the program committee at the Second International Workshop on Programming Paradigms for Grids and Metacomputing Systems (PGaMS'05), Atlanta, Georgia, USA, May 22 - 25, 2005
> Member of the program committee of the International Conference on Computational Science 2005 (ICCS 2005), Atlanta, Georgia, USA, May 22 - 25, 2005

Rainer Keller

> Member of program committee of International Conference on High Performance Computing and Communications 2005 (HPCC), Sorrento, Italy, September 21 - 23, 2005

Matthias Müller

> Program committee member of HPC Asia 2005, Beijing, China, November 30 - December 03, 2005
> Member of the program committee of the 10th International Workshop on High-Level Parallel Programming Models and Supportive Environments, held in conjunction with the IPDPS 2005, Denver, Colorado, USA, April 04 - 08, 2005

Rolf Rabenseifner

> Program committee member for EuroPVM/MPI (since 2002)
> Program committee member of the Cray User Group (since 2000)
> Program committee member for PPGaMM Workshop at ICCS (since 2004)
> Program committee member of ParCo 2005, Malaga, Spain, 2005
> Program committee member of ISPA'05, Nanjing, China, 2005
> Member of the HPC Challenge Benchmark Award Committee (since 2005) (award at Supercomputing Conference Series)

Michael Resch

> Member of the Scientific Advisory Board of the Swiss Center for Scientific Computing (CSCS), Switzerland

- Member of the board of the Center of Competence for HPC of the State of Baden-Württemberg (hkz-bw), Germany
- Member of the steering committee of the German e-science initiative d-grid
- Member of the Board of the Computer Science Network Stuttgart / Informatik Verbund Stuttgart
- Chairman of the NEC User Group (NUG)
- Member of the board of the Virtual Dimension Center Fellbach (VDC)
- Reviewing for the European Commission
- Program committee member of the OECD Global Science Forum Workshop on Grids and Basic Research Programs, Sydney, Australia, September 25 - 27, 2005
- Program committee member of ParCo 2005, Malaga, Spain, September 13 - 16, 2005
- Scientific committee member of International Conference on Computational Science and Engineering (ICCSE), Istanbul, Turkey, June 27 - 30, 2005
- Program committee member of European Grid Technology Day, Brussels, Belgium, May 31, 2005
- Chairman of the award committee for the ISC'2005 Award, Heidelberg, Germany, June 21 - 24, 2005
- Co-Chairman of the 2nd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, Stuttgart, Germany, March 14 - 16, 2005
- Co-Chairman of the 1st Kazakh-German Advanced Research Workshop on Computational Science and High Performance Computing, Almaty, Kazahkstan, September 25 - October 01, 2005
- Co-Organizer and program chair of the 8th HLRS Metacomputing Workshop, Stuttgart, Germany, March 07 - 09, 2005

Sabine Roller

- Reviewing for Journal of Computational Physics

Stefan Wesner

- Program committee of Akogrimo workshop at Practical Aspects of Knowledge Management 2005, Vienna, Austria, December 02 - 03, 2005
- Program committee of GSEM 05 (Grid Services Engineering and Management), Erfurt, Germany, September 19 - 22, 2005
- Program committee of eChallenges e-2005, Ljubljana, Slovenia, October 19 - 21, 2005

8 List of Staff

Höchstleistungsrechenzentrum Stuttgart (HLRS)

> Mailto: <***nachname***>@hlrs.de
> www.hlrs.de
> fax: +49-711-68587209

		+49-711-685-
Director	Prof. Dr.-Ing. Michael ***Resch***	87200
Office	Margot ***Megerle***	87269
Deputy Director	Dipl.-Ing. Thomas ***Beisel***	87220
	Agnes ***Lampke***	87210
	Dipl.-Ing. Stefan ***Wesner***	64275
Staff Unit	Dipl.-Inform. Natalia ***Currle-Linde***	65801
	Dipl.-Ing. Isabel ***Loebich***	87207

HLRS-Administration

Head	Agnes ***Lampke***	87210
Staff	Ina ***Arnold***	87211
	Wolfgang ***Gerner***	87213
	Vera ***Kebsch-Müller***	65951
	Almuth ***Leeck***	87212
	Anja ***Schnepf***	87214

PR, Documentation, Library

	F. Rainer ***Klank***	62506

Department Software & Systems

Head	Dipl.-Ing. Thomas ***Beisel***	87220

> HPCN Production

Head	Dipl.-Ing. Thomas ***Beisel***	87220
Staff	Heinz ***Braun***	65978
	Dipl.-Ing. ***Peter Haas***	87223
	Dipl.-Ing. ***Bernd Krischok***	87221
	Dipl.-Ing. Dieter ***Raith***, Akad. Oberrat	87224
	Dipl.-Ing. (FH) Thomas ***Reissner***	65533
		87255
	Rolf A. ***Supper***	87225

> Numerical Methods and Libraries

Head	Dipl.-Math. Uwe ***Küster***	87232
Staff	Denis ***Altmann***	87230
	Tünde ***Erdei***	87234
	Elke ***Krumrück***	87231
	Dr.-Ing. Peter ***Lammers***	87233
	Dr.-Ing. Nina ***Shokina***	87236
	Manuela ***Wossough*** (on maternal leave)	

> Parallel Computing - Training & Application Services

Head	Dr. Rolf ***Rabenseifner***	65530
Staff	Dr.-Ing. Panagiotis ***Adamidis***	65529
	Dipl.-Ing. Dipl.-Phys. Norbert ***Ibold***	65803
	Dipl.-Ing. Hermann ***Knapp***	64542
	Dr. rer.nat. Heinz ***Pöhlmann***	65992
	Dipl.-Ing. Martin ***Winter***	65532

> Project & User Management, Accounting

Head:	Dipl.-Inform. Thomas ***Bönisch***	87222
Staff	Dirk ***Kröller***	65576
	Dipl.-Inf. Sedigeh ***Morrovat Pour***	65964
	Dr. rer.nat. Frank ***Zeller***	65932

Department Applications & Visualization

Head	Dipl.-Ing. Stefan ***Wesner***	64275

> Distributed Systems

Head	Dipl.-Ing. Stefan ***Wesner***	64275
Staff	Dipl.-Ing. Hubert ***Hérenger***	63894
	Dipl.-Inform. Bastian ***Koller***	63894
	Dipl.-Inform. Aenne ***Löhden***	64823
	Dipl.-Ing. Ignaz ***Müller***	64549
	Dipl.-Phys. Robert ***Piotter***	63824
	Dipl.-Inform. Lutz ***Schubert***	63894
	Dipl.-oec. Konrad ***Wulf***	65802

> Visualization

Head	Dipl.-Ing. Uwe ***Wössner***	65790
Staff	Dipl.-Ing. Martin ***Becker***	65982
	Dipl.-Inform. Michael ***Braitmaier***	65996
	Dipl.-Inform. Blasius ***Czink***	65805
	Dipl.-Inform. Andreas ***Kopecki***	65789
	Jutta ***Sauer***	65798
	Uwe ***Zimmat***	65968

> Applications, Models & Tools

Head	Dipl.-Inform. Rainer ***Keller***	65858
Staff	Dipl.-Math.Techn. Katharina ***Benkert***	65892
	Dipl.-Math. Bettina ***Krammer***	65890
	Dipl.-Ing. Peggy ***Lindner*** (on maternal leave)	
	Dr.-Ing. Sabine ***Roller***	65734
	MSc. Sunil Reddy ***Tiyyagura***	65799

hww

Managing Director	Prof. Dr.-Ing. Roland ***Rühle***	87263

High Performance Computing Center Stuttgart

Nobelstrasse 19 • 70569 Stuttgart, Germany

phone: +49-711-685-87269

fax: +49-711-68587209

info@hlrs.de • www.hlrs.de