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7.1.5.5 5th HLRS/hww Workshop on Scalable Global Parallel File Systems and HNF Europe Spring Meeting 2006 and OpenIB/RDMA Track
7.1.5.6 Cluster OpenMP Workshop
7.1.5.7 9th HLRS Metacomputing and Grid Workshop
7.1.5.8 High Performance Computing in Science and Engineering – The 9th and 10th Results and Review Workshop of the HPC Center Stuttgart (HLRS)
7.1.5.9 5th Teraflop Workshop
7.1.5.10 6th HLRS-NEC Teraflop Workshop
7.1.5.11 2nd D-Grid Security Workshop
7.1.5.12 6th HLRS/hww Workshop on Scalable Global Parallel File Systems HNF Europe Spring Meeting 2007 and OpenFabrics
7.1.5.13 16th CCSE Workshop on High Performance Computing on Vector-based Architectures - Recent Achievements and Future Directions
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I. OVERVIEW

Welcome to the bi-annual report of the High Performance Computing Center Stuttgart / Höchstleistungsrechenzentrum Stuttgart (HLRS). We are trying to give you a comprehensive overview about the years 2006 and 2007.

After having published annual reports over the last years we have decided to go for a bi-annual report. The reasons are mainly two: HLRS does a lot of publications of its scientific results every year. A summary of the most interesting results of our users is published as Transactions of the High Performance Computing Center Stuttgart at Springer every year. The book is a collection of about 40 papers that describe the work of our user community for every year. Meanwhile the series runs successfully for ten years. Over the last years we have complemented this series by other scientific publications as Proceedings of the High Performance Computing Center Stuttgart. These Springer publications summarize the research activities of HLRS and partner in the field of Teraflop computing and tools for High Performance Computing.

Given the growing number of annual report that mainly give a quantitative overview of activities we decided to summarize our main figures for the public every second year. This should still give a good overview of what is happening at HLRS.

The last two years covered by this report (2006-2007) were marked by a change in concept of High Performance Computing in Europe and Germany. With the idea of European HPC centers all European countries had to rethink their national strategies. In Germany over the last two years intensive discussions took place and have led to the founding of the Gauss Center for Supercomputing in 2007.

The GCS brings together the national HPC centers of Germany (Jülich, Munich and Stuttgart) into a single virtual organization supporting both users and research in HPC. For HLRS the creation of the GCS will intensify the level of national collaboration. Rest assured that our international activities both in Europe and abroad will not suffer from this.

At the same time the national Grid project D-Grid has initiated the creation of a national IT infrastructure in which large and small centers can be integrated seamlessly. For HLRS this again has triggered a closer collaboration with the overall German HPC community. HLRS has established itself as an important Grid-node in Germany both for HPC and beyond. Being the project leader for the D-Grid subproject InGrid HLRS has emphasized its leading role in engineering simulation on HPC systems.

With this I hope that our bi-annual report 2006/2007 is of interest to you and hope that you will support us in the coming years in creating better tools for simulation on High Performance Computing Systems.

Prof. Dr.-Ing. Michael M. Resch, Director of HLRS
2. LAND OF IDEAS / LAND DER IDEEN

When the Soccer World Championship 2006 drew attention to Germany in 2006 from sports fans all over the world Germany was proud of it but felt that the country should also show its potential for innovation to the outside world. As a consequence the president of Germany Dr. Horst Köhler and the Deutsche Bank initiated the concept of “land of ideas”. Every single day of 2006 one place in Germany would present its ideas to highlight innovations in every field in Germany and would be honored by an award. The program was so successful it was continued since.

In 2007 HLRS was chosen as one site of the land of ideas to present its work in the field of High Performance Computing to the general public. Together with its partners from research and industry HLRS opened its doors on July 21st 2007. HLRS was honored to welcome State Secretary of Science from the state of Baden-Württemberg Dr. Dietrich Birk, Mayor Gabriele Müller-Trimbusch from the city of Stuttgart, Dr. Rainer Grünenwald from Deutsche Bank and the president of the University of Stuttgart Prof. Dr. Wolfram Ressel for the awarding ceremony. The presentations of the open day - first shown to the guests of honor and opened to the general audience - focused on the usage of High Performance Computing in a variety of fields. Applications were shown using five virtual reality environments. The history of supercomputing at HLRS was presented showing the front panels of all systems that had been installed at Stuttgart over the last 20 years. Visitors were also shown to the computer room.

The open day was supported by children’s activities and drew a surprising large attention. Within a day more than 1000 visitors were shown the work of HLRS and partners. They had a chance to see Europe’s fastest supercomputer, drive a virtual Porsche and fly through applications in engineering, physics, chemistry, and medicine.
3. ORGANIZATION

The High Performance Computing Center Stuttgart (HLRS) of the University of Stuttgart supports researchers and industry with leading edge supercomputing technology. Services are supplied in collaboration with scientific and industrial partners through hkz-bw and hww GmbH. In European, national, and industrial projects HLRS conducts basic and applied research in HPC together with partners from research and industry.
3.1 STRUCTURE

Institut für Höchstleistungsrechnen
Software & Systems
 Thomas Beisel
BeWi
HPCN Production
Numerical Methods & Libraries
Project & User Management, Accounting
Parallel Computing, Training & Application Services

Applications & Visualization
Stefan Wesner
Applications, Models & Tools
Intelligent Service Infrastructures
Scalable Computing & Coupled Systems
Service Management & Business Processes

Director
Prof. Dr.-Ing. Michael Resch

Staff Unit

Administration
Agnes Lampke

Visualization

Head Office

Intelligent Service Infrastructures

Staff Finances

Public Relations

35 Research Ass. (Students)
27 Permanent Staff
47 Third Party funded Staff
3.2 STAFF

In 2006 and 2007 the staff numbers rise continuously. This is mainly due to an increase in external funding through projects while the number of permanent staff decreased substantially.

<table>
<thead>
<tr>
<th></th>
<th>Scientist</th>
<th>non Scientist</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>male</td>
<td>54</td>
<td>20</td>
<td>74</td>
</tr>
<tr>
<td>female</td>
<td>83</td>
<td>17</td>
<td>100</td>
</tr>
</tbody>
</table>

3.2.1 GENERAL INFORMATION

HLRS staff including students now totals 109 of which 2 are currently on parental leave. A breakdown of gender shows that percentage of female scientists is about a quarter. 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. Remarkable is, that in the last two years the number of applicants from female PhD students got back.

3.2.2 KEY STAFF CHANGES

DR. SABINE ROLLER

Dr. Sabine P. Roller is head of the Scalable Computing & Coupled Systems (SCCS) group since December 2006. The group is concerned with High Performance Computing, especially the Teraflop workbench project, the development of BLIS, and further user support on HPC applications. The other focus is on Grid computing, here especially the projects InGrid and bwGrid are to be mentioned. Dr. Sabine Roller studied Technical Mathematics at Universität Karlsruhe (TH), focussed on numerical methods for fluid flows and computer science. She got here PhD (Dr.-Ing.) in aerospace engineering from the faculty of Aerospace Engineering and Geodesy, University of Stuttgart in 2004. Her expertise is in all aspects of engineering applications on High Performance Computers. Special emphasis currently is on coupled applications [multi-scale and/or multi-physics] on hybrid systems.

BASTIAN KOLLER

Mr. Bastian Koller has joined HLRS in 2004 after receiving his diploma degree in computer science. He initially worked in the Distributed Systems group by Stefan Wesner and was assigned head of the Service Management and Business Processes group in 2007, which is involved in multiple EC research projects, namely BREIN, BeInGrid and NextGRID, as well as the FinGrid initiative. His main expertise is in the area of Service Level Agreements, where he is involved in many activities, within HLRS’ projects as well as in standardization bodies as the OGF Workinggroup GRAAP.

LUTZ SCHUBERT

Mr. Lutz Schubert holds a diploma in computer science from the University of Stuttgart. He joined HLRS back in 2004 as a research assistant of the Distributed Systems group by Stefan Wesner. Since 2007 he is head of the Intelligent Service Infrastructures group which is involved in various EC research projects, namely AkGoRiM0, BREIN, CoSpaces, ELeGi, ViRoLab and furthermore in the bwGrid initiative. His expertise lies in the domain of Service Oriented Architecture and Service Infrastructures.
3.2.3 Guest Scientists

- **October 1st – September 30th 2007**, 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.

- **January 16th – March 24th 2006**, Dr. Viktor Bannidi
  Faculty of Material Science and Engineering, University of Miskolc, Hungary. Guest in the HPC-Europa project collaborating with Dr. Panagiotis Adamidis. His work has the title "Simulation of transient heat conductivity under microgravity conditions".

- **March 1st – April 4th 2006**, Prof. Volodymyr SvJatny
  National Technical University Donetsk, Faculty for Computer Science Donetsk, Ukraine, was visiting as guest scientist working on his thesis.

- **March 6th – April 13th 2006**, Dr. Artur Marczewski
  Institute of Fundamental Technological Research, Polish Academy of Sciences, Poland, HPC-Europa guest. For the use of HPC systems, he was parallelizing his simulation software on numerical fatigue analysis of the cracked rotor and of hydraulic cylinders.

- **June 1st – August 31st 2006**, Hatem Ltaief
  Department of Computer Science, University of Houston, USA. Guest scientist working together with Prof. Marc Garbey on new algorithms in Metacomputing within the group “Applications, Models & Tools”.

- **July 1st – July 31st 2006**, Dr. Federico Boschetti
  Dipartimento di Scienze e Tecnologie della Salute, Trento University, Italy. HPC-Europa guest working at HLRS within the group “Applications, Models & Tools” on parallelizing Tiger-Search, developed at IMS, aiming at distributed and shared memory machines.

- **August 1st – October 30th 2006**, Dr. Alejandro Calderon Mateos
  Computer Science Department, University of Miskolc, Hungary. Guest in the HPC-Europa project collaborating with Dr. Panagiotis Adamidis. His work has the title "Simulation of transient heat conductivity under microgravity conditions”.

- **September 18th – September 29th 2006**, Joachim Zottl
  Multimedia and Distributed Systems, University of Vienna. HPC-Europa guest working in the group “Applications, Models & Tools” together on his parallel Eigensolver used for his PhD thesis.

- **November 27th – December 1st 2006**, Dr. Lars Grasedyck
  PI für Mathematik in den Naturwissenschaften, Leipzig.

- **February 1st – April 30th 2007**, Natalia B. Melnikova
  St. Petersburg State Polytechnical University, Department of Computer Technologies in Engineering, has worked as a guest scientist in parallelization of a large FEM program. She was also participating in the Parallel Programming Workshop at HLRS.

- **March 2nd – March 13th 2007**, Dr. Xing Cai
  Dr. Xing Cai of the Simula Research Center, Norway was visiting the working group “Applications, Models & Tools”, working with Rainer Keller to evaluate and optimize the performance of his hybrid Tsunami simulation, an MPI parallel application written in C++.

- **March 5th – May 31st 2007**, Enol Fernandez
  Mr. Fernandez is a researcher at the Autonomous University of Barcelona (UAB) and was working with Sven Stork of the working group “Applications, Models & Tools” within the frame of the INT.EU.Grid project.

- **April 16th – May 11th 2007**, Margarida Boiarciuc
  Mrs. Boiarciuc, a researcher of the University of Orleans, collaborated with Alexander Schulz to performance-analyse her application using Paraver.

- **June 1st – July 4th 2007**, Prof. Marc Garbey
  University of Houston, Texas, USA, works on fault tolerant simulation techniques and coupling decomposed domains by special operators reducing the amount of data to be transferred. Other parts of his work are dedicated to the fast simulation of the blood flow in the human body vessel systems directly using the data from computer tomograph scans.

- **July 1st – July 31st 2007**, Prof. Barbara Chapman
  Dr. Chapman of the University of Houston has been visiting the HLRS to work with Rainer Keller and Rolf Rabenseifner on various items of the OpenMP standard. She has been integrated into the working group “Applications, Models & Tools”.

- **September 30th – December 14th 2007**, Javier Garcia
  Mr. Garcia is a researcher of the HPC-Europa project visiting the the working group “Applications, Models & Tools”, working with Alexander Schulz, Rainer Keller and Rolf Rabenseifner on parallel filesystems.

- **November 2nd – January 3rd 2007**, Margarita Boiarciuc
  Mrs. Boiarciuc, a researcher of the University of Orleans, collaborated with Alexander Schulz to performance-analyse her application using Paraver.
4. SYSTEMS

HLRS offers his clients of the scientific and industrial area a variety of supercomputers. Today the IBM BladeCenter with 428 nodes and a capacity of 29.32 TFlop/s is the most efficient one. Additive HLRS is the owner of the fastest vector computer NEC SX-8 with 576 processors and 12 TFlop/s. This section describes systems that are available to the users of the HLRS.
4.1 NEC SX-8 576 M72
HLRS builds a supercomputer by clustering NEC SX-8 nodes using NEC’s high performance crossbar interconnect. This system will deliver more than 5 TFLOPS sustained performance on a HLRS customers CFD application. System production started on March 23rd, 2005. The specification of the system is:

<table>
<thead>
<tr>
<th>CPU</th>
<th>NEC SX-8 2GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of CPUs</td>
<td>8 per node total of 576</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>12.7 TFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>9.2 TB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>NEC IXS 16 GB/s bidirectional</td>
</tr>
<tr>
<td>Disk Space</td>
<td>160 TB</td>
</tr>
</tbody>
</table>

In December 2007 an additional NEC SX-8R node has been installed. This system has double the functional units and offers a peak performance of 280 GFLOPS.

4.2 NEC SX-6 40
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.

<table>
<thead>
<tr>
<th>CPU</th>
<th>NEC SX-6 565 MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of CPUs</td>
<td>8 per node total of 40</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>361 GFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>512 GB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>NEC IXS 16 GB/s bidirectional</td>
</tr>
<tr>
<td>Disk Space</td>
<td>160 TB</td>
</tr>
</tbody>
</table>

4.3 D-GRID COMPUTING ENVIRONMENT
In December 2006 HLRS installed a computing environment in the frame of the D-GRID initiative. This environment consists of three parts:

- Storage system with 100 TB Raid
- Compute cluster 28 node Intel Woodcrest @ 2,8 GHz
- IBM Cell blades 7 nodes IBM Cell processor blades

In December 2007 the compute cluster has been upgraded:

<table>
<thead>
<tr>
<th>CPU</th>
<th>Intel Harpertown 2.6 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Cores</td>
<td>3472</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>~36 TFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>6.8 TB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Infiniband DDR</td>
</tr>
</tbody>
</table>

4.4 OPTERON CLUSTER
The service of the Cray Opteron Cluster installed in 2Q 2004 has been terminated in 4Q 2007. In co-operation with the industrial partner Porsche AG, HLRS established a new cluster based on AMD’s server processor. Due to different needs of automotive applications, the cluster has different types of interconnects and nodes.

<table>
<thead>
<tr>
<th>CPU</th>
<th>AMD Opteron 2.8 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of CPUs</td>
<td>96</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>540 GFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>192 GB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>RapidArray</td>
</tr>
</tbody>
</table>

4.5 CRAY XDI
Due to the high usage of industrial partners and increasing demands for crash simulation HLRS extended this System.

<table>
<thead>
<tr>
<th>CPU</th>
<th>AMD Opteron 2.8 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of CPUs</td>
<td>96</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>540 GFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>192 GB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>RapidArray</td>
</tr>
</tbody>
</table>
4.6 INTEL CLUSTER PLATFORM

Together with its partners NEC and Intel, HLRS replaced 32 Nodes with dual core CPUs of the latest server processor family. The specifications of the system are:

<table>
<thead>
<tr>
<th>CPU</th>
<th>Intel Xeon EM64T, 3.2 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Cores</td>
<td>460</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>3,7 TFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>618 GB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Infiniband</td>
</tr>
<tr>
<td>Disk Space</td>
<td>1 TB</td>
</tr>
</tbody>
</table>

4.7 D-GRID STORAGE

In addition to the computing hardware, a storage system was installed as a part of the distributed D-Grid storage environment. It consists of two storage servers and a Datadirect Networks high performance storage device.

<table>
<thead>
<tr>
<th>Storage Servers</th>
<th>Intel Xeon 5130</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU</td>
<td>2x2 cores per server, 8 in total</td>
</tr>
<tr>
<td>Memory</td>
<td>2x16 GB GB</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Infiniband</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Storage System</th>
<th>DDN 9550 Couplet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head</td>
<td>Infiniband</td>
</tr>
<tr>
<td>Host Interconnect</td>
<td>Fibre Channel</td>
</tr>
<tr>
<td>Drive Interconnect</td>
<td>SATA</td>
</tr>
<tr>
<td>iDrive Technology</td>
<td>120 TB</td>
</tr>
</tbody>
</table>

4.8 COMMON SERVER CUSS

The Common Ulm Stuttgart Server CUSS is a common effort of the Communication and Information Center Ulm (KIZ) and HLRS to provide the users of both universities with general purpose computing power. The co-operation lasts since 2001. The machines are located and operated in Ulm. The users have access to a large variety of packages. The actual equipment consists in 36 IBM-AMD-Opteron servers, 4 SunFire 2900 and 2 SunFire V40z.
5. USER SUPPORT

The goal of HLRS is to offer the optimal supercomputer to different user groups of the scientific and industrial area and to support programmers and users with the optimal usage of them. Therefore HLRS offers the necessary infrastructure as well as user and programming support.
5.1 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 blood flow simulations as well as traditional engineering as 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 years 2006 and 2007 is due to the lack of a competitive system for other fields. As part of the collaboration of NEC and HLRS increased user support for other fields in tuning codes for vector based systems is provided.

5.1 USER PROJECTS

In total 72 (2006) / 61 (2007) research projects were active on the national supercomputer systems of HLRS and actively managed and administrated. Of these 49 / 54 were running projects and 23 / 7 were new projects in the years 2006 and 2007.

Additionally 12 (2006) / 12 (2007) research projects from industry in the area of Computational Fluid Dynamics and 2 / 1 research projects from industry in the area of Structural Mechanics reveal our close co-operation with industrial partners in the years 2006 and 2007.
5.2 USAGE OF THE SYSTEMS

5.2.1 SYSTEM USAGE BY FIELD

The strong role of CFD is emphasized again when looking at system usage. In the years 2006 and 2007 more than 75% go to projects in this field. The second strongest field is solid state physics together with physics, followed by chemistry. The reader has to keep in mind, however, that the NEC SX-8 has a far higher level of performance than the Cray Opteron Cluster. Hence the percentage of CPU time used on the NEC SX-8 is about 94% of the total CPU time provided in 2006. It is interesting to note that the system usage in non-CFD fields has doubled compared to 2005. It was one of the goals of the Teraflop Workbench Project to achieve efficient usage of the NEC SX-8 system for a broader range of codes.

5.2.2 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 nationwide 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 (7.0%, more than tripled in 2006) indicates the international role of HLRS.

2006

System usage by state (percentage)

- Baden-Württemberg
- Bayern
- European Union
- Federal Research Center
- Hessen
- Niedersachsen
- Nordrhein-Westfalen
- Sachsen
- Schleswig-Holstein
- Thüringen

2007

System usage by state (percentage)

- Baden-Württemberg
- Bayern
- European Union
- Federal Research Center
- Hessen
- Niedersachsen
- Nordrhein-Westfalen
- Sachsen
- Schleswig-Holstein
- Thüringen
5.3 PARALLEL DEVELOPMENT TOOLS

In order to provide its users better support for the program development, HLRS has improved its Parallel Programming Tools support. This ranges from various tools in the area of debugging to performance analysis, but also includes several underlying communication libraries and communication paradigms.

The following table lists the available and supported software on various platforms. Please consult the “Services”-Webpage http://www.hlrs.de/organization/amt/services for further information on installation and usage of the software tools.

<table>
<thead>
<tr>
<th>Debugging &amp; Parallel Verification Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>DDT</td>
</tr>
<tr>
<td>Totalview</td>
</tr>
<tr>
<td>Thread Checker</td>
</tr>
<tr>
<td>Marmot</td>
</tr>
<tr>
<td>Valgrind</td>
</tr>
<tr>
<td>OPT</td>
</tr>
<tr>
<td>Vampir + VampirNG</td>
</tr>
<tr>
<td>Paraver</td>
</tr>
<tr>
<td>Trace Collector and Analyzer [Intel Cluster Tk]</td>
</tr>
<tr>
<td>Thread Profiler</td>
</tr>
<tr>
<td>Vtune</td>
</tr>
<tr>
<td>Kojak</td>
</tr>
<tr>
<td>Eclipse</td>
</tr>
<tr>
<td>OpenMP in various compilers</td>
</tr>
<tr>
<td>UPC</td>
</tr>
<tr>
<td>Open MPI</td>
</tr>
<tr>
<td>Intel MPI [Intel Cluster Tk]</td>
</tr>
<tr>
<td>Global Arrays</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Performance Libraries and Analysis Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>OPT</td>
</tr>
<tr>
<td>Vampir + VampirNG</td>
</tr>
<tr>
<td>Paraver</td>
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<tr>
<td>Trace Collector and Analyzer [Intel Cluster Tk]</td>
</tr>
<tr>
<td>Thread Profiler</td>
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<tr>
<td>Vtune</td>
</tr>
<tr>
<td>Kojak</td>
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<tr>
<td>Eclipse</td>
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<tr>
<td>OpenMP in various compilers</td>
</tr>
<tr>
<td>UPC</td>
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<tr>
<td>Open MPI</td>
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<tr>
<td>Intel MPI [Intel Cluster Tk]</td>
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<tr>
<td>Global Arrays</td>
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<table>
<thead>
<tr>
<th>Development Environment</th>
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<tbody>
<tr>
<td>Parallel Programming Compilers and Libraries</td>
</tr>
</tbody>
</table>

5.4 APPLICATION PACKAGES

The HLRS also provides a strong support in application software packages. These packages are used partially for pre and post processing but also as standalone simulation software. On HLRS supercomputers, clusters, pre-processors and the CUSS system following packages are available:

#### COMPUTATIONAL FLUID DYNAMICS
- CFX, FIDAP, FIELDVIEW, FIRE, FLUENT, FLUXEXPERT, GAMBIT, GRIDGEN, ICEM-CFD, POLYFLOW, STAR-CD, SWIFT, TGRID

#### STRUCTURAL MECHANICS
- ABAQUS, ANSYS, HyperWorks, LS-DYNA, MSC.Patran, PERMAS

#### COMPUTATIONAL CHEMISTRY
- GAMESS-US, GAUSSIAN, MOLPRO, MOPAC, TURBOMOLE

5.5 USER WORKSHOPS

<table>
<thead>
<tr>
<th>Date</th>
<th>Organizer</th>
<th>Location</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mar. 01-03, 2006</td>
<td>ZIH</td>
<td>Dresden</td>
<td>Parallel Programming</td>
</tr>
<tr>
<td>Mar. 13-17, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Iterative Linear Solvers and Parallelization</td>
</tr>
<tr>
<td>Mar. 20-21, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>NEC SX-8 Usage and Programming</td>
</tr>
<tr>
<td>Apr. 03-07, 2006</td>
<td>Fak. Math. &amp; Inf.</td>
<td>Kassel</td>
<td>Introduction to Computational Fluid Dynamics</td>
</tr>
<tr>
<td>Aug. 28-Sep. 08, 2006</td>
<td>ICT, HLRS</td>
<td>Novosibirsk, Russia</td>
<td>3rd Russian-German School on Parallel Programming using High Performance Computation Systems</td>
</tr>
<tr>
<td>Aug. 23-25, 2006</td>
<td>CSCS</td>
<td>Manno Switzerland</td>
<td>Parallel Programming</td>
</tr>
<tr>
<td>Sep. 13-17, 2006</td>
<td>LRZ</td>
<td>Garching</td>
<td>Iterative Linear Solvers and Parallelization</td>
</tr>
<tr>
<td>Sep. 18-22, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Introduction to Computational Fluid Dynamics</td>
</tr>
<tr>
<td>Sep. 25-26, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Parallel Programming with MPI</td>
</tr>
<tr>
<td>Sep. 27, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Shared Memory Parallelization with OpenMP</td>
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<tr>
<td>Sep. 28-29, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Advanced Topics in Parallel Programming</td>
</tr>
<tr>
<td>Nov. 27-29, 2006</td>
<td>NIC</td>
<td>Jülich</td>
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<td>Feb. 12-15, 2007</td>
<td>ZIH</td>
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<td>Mar. 05-09, 2007</td>
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<td>Mar. 28-29, 2007</td>
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<td>Stuttgart</td>
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<td>Aug. 08-10, 2007</td>
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<td>Manno Switzerland</td>
<td>Parallel Programming</td>
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<tr>
<td>Sep. 17-21, 2007</td>
<td>LRZ</td>
<td>Garching</td>
<td>Iterative Linear Solvers and Parallelization</td>
</tr>
<tr>
<td>Oct. 08-09, 2007</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Distributed Memory Parallelization with MPI</td>
</tr>
<tr>
<td>Oct. 10, 2007</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Shared Memory Parallelization with OpenMP</td>
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<tr>
<td>Oct. 11-12, 2007</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Advanced Topics in Parallel Programming</td>
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<tr>
<td>Oct. 15-19, 2007</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Introduction to Computational Fluid Dynamics</td>
</tr>
<tr>
<td>Nov. 26-28, 2007</td>
<td>NIC</td>
<td>Jülich</td>
<td>Parallel Programming</td>
</tr>
</tbody>
</table>
In these workshops in 2006 and 2007, each year 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 directive of OpenMP, of iterative solvers or Computational Fluid Dynamics.

### SHORT DESCRIPTIONS OF WORKSHOPS

#### 5.5.1 INTRODUCTION TO PARALLEL PROGRAMMING

Mar. 01-03, Aug. 23-25, Nov. 27-29, 2006, Feb. 12-15, Aug. 08-10 and Nov. 26-28, 2007 at ZIH, CSCS and NIC: 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) and NIC/ZAM (Jülich), and CSCS (Manno) in collaboration with HLRS. Course language is German at ZIH and NIC, and English at CSCS.

#### 5.5.2 ITERATIVE LINEAR SOLVERS AND PARALLELIZATION

Mar. 13-17, 2006, Mar. 12-16, 2007 at HLRS and Sep. 13-17, 2006, Sep. 17-21, 2007 at LRZ: 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.

#### 5.5.3 NEC SX-8 USAGE AND PROGRAMMING

Mar. 20-21, 2006 and Mar. 28-29, 2007 at HLRS: The focus is on vectorization and optimization on the NEC SX-8 system at HLRS (1st day), and on I/O and optimization of iterative solvers (2nd day). The participants learn about the configuration of the multi-teraflop NEC SX-8 system at HLRS and how to use this cluster of vectorizing shared memory nodes. One focus is an introduction in vectorization. More experienced users can learn how to optimize programs based on performance measurements. The second day is focused on I/O and the optimization of application programs.

#### 5.5.4 INTRODUCTION TO COMPUTATIONAL FLUID DYNAMICS

Apr. 03-07, Sep. 18-22, 2006, Mar. 05-09 and Oct. 15-19, 2007 at University of Kassel and 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).
5.5.5 PARALLEL PROGRAMMING WORKSHOP

Sep. 25-26, 2006 and Oct. 08-09, 2007 at HLRS: Parallel Programming on distributed memory systems with the Message Passing Interface (MPI-1 and MPI-2), domain decomposition, load balancing and parallel debugging is presented. Hands-on sessions (in C and FORTRAN) allow users to immediately test and understand the basic constructs of the MPI. Course language is English.

Sep. 27, 2006 and Oct. 10, 2007 at HLRS: Shared Memory Parallelization with OpenMP, verification and tuning of the parallelization is presented. Hands-on sessions (in C and FORTRAN) allow users to immediately test and understand OpenMP and verification and profiling tools. Course language is English.

Sep. 28-29, 2006 and Oct. 11-12, 2007 at HLRS: The focus is on advanced parallel programming with MPI and OpenMP. Hands-on sessions are included. Course language is English.

5.5.6 RUSSIAN-GERMAN SUMMER SCHOOLS

Jun. 28-Sep. 08, 2006, Novosibirsk, Russia: The third school was jointly organized by the Institute for Computational Technologies (ICT), Russian Academy of Sciences, Siberian Branch and HLRS. The school was given in two parts, a one week basic introduction to parallel programming and second week covering advanced topics of 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. Many participants gave also a short introduction of their current scientific work. Additionally, practical sessions on the cluster of ICT allowed the participants to deepen their new knowledge. The attendees came from all over Russia as well as from several east European countries like Georgia and Belarus.

Jul. 09–20, 2007, Novosibirsk, Russia: The forth school was again organized by the Institute for Computational Technologies (ICT), Russian Academy of Sciences, Siberian Branch and HLRS. The already proven setup with two parts, one week of basic introductions to parallel programming and a second week covering advanced topics was kept. The focus of the second week in the forth school 2007 has been coupled applications. Thus, all relevant topics from a view point of parallel programming on coupled applications have been covered. For the second week, participants of last years schools have shown again interest in this years topic and attended the advanced part.

5.6 SOFTWARE VENDER PRESENTATIONS

Furthermore, several area-specific software vendor presentations and workshops took place at HLRS:

<table>
<thead>
<tr>
<th>Date</th>
<th>Topic</th>
<th>Short Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nov. 29, 2007</td>
<td>AVL-FIRE</td>
<td>Modelling of complex flows</td>
</tr>
<tr>
<td>Nov. 19, 2007</td>
<td>Pointwise V16</td>
<td>Mesher methods</td>
</tr>
<tr>
<td>Jun. 12, 2007</td>
<td>COMSOL V3.3</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
<tr>
<td>Jun. 11, 2007</td>
<td>COMSOL V3.3</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
<tr>
<td>Feb. 07, 2007</td>
<td>Gridgen</td>
<td>Hybrid meshing methods</td>
</tr>
<tr>
<td>Dec. 13, 2006</td>
<td>COMSOL V3.3</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
<tr>
<td>Dec. 12, 2006</td>
<td>COMSOL V3.3</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
<tr>
<td>Jul. 11, 2006</td>
<td>ANSYS-CFX</td>
<td>Multi-purpose CFD program, fluid structure interaction</td>
</tr>
<tr>
<td>May 23, 2006</td>
<td>COMSOL V3.2</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
<tr>
<td>May 22, 2006</td>
<td>COMSOL V3.2</td>
<td>Multi-physics CFD, chemistry, etc. and user specific part</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Lecturer</th>
<th>Title of Lecture</th>
<th>Semester</th>
<th>University</th>
</tr>
</thead>
<tbody>
<tr>
<td>Martin Bernreuther</td>
<td>Molecular Dynamics and Lattice-Boltzmann Methods</td>
<td>WS 2007/2008</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Peter Haas</td>
<td>Microprocessors</td>
<td>WS 2006/2007</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Uwe Küster</td>
<td>Numerical Methods for Supercomputers</td>
<td>WS 2006/2007</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Matthias Müller</td>
<td>C++ for Scientific Computing</td>
<td>SS 2006</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science III in Mechanical Engineering</td>
<td>SS 2006, SS 2007</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science III in Automotive Engineering</td>
<td>SS 2006, SS 2007</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science III in Technology Management</td>
<td>SS 2006, SS 2007</td>
<td>Univ. of Stuttgart</td>
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<td>Michael Resch</td>
<td>Simulation on Supercomputers</td>
<td>SS 2004, SS 2007</td>
<td>Univ. of Stuttgart</td>
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<tr>
<td>Sabine Roller, Mark Haas [IAG]</td>
<td>Computer Practical on Numerical Gasdynamics</td>
<td>SS 2007</td>
<td>Univ. of Stuttgart</td>
</tr>
</tbody>
</table>

Sabine Roller, Mark Haas [IAG]

Computer Practical on Numerical Gasdynamics
SS 2006
WS 2005/2006
Univ. of Stuttgart

Michael Schliephake

Distributed Systems
WS 2007/2008
Univ. of Cooperative Education Stuttgart

Stefan Schwarzer, Hubert Hérenger

C++ for Scientific Computing
SS 2007
Univ. of Stuttgart

Stefan Wesner, Robert Piotter, Michael Resch

Software Development for Scientific and Technical Applications
WS 2006/2007
WS 2007/2008
Univ. of Stuttgart

Uwe Wössner

Visualization of Technical and Scientific Data
WS 2006/2007
WS 2007/2008
Univ. of Stuttgart
6.2 PHD THESSES

1. THOMAS BÖNISCH
The PhD thesis was developed in the frame of the collaborative research center 256 (Sonderforschungsbereich 256) which was focussed on re-entry phenomena of reusable space vehicles. The work presents the parallelization of a flow simulation code which was ported to several parallel systems at HLRS. In order to handle complex geometries a multi-block approach was chosen. This allows keeping the regular data structures of the original sequential code and at the same time model complex geometries. Load balancing for the multi-block codes was handled as well as communication problems.

2. NATALIA CURRLE-LINDE
As to possible applications in industry, there is a particular demand for Grid technology in sectors which require high processing capacities and where tasks can be easily parallelized. Here Grid technology assumes a strategic character and might in the near future be established in many sectors as a universal computing instrument. However, the utilization of Grid technology in science and industry is not that easy. On the one hand, there are only few Grid infrastructures which are really functional and in production state, and in many cases the time required to develop and validate programs of complex experiments for the Grid would exceed the actual execution time of the experiment itself. On the other hand, the generation of Grid configurations requires a comprehensive knowledge in the fields of programming and Grid technology, so that complex programs for Grid experiments usually cannot be developed by the scientist themselves. This work presented a powerful integrated system for the creation and execution of complex modeling experiments in the Grid. The integrated system is composed of GriCoL, an abstract language for the description of Grid experiments, and SEGL, a problem solving environment capable of utilizing the resources of the Grid to execute and manage complex scientific Grid applications. The new technology has a sufficient level of abstraction to enable a user, without knowledge of the Grid or parallel programming, to efficiently create and execute complex modeling experiments.

3. PEGGY LINDNER
This work presents the concept and implementation of a Grid Configuration Manager (GCM), a tool developed to hide some of the complexity of Grid environments from the end-user. The central objective of GCM is to ease the handling of computational Grid environments for end-users and application developers, by abstracting the steps necessary for submitting computational jobs and implementing them for various Grid software environments. The GCM assists users during three phases of the execution of an application: definition of a Grid configuration, job submission and monitoring. Furthermore, GCM supports the generation and management of distributed multi-site jobs on the basis of the communication library PACX-MPI. The Grid Configuration Manager integrates a performance based resource brokering mechanism. Under consideration of predicted application performance for a given pool of machines, the GCM can decide which combination of machines to use. The Grid Configuration Manager was tested and deployed in various scenarios. It has been shown, that the handling of scientific, computational jobs in heterogeneous Grid environments was significant easier and the determination of the execution environment was facilitated for users by utilization of the GCM.
In total 20 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.


8. Eduard Burghardt: Erweiterung eines Strömungslösers von 2D auf 3D.


15. Dominik Rössler: Optimierung eines MD-Simulationsprogramms für inhomogene Molekülverteilungen.


a) at the VIS (Prof. Ertl) and IPVS/SgS in co-operation with HLRS
b) at the IPVS-SgS (Prof. Bungartz / Prof. Bastian) in co-operation with HLRS and Bosch GmbH
c) at the IPVS-/SgS (Prof. Bungartz / Prof. Bastian) in co-operation with HLRS
d) COMMAS master thesis, in co-operation with HLRS
e) at the VIS (Prof. Ertl) in co-operation with HLRS
f) at the IPVS-SgS (Prof. Bastian) in co-operation with HLRS.
6.4 STUDENT RESEARCH PROJECT THESES

1. LARS FRENZEL: Konzeption und Entwicklung eines objektorientierten Particle Tracers

2. KASPAR SCHMOLL: Visualisierung des Schaltverhaltens von schweren Nutzfahrzeugen mit automatisiertem Schaltgetriebe durch VRML und JavaScript

3. PAUL ILLEG: Modellierung und numerische Simulation hydraulischer und pneumatischer Ventilströmungen zur Quantifizierung des Einflusses von Fertigungsstreuungen

4. ALEXANDER GROMER: Verbesserung der Prognosegüte von Verzögerungssignalen und Auslegung von Sensororten zur Crashschwereunterscheidung beim Seitenkollision

5. PATRICK MONTHEU: Realisierung einer Erweiterung des Axis Toolkits zum Transport von Kontextdaten Realising an Extension of the Axis Toolkit to Transport Context Data

6. MIRIAM PULZ: Realisierung einer grid-basierten Web Service-Anwendung zur Anbindung verschiedener vertreiter Datenquellen Design and Implementation of a grid-based Web Service Application to manage different distributed Data Resources

7. JIN GONG: Bestimmung der Eingangsimpedanz einer Abgasanlage: Entwurf eines Prüfstands und Entwicklung einer Auswertesoftware measurement of the input impedance of an exhaust system: design of an experimental setup and development of an analysing software

8. MELANIE STRAUCH: Textur-Analyse mit Gabor Wavelets

9. JIANG LONG: Planung und Implementierung eines Prüfsignalgenerators mit Matlab/Simulink und xPC-Target Conception and Implementation of a Test Signal Generator using Matlab/Simulink and xPC-Target

10. ARMIN ZIRKEL: Untersuchung von Geometrie- und Treibmengevariationen bei einer Saugstrahlpumpe

11. SASCHA KRETER: Modellierung und Simulation des Wärme- und Stoffübergangs bei der Herstellung von Preparats für faserverstärkte Metal Matrix Composites [MMC] durch thermische Spritzverarbeitung

12. HUANG JIANYE: Entwicklung eines Werkzeugs für automatisierte Datenreduktion mittels Kurvenanpassungsmethoden

13. MANUEL HASERT: Interpolations- und Ortsbestimmungsmethoden auf unregelmäßigen Netzen

14. FLORIAN SEYBOLD: Parallele Partikel-schwarm Optimierungsalgorithmen unter Verwendung von eindimensionalen Suchmethoden
7. RESEARCH

HLRS is involved in a variety of scientific projects in the international and national field. This section covers in more detail the projects that were running or newly started in 2006. A complete list of currently running projects includes.
## 7.1 Projects

<table>
<thead>
<tr>
<th>Project</th>
<th>Funded by</th>
<th>Duration</th>
<th>Web Page</th>
<th>Project</th>
<th>Funded by</th>
<th>Duration</th>
<th>Web Page</th>
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<td>European Commission</td>
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<td>Akogrimo</td>
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<td>01.07.2004-30.06.2007</td>
<td><a href="http://www.mobilegrids.org">http://www.mobilegrids.org</a></td>
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<td>NextGRID</td>
<td>European Commission</td>
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<td>TrustCoM</td>
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<td>01.02.2004-31.01.2007</td>
<td><a href="http://www.eu-trustcom.com">http://www.eu-trustcom.com</a></td>
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<td>BEInGRID</td>
<td>European Commission</td>
<td>01.06.2006-30.11.2009</td>
<td><a href="http://www.beingrid.eu">http://www.beingrid.eu</a></td>
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<td>CoSpaces</td>
<td>European Commission</td>
<td>01.05.2006-31.10.2009</td>
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</tbody>
</table>
7.1 NATIONAL

7.1.1 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 geo-thermic project in Bad Urach and the test-case South in Stuttgart.

PARTNERS
Center for Applied GeoScience, University of Tübingen, HLRS

7.1.2 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 Aerothermodynamik, Universität Stuttgart; IHS Universität Stuttgart

7.1.3 DISSIPATIVE-PARTICLE-CODE

ABSTRACT
Dissipative-Particle-Dynamics is capable for simulation of production relevant mechanisms like filling, coating and 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); Höchstleistungsrechenzentrum der Universität Stuttgart (HLRS)

7.1.4 SFB 716 DYNAMIC SIMULATION OF SYSTEMS WITH LARGE NUMBERS OF PARTICLES

ABSTRACT
The collaborative research programme SFB716 is a project working on dynamic simulations of systems with large numbers of particles. In total nine institutes of various research areas at the University of Stuttgart are working together to solve new scientific challenges on high-performance computers. The HLRS is participating with two sub-projects, D.1 and D.2, which are working on new software approaches to adapt to large numbers of particles. One is more in the algorithmic approach to handle large-scale simulations, while the latter is working on porting and optimizing molecular dynamics simulations onto new multi-core hardware architectures, such as the IBM Cell processor.

PARTNERS
Fraunhofer-Institut für Werkstoffmechanik (IWM); Institut für Mikrosystemtechnik, Albert-Ludwigs-Universität Freiburg (IMTEC); Höchstleistungsrechenzentrum der Universität Stuttgart (HLRS)

7.1.5 SFB 374 RAPID PROTOTYPING

ABSTRACT
The SFB 374’ 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.

PARTNERS

7.1.6 INGRID

ABSTRACT
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 Information Technology, University of Siegen, Computer Science, Philipps-University of Marburg, Wasy Gesellschaft für wasserwirtschaftliche Planung und Systemforschung, Access e.V.

7.1.7 FINGRID

ABSTRACT
FinGrid is one of the projects of the German D-Grid Initiative, funded by the Ministry for Education and Research (Bundesministerium für Bildung und Forschung).
The aim of FinGrid (Financial Business Grid) is
to identify and develop financial services and
business processes of the financial sector
that can be supported and simpler handled
by basing them on grid based applications.
Furthermore it is aimed to identify business
sectors in the financial environment, which
are currently not yet targeted by applications
but could be of high value when enabling
them with grid technology.
The FinGrid project envisages two main as-
psects. The first aspect is to evaluate the eco-
nomic potential of grid applications by em-
pirical analysis and to generate new aspects
of knowledge out of this. The second aspect
is to develop three prototypes which refer to
the exposed potential to give a proof-of-con-
cept. Hereby, the new theoretical knowledge
for grid applications for the financial sector
becomes practical appropriable.
Research in this project is split up into different
clusters, closely interconnected which each
other, to ensure a consolidated result at the
end of the project. HLRS is leading the Cluster
for research in the Service Level Agreement
topic. The current understanding of SLAs in
the community is limited to express certain
Quality of Service boundaries for the pro-
vision of the service. However the problem
that needs to be solved for deploying SLAs
in the area of financial services provision is
to leverage the SLAs between consumer and
provider on the level of electronic contracts
rather than low level infrastructure metrics.
For that purpose a SLA-Management-System
targeting all the requirements of a financial
business grid will be developed.
PARTNERS
The FinGrid consortium consists of five
research partners and six business partners.
Research partners: Johann Wolfgang Goethe-
University of Frankfurt and the E-Finance Lab
(Project Leader), High Performance Com-
puting Center Stuttgart (HLRS), Philipps-
University of Marburg, University of Siegen.
Business Partners: Data Synapse, Deutsche
Bank, Dresdner Bank, Finanz IT, PA Consulting
Group, IBM
7.I.8 DAAD EXCHANGE PROGRAMME
In order to strengthen the collaboration of
HLRS and the University of Tennessee, Knox-
ville [UTK] in the area of MPI-development, a
collaborative initiative has been started with
the help of the German Academic Exchange
Service (DAAD). In the frame of the project,
Dr. Graham Fagg has visited HLRS, while
Bettina Krammer and Rainer Keller from
HLRS have visited UTK to work on Marmot
and Open MPI.
7.1.2 INTERNATIONAL (EUROPEAN AND OTHERS)

7.1.2.1 HPC-EUROPA

ABSTRACT
The HPC-Europa project was an EU-funded project within the 6th Framework Programme (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 programme (TA), accompanied by several networking activities (NA) and joint research activities (JRA).

While the first and biggest part is the visitor programme, the other two parts go hand in hand with this activity by developing new solutions, from 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.

Overall 120 guest scientists from European and other countries have been working in Germany at various institutions using computers at HLRS. Most of the visitors were hosted at institutes of the University of Stuttgart, some visitors also went to Freiburg, Karlsruhe, Munich and also the RWTH Aachen. The largest fraction of computational time was spent on the large clusters, while professional users utilizing the resources of the Grid to execute and manage complex scientific Grid applications. HLRS mainly contribute with its experience in the area of programming models and of Grid Systems. HLRS has developed a powerful integrated system for the creation, execution and monitoring of complex modelling experiments in the Grid. The integrated system is composed of GriCoL, a universal abstract language for the description of Grid experiments, and SEGL, a problem solving environment capable of utilizing the resources of the Grid to execute and manage complex scientific Grid applications.

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

7.1.2.2 INT.EU.GRID

ABSTRACT
The main purpose of this project is, as suggested by its name, to support large-scale interactive, parallel applications within a European Grid, allowing computation on distributed compute resources, as well as interactive visualization and simulation steering on selected applications using the Migrating Desktop (MD) software. The major focus with regard to the Grid-software stack deployed is compatibility and interoperability at the middleware-level with LCG and the EGEE-II project, based on gLite-3.0. The computational infrastructure operating at the eleven computational sites includes several production clusters based mainly on Intel Xeon and dual AMD Opteron clusters with a total of around 500 processors. The Message Passing Interface (MPI) will be used as the main parallelization paradigm for intra- and inter-cluster computing.

HLRS, being a partner in the Open MPI consortium, will be responsible for the integration and support of the MPI infrastructure in the testbed and production clusters. As parallel middleware libraries, Open MPI, PACX-MPI and the analysis and checking tool Marmot will be supported on the platforms.

PARTNERS
CSIC, LIP, PSNC, FZK, UAB, CYFRONET, GUP, TCD, CESGA, IISAS, ICM, BIFI, HLRS

7.1.2.3 COREGRID

ABSTRACT
The European Research Network on Foundations, Software Infrastructures and Applications for large scale distributed, Grid and Peer-to-Peer Technologies. 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 (161 permanent researchers and 164 PhD students) from 41 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
- architectural issues: scalability, dependability, adaptability
- Grid information, resource and workflow monitoring services
- resource management and scheduling
- Grid systems, tools and environments

HLRS mainly contribute with its experience in the area of programming models and of Grid Systems. HLRS has developed a powerful integrated system for the creation, execution and monitoring of complex modelling experiments in the Grid. The integrated system is composed of GriCoL, a universal abstract language for the description of Grid experiments, and SEGL, a problem solving environment capable of utilizing the resources of the Grid to execute and manage complex scientific Grid applications.

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

7.1.2.4 DEISA AND EDEISA

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. 2006, the project was extended by eDEISA to cover additional efforts in networking, middleware deployment and user support.

PARTNERS
IDRIS, FZJ, RZG, CINECA, EPCC, CSC, SARA, ECMWF, LRZ, BSC, HLRS
7.1.2.5 GRIDCOORD

ABSTRACT
The GridCoord project aims at strengthening the co-operations amongst the European funding authorities and Grid projects in order to improve the co-ordination 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: DIIST, UP, HLRS, QUB, EPSRC, INRIA, UNSA, ZIB, UvA, MTA, SZTAKI, UPM, PSNC, OMII.

7.1.2.6 NEXTGRID

ABSTRACT
The NextGRID project is an integrated project in the 6th 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:

- Meeting the needs of business users
- Enabling participation by the public
- Consolidating and standardizing

The development of the next generation Grid will result in a collection of new architectural designs, key middleware components, application support mechanisms, know-how and standards that will underpin the next generation Grid.

HLRS contributed in particular to the realization of the Service Level Agreement subsystem, leading the task on Virtual Organizations and contributed to the definition and the Next Generation Grid architecture.

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

7.1.2.7 AKOGRIMO

ABSTRACT
The Akogrimo (Access to knowledge through the Grid in a mobile world) project was 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 7M€. Akogrimo developed a framework which expedites a breakthrough in current Grid practices by making a distributed, mobile, and pervasive environment a business proposition. In such an integrated world based on Grid and mobile communication concepts, network and service operators can develop new business activities and provide new services. Akogrimo’s results were validated through scenarios from different domains, focussed on eHealth and disaster/crisis handling.

Akogrimo’s inventions cover:
- Integrated approach for network and Grid service accounting across several providers
- Joint treatment of context information from different sources and types across technology layers as well as context change notification
- Interoperable identity management with user attributes shared between network and Grid layers and across organizations
- Mobile collaborative business service provision driven by workflows, also enabling direct services invocation, adaptive to changing contexts
- Integration of requirements modelling, system architecture and design modelling, and knowledge modelling

Akogrimo’s framework was demonstrated repeatedly to the public, the most prominent events being the IST in 11/2006 in Helsinki/Finland where Akogrimo exhibited the eHealth prototype in the Stuttgart University Science Truck within the exhibition hall, and Akogrimo’s final demonstration showcase of the disaster/crisis handling prototype in 11/2007 in Madrid/Spain.

HLRS technically co-ordinated the overall project and led several large activities such as the architecture and Grid infrastructure services layer. This project was performed in collaboration with Rechenzentrum Universität Stuttgart [RUS] being responsible for the network oriented aspects.

PARTNERS
TID, HLRS, UPM, ATOS, CRMPA, BOC, IT-aweiro, UniZH, STFC, TN, ICCS/NTUA, DM, UHOH, QQ, IT Innovation.

7.1.2.8 TRUSTCOM

The TrustCom project has developed a framework for trust, security, and contract management for secure, collaborative business processing and resource sharing in dynamically-evolving virtual organizations. The framework incorporates the conceptual models required to understand the issues involved, an architecture to manage the risks that arise from business collaborations, and profiles of standards defining the subsets which interoperate, and proposing extensions where required. Legal analyses of the issues relating to contracts for virtual organizations, and the management of the business throughout its lifecycle have been incorporated into the framework along with social science and economic analysis of the trust judgments of the actors involved, and the best practice in supplier qualification analysis to select the collaborating partners.

The service oriented architecture implemented as web services incorporating recent standards for security and trust has been produced in a reference implementation. Two demonstrators have been implemented and evaluated to show the user and business benefits to the supply chain management of large organizations operating their own collaboration infrastructure, and to consortia of small organizations hosted by a trusted third party network service provider.

Many of the project results are available as open source software, some are already available in commercial products, while consortium member organizations plan to exploit others in future products and services which will have a significant impact on the ability of European companies to collaborate to provide the large value propositions that they need to compete in the global marketplace.

HLRS’ main roles in the project consisted in leading the architecture work of the framework and contributing to the implementation integration from this stance. HLRS was further-more involved in designing and developing a service level agreement management framework and the cross-organization notification support.

The project started in February 2004 and ended in May 2007.
PARTNERS
Atos Origin, British Aerospace (BAE), British Telecom (BT), EMIC, HLRS, IBM, Imperial College, Kings College, NRCCL, SAP, SICS, SINTEF, Science and Technology Facilities Council (STFC, former CCLRC), University of Kent, University of Milano

7.1.2.9 ELeGI
ABSTRACT
The European Learning Grid Infrastructure (ELeGI) project is an integrated project in the 6th 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 experimental, 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 implementation activity for the ELeGI learning infrastructure and is contributing to the architecture activity designing the overall system.

PARTNERS
AIT, Atos Origin, CCLRC, CEMSAC, CNRS, CRMPA, CRSA, CS-SI, Microsoft EMIC, FAU Erlangen, FUNDP, HOU, Kaunas TU, Open University KFU-Graz, RU Bochum, UM2-Montpellier, University of Dundee, University of Southampton, UPPA, University of St. Andrews, HLRS

7.1.2.10 BREIN
ABSTRACT
In today’s world, enterprises, independent of their size, have to co-operate closely with other companies to keep their competitiveness, as no company is capable of fulfilling all requirements alone. But setting up these collaborations is still difficult and extremely costly, difficult to realize and manage and often highly risky for all involved parties. Especially for SMEs these collaborations are not really cost-efficient, as they have to put in high efforts to be able to compete on the market with other players.

BREIN will enable service providers to reduce costs whilst maximizing profit. The framework will automatically adapt to changes in individual business needs and/or environment in an intelligent manner. Cost and effort for service provisioning will be greatly reduced by simplifying business goal definition, intelligent optimization and decision making support.

BREIN will revolutionise electronic business collaborations by taking the classical Grid approach to the next level by

- realizing intelligent, autonomous resources
- supporting complex business definitions
- simplifying communication
- meeting security, confidentiality & privacy issues
- automating collaboration management
- intelligently optimizing business execution

BREIN will combine the flexibility and stability of Grid-technologies with the autonomy of Multi Agent concepts and enhance it with the intelligence and adaptability of AI systems. It will furthermore make extensive use of semantic web’s knowledge management capabilities and embed security technologies into these approaches – all to deliver the powerful business grid of tomorrow.

HLRS is technically managing the overall project and besides this involved in several areas like architecture definition and implementation. The project started in September 2006 and with a duration of 36 months is planned to end in August 2009.

PARTNERS
HLRS, UNIMAN, TID, UHOH, IT Innovation, Elsag Datamat, EMIC, ADEI, ANSYS Europe, MTA Sztaki, CRMPA, PSNC, FSG, ATOS Origin, BSC, BOC
7.1.2.11 BEingRID

ABSTRACT

The mission of BEingGRID – Business Experiments in Grid – is to establish effective routes to foster the adoption of Grid technologies across the EU and to stimulate research into innovative business models using Grid technologies.

It is well known that the point of greatest peril in the development of a market for new technology, such as the Grid, lies in making the transition from an early market dominated by a few visionary customers to a mainstream market dominated by a large block of customers who are predominantly pragmatists in orientation. The gap between these two markets is so significant as to warrant being called a chasm. Crossing this chasm must be the primary focus of any long-term high-technology marketing plan. A successful crossing is known to lead to success. Therefore, the strategic objectives of BEingGRID are:

- Understanding the requirements for Grid uptake in the commercial environment
- Enabling and validating the adoption of Grid technologies by business
- Designing and building a Grid toolset repository with components and solutions based on the main Grid software distributions
- Developing and deploying a critical mass of Grid-enabled pilots, embracing a broad spectrum of economic sectors with different needs and requirements in terms of technological Grid challenges

To meet these objectives, BEingGRID is undertaking a series of targeted Business Experiments (BEs) designed to implement and deploy Grid solutions across a broad spectrum of European business sectors (including the media, financial, logistics, manufacturing, retail and textile sectors). Eighteen Business Experiments were launched at the outset of the project with a second competitive call (2M€) for a second wave of BEs starting in early 2008.

Gridipedia is the showcase through which this information is made available to interested parties such as industry, researchers, journalists and technology organizations. The repository is also open to external contributors keen on offering high-level services, new tools and innovative Grid application solutions. The creation of this Gridipedia toolset repository will result in a “Grid marketplace” enabling individuals and organizations to create, provide and use Grid technologies to meet their business challenges.

Employees of the HLRS take part in the technical common cross activities, in building up the toolset repository Gridipedia, and we are leading the sixth Business Experiment of Phase I (BE06) about Groundwater Modeling. We also preside over the architecture and interoperability work package, which is part of the technical common cross activities.

PARTNERS

BEingGRID is a Consortium of 99 partners led by ATOS Origin and drawn from across the European Union. This Consortium is structured in two groups: the Core Team Members and the Business Experiments Partners. The Core Team Members are Atos Origin, BT, EPPC, LogicaCMG, CETIC, HLRS, T-Systems, CRMPA, SCAI, ENEA, Universität St. Gallen, ECP, AUEB, NTUA, ICRI, Telefonica

7.1.2.12 CoSpaces

ABSTRACT

CoSpaces is an IP project funded by the EC under the IST Programme of the FP6, which overall objective is to develop organizational models and distributed technologies supporting innovative collaborative workspaces for individuals and project teams within distri-
buted virtual manufacturing enterprises. Thus, CoSpaces results will enable effective partnerships, collaborate, be creative, improve productivity, reduce the length of design cycles and take a holistic approach to implementing product phases.

This will be achieved through enhanced human communication, innovative visualization, knowledge support and natural interaction and will transform the current working practices to be more competitive in the global market. CoSpaces proposes to validate these collaborative workspaces against three sectors: aerospace, automotive and construction. However, the impact of this research will go beyond these three sectors due to the generic nature of the technologies. CoSpaces will undertake the ambitious challenge of developing the technical, organizational and human networks to build collaborative workspaces. This will be achieved through a systematic and integrated programme of RTD activities, dissemination, training, demonstration and exploitation activities, led by a consortium of European experts who are committed to this mission.

HLRS role in this project is twofold. First HLRS is realizing the Dynamic Session Management within the CoSpaces Framework being responsible for the dynamic, ad-hoc setup of collaborative working sessions as well as application-centric services and is providing the design and implementation of the security concepts necessary to work in inhomogeneous and otherwise unprotected environments. Second, the HLRS contributes its simulation and visualization platform CO-VISE to the project and therefore provides a sophisticated engineering environment that will be extended to fit seamlessly into the CoSpaces framework to support collaborative engineering tasks as well as to access CoSpaces from within virtual immersive environments.

**PARTNERS**
Open Group, USAL, CARSA; UNOTT, FIT, TELIN, UKOELN, NTUA, Frietuna, UNINOVA, ESoCE-Net, COWI, CIMPA, CERFACS, VDC, VARINEX, TANet, FILAS, Pragmatics, AKM, ULEIDEN, CLARS, HLRS

### 7.1.2.13 VIROLAB

**ABSTRACT**

The Virolab project is funded by the EC as a STREP in the area of integrated biomedical information for better health. Its duration is determined for three years from March 2006 until February 2009.

Virolab’s mission is to provide researchers and medical doctors in Europe with a virtual laboratory for infectious diseases. As a prototype for this laboratory, the problem of HIV drug resistance was chosen. HIV drug resistance is increasing in Europe, with failure of complete virus suppression for many HIV infected persons and HIV drug resistance is one of few medical areas where genetic information is widely used for many years and related data is available.

These available clinical and patient databases can be used to relate genotype to drug-susceptibility phenotype. The data spans all temporal and spatial scales from the genome to the clinical data and is distributed over various sources in different formats (virological, clinical, drug databases) that change over time. Using a Grid-based service-oriented architecture, Virolab ‘vertically’ integrates biomedical information from viruses (proteins, mutations), patients (e.g. viral load), and literature (drug resistance experiments).

The virtual laboratory furthermore supports tools for statistics, visualization, modelling and simulation, as well as data integration and mining, to predict the temporal virological and immunological response of viruses with complex mutation patterns to drug therapy. The laboratory provides medical doctors with a decision support system to rank drugs targeted at patients. It helps virologists to study trends on individual, population, and epidemiological level.

The main objectives of the Virolab project can be summarized as followed:

- Develop a virtual organization, providing the “glue” for binding the various components of the Virolab virtual laboratory and guaranteeing a maximum of security and trustworthiness.
- Develop a virtual laboratory system infrastructure for transparent workflow, data access, experimental execution, and collaboration support.
- PVirtualise and enhance state-of-art in genotype resistance interpretation tools and integrate them directly into the virtual laboratory infrastructure.
- Establish epidemiological validation that Virolab correctly and quantitavely predicts virological and immunological outcome and disseminate the results of Virolab to medical experts worldwide.

**HLRS’ main contribution is to provide a centralized data access point virtualizing the diverse involved data sources and guaranteeing secure, efficient and resource-independent access. The centralized data access point is intended to be based on OGSA-DAI technology.**

**PARTNERS**
UVA, UMCG, HLRS, UCSC, IRSICAIXA Foundation, UNIBS, K.U. Leuven, ELTE, Gridwise Tech, ACK Cyfronet AGH, UCL, VE

### 7.1.2.14 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 Garbev, 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**
The Partners in the project are Intel GmbH and HLRS

#### 7.1.3.2 MICROSOFT HPC INSTITUTE

**ABSTRACT**

HLRS and Microsoft work together in the MS HPC Institutes program. The first period of the project ended with SC2007 in Reno, but HLRS continues to work with Microsoft in a renewed HPC Institutes project. Microsoft recently launched Windows HPC Server 2008 which adds a job scheduler, MPI and other cluster tools to Windows Server 2008. The subject of our new engagement will be parallel visualization, GPU postprocessing, parallel rendering and interactive simulation under Windows HPC Server 2008.
PARTNERS
The Partners in the project are Microsoft and HLRS

7.1.3.3 MICROSOFT TCI
ABSTRACT
HLRS and Daimler AG are collaborating in the field of Augmented Reality to support quick and visual evaluations in vehicle development. In selected applications, Augmented Reality tools are investigated, optimized and evaluated in a real engineering environment. Consultations and surveys with specialists at Daimler AG take place in order to assure that the research results can later be applied in real engineering environments.

In order to support the engineer in a homogeneous computing environment, the Open MPI implementation is ported and optimized for the Microsoft Windows Compute Cluster platform, including the integration in the CCS scheduler. In the frame of this project, additional memory debugging capabilities are implemented into the library.

PARTNERS
The Partners in the project are HLRS, Daimler AG and Microsoft

7.1.3.4 MICROSOFT MARMOT
ABSTRACT
Together with the Technical University of Dresden, HLRS is porting further developing Marmot to the Microsoft Windows platform to integrate it into the Microsoft Visual Studio programming environment. This will allow application developers to easily find bugs in MPI-parallel programs, pinpointing directly to the source of error. Through the tight integration into VS, the programmer has additional help menus and may immediately detect e.g. non-standard MPI usage in the application.

PARTNERS
The Partners in the project are NEC GmbH and HLRS

7.1.3.5 TERAFLP WORKBENCH
ABSTRACT
The Teraflop Workbench is a co-operation between HLRS and NEC, the Japanese vendor of High Performance Computing platforms. Its goal is to demonstrate the efficiency of NEC SX vector systems and that these systems 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. An application has to demonstrate scientific merit as well as suitability and demand for Teraflop performance in order to qualify. The applications come from areas like Computational Fluid Dynamics, Bioinformatics, Structural Mechanics, Chemistry, Physics, Combustion, Medical Applications and Nanotechnology.

Secondly, NEC Linux clusters and SMP systems will 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. 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.

PARTNERS
The Partners in the project are NEC GmbH and HLRS
7.2 SCIENTIFIC CO-OPERATIONS

7.2.1 CO-OPERATIONS CONTINUED IN 2006 AND 2007
- Japan Atomic Energy Agency (JAEA), 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: 13 members, among them Los Alamos National Labs (LANL), Indiana University (IU), but also Industrial members, such as IBM, Cisco and Qlogic
- University of Tennessee, Knoxville (UTK)

7.2.2 NEW CO-OPERATIONS ESTABLISHED IN 2006 AND 2007
Co-operation with University of Tohoku/Sendai, Japan
The HLRS is collaborating since 2006 with the CyberScienceCenter of the University of Tohoku at Sendai, Japan. We share a common interest in the usage of vector systems. The University of Tohoku is one of the leading users of NEC SX systems and has a close collaboration with NEC in the development of vector systems. The collaboration with HLRS includes the organization of teraflop workshops that take place in Stuttgart and Sendai alternately. Both sides also closely collaborate in the investigation of the potential of vector supercomputers and their application in engineering applications.

7.3 SCIENTIFIC WORKSHOPS

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<thead>
<tr>
<th>Date</th>
<th>Organizer</th>
<th>Location</th>
<th>Topic</th>
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<tbody>
<tr>
<td>Mar. 06, 2006</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Akogrimo Public Workshop</td>
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<tr>
<td>Mar. 21-22, 2006</td>
<td>HLRS, University of Göttingen, University of Hannover, DFN Verein</td>
<td>Göttingen</td>
<td>D-Grid Security Workshop</td>
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<td>Mar. 30-31, 2006</td>
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<td>Stuttgart</td>
<td>5th HLRS/hww Workshop on Scalable Global Parallel File Systems</td>
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<td>May 19, 2006</td>
<td>HLRS, Intel</td>
<td>Stuttgart</td>
<td>Cluster OpenMP Workshop</td>
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<td>Jul. 26-28, 2006</td>
<td>HLRS</td>
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<td>9th HLRS Metacomputing and Grid Workshop together with 10th Anniversary of HLRS</td>
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<td>Nov. 20-21, 2006</td>
<td>Tohoku University, HLRS</td>
<td>Tohoku University Sendai Japan</td>
<td>5th Teraflop Workshop</td>
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<td>Mar. 26-27, 2007</td>
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<td>6th Teraflop Workshop</td>
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<td>Apr. 23, 2007</td>
<td>JAEA</td>
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<td>Jul. 09-10, 2007</td>
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<td>Stuttgart</td>
<td>1st HLRS Parallel Tools Workshop</td>
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<td>Jul. 23-27, 2007</td>
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<td>Novosibirsk, Russia</td>
<td>3rd Russian-German Advanced Research Workshop on Computational Science and High Performance Computing</td>
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<td>Sep. 10-15, 2007</td>
<td>TU Donezk</td>
<td>Sevastopol, Russia</td>
<td>International Research Seminar on Problems in Parallel Modelling and Simulation</td>
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## Research

<table>
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<th>Date</th>
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<td>Oct. 25, 2007</td>
<td>HLRS, T-Systems SfR</td>
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<td>Industrial Grids Meeting</td>
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<tr>
<td>Nov. 21-22, 2007</td>
<td>HLRS</td>
<td>Sendai</td>
<td>7th Teraflop Workshop</td>
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### 7.3.1 1st HLRS COVISE WORKSHOP
February 14-15, 2006, Stuttgart, Germany

COVISE users from academia and industry came to the HLRS to learn more about CFD visualization with COVISE, new features and how to configure Virtual Reality projection environments. The application sessions by Martin Becker were followed by an introduction to programming of COVISE modules and plugins for the VR-Environment OpenCOVER. Andreas Kopecki gave an introduction to the COVISE configuration file API and Uwe Wössner finished the workshop with an introduction to modelling virtual worlds for OpenCOVER with 3ds Max.

### 7.3.2 AKORIMO PUBLIC WORKSHOP
March 06, 2006, Stuttgart, Germany

This workshop was open to the public and was particularly addressing research and industry looking into the integration of context, knowledge and networks with Grid concepts. The purpose is to present selected results from the Akorimo project together with results achieved in other relevant projects in order to provide the audience an overview of the results achieved and how they fit in a larger context. Becker were followed by an introduction to programming of COVISE modules and plugins for the VR-environment OpenCOVER. Andreas Kopecki gave an introduction to the COVISE configuration file API and Uwe Wössner finished the workshop with an introduction to modelling virtual worlds for OpenCOVER with 3ds Max.

### 7.3.3 D-GRID SECURITY WORKSHOP
March 21-22, 2006, Göttingen, Germany

On March 21 - 22, 2006, the joint D-Grid workshop on security was held by InGrid, MediGrid and DGI. D-Grid is the German Grid initiative, funded by the Ministry for Education and Research [Bundesministerium für Bildung und Forschung], InGrid and MediGrid the engineering and medical community projects respectively.

Security issues and trust in the installed security mechanisms are topics of wide importance for the common use of distributed resources. Aim of the workshop was to inform the communities about the current and ongoing work done on the security topic.

It aims also to bring those together who work on security themes. About 55 participants discussed a wide range of topics related to security aspects in Grid.

### 7.3.4 4th HLRS-NEC TERAFLOP WORKSHOP
March 30-31, 2006, Stuttgart, Germany

The Teraflop Workshop is part of the Teraflop Workbench co-operation between NEC and HLRS. With more than 40 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 Hiroaki Kobayashi (Tohoku University) and Leonid Oliker (LBL) talked about performance and applications on scalar and vector systems, experts like Alice Koniges (LLNL) and Thomas Schulthess (ORNL) discussed the use of high performance systems especially in material science and their expectations and problems using future supercomputer architectures. Computational scientists of different fields presented their current work and their results obtained using the SX-8 system.
7.3.5 5th HLRS/HWW WORKSHOP ON SCALABLE GLOBAL PARALLEL FILE SYSTEMS AND HDF EUROPE SPRING MEETING 2006 AND OPENIB/RDMA TRACK
April 03-05, 2006, Stuttgart, Germany
Under the subtitle “Getting on Top of the Storage Cube” more than 100 participants met at HLRS in Stuttgart to discuss the current state and future of Distributed Storage Technology. One focus in this year’s workshop were cluster file systems. The keynote 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.

7.3.6 CLUSTER OPENMP WORKSHOP
May 19, 2006, Stuttgart, Germany
In this one day workshop, organized by HLRS, participants joined from all over Germany, including various university institutions and industry. Larry Meadows and James Cowie (both Intel) and Dr. Georg Hager (University of Erlangen) presented the features of Intel’s the newly available product Cluster OpenMP. Demonstrations and practical experience as hands-on-sessions were being done on the HLRS cacau-cluster. Further information may be found on http://www.hlrs.de/news-events/events/2006/metacomputing

7.3.8 HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING – THE 9TH AND 10TH RESULTS AND REVIEW WORKSHOP OF THE HPC CENTER STUTTGART (HLRS)
October 19-20, 2006 and October 04 - 05, 2007, Stuttgart, Germany
The 9th and 10th Results and Review Workshop of the HLRS brought together more than 50 participants from German research institutions, the steering committee and scientific support staff of HLRS. In both workshops more than 30 sophisticated talk and poster presentations were selected in advance from the steering committee out of the yearly supercomputer project reports and presented at the Results and Review Workshop. State-of-the-art scientific simulations on the supercomputer systems of HLRS again emphasized the world-class research done at the center obtaining outstanding results in achieving highest performance for production codes which are of particular interest for both scientists and engineers. The presentations covered all fields of computational science and engineering ranging from CFD via computational physics and chemistry to computer science with a special emphasis on industrially relevant applications. Every year the three most outstanding projects are honoured by the Golden Spike Award which is awarded by the steering committee of HLRS. The laureates of 2006 and 2007 and their project titles are:

2006:
- Jens Harting, Institute for Computational Physics, University of Stuttgart, “Rheological properties of binary and ternary amphiphilic fluid mixtures”
- Andreas Marek, Max-Planck Institute for Astrophysics, Garching, “The SuperN-Project: Understanding core collapse supernovae”
- Sven Ganzenmüller, Department of Computer Engineering, University of Tübingen, “Object-Oriented SPH-Simulations with Surface Tension”

2007:
- Rainer Stauch, Institute for Technical Thermodynamics, University of Karlsruhe, “Ignition of Droplets in a Laminar Convective Environment”
- Janina Zimmermann, Fraunhofer Institut für Werkstoffmechanik, Freiburg, “DFT Modelling of Oxygen Adsorption on CoCr-Surfaces”
7.3.9 5th TERAFLIP WORKSHOP
November 20–21, 2006, Tohoku University, Sendai, Japan
The 5th Teraflop Workshop was held in cooperation with NEC and the Information
Synergy Center of Tohoku University at Tohoku. More than 70 participants from
Europe and Asia came together and discussed HPC applications of different fields and the
steps towards petaflops computing. Speakers like Ryutaro Himeno (Riken Next Generation
Supercomputer R&D Center) gave an overview about current hardware developments
for the next generation of HPC systems and experts like Seiji Tsuoi (Institute for
Research on Earth Evolution, JAMSTEC) talked about applications with a sustained high
performance. Specialists of different fields presented their research and the results obtained using today’s HPC systems.

7.3.10 6th HLRS-NEC TERAFLIP WORKSHOP
March 26–27, 2007, Stuttgart, Germany
The 6th Teraflop Workshop continues a series of workshops which are held twice a year,
alternatingly in Japan and at HLRS. The 2007 was focusing on the applications perspective of high end computer systems. Special attention was paid to coupled systems applications combining different physical phenomena with possibly distinct requirements on computer architectures. Sessions were dedicated to developments in architectures and performances achievements on the one hand, to applications on High Performance Computing platforms on the other, focussing especially on coupled multi-scale / multi-physics applications.

7.3.11 2nd D-GRID SECURITY WORKSHOP
March 27–28, 2007, Göttingen, Germany
On March 27–28, 2007, the 2nd Joint D-Grid Workshop on Security was held by In-Grid, MediGrid and DGI. Participants from In-Grid, MediGrid, DGI, as well as from C3, TextGrid, and Astro discussed a wide range of topics related to security aspects in Grid. More than 50 participants contributed to the workshop with talks, comments and experience. Additionally, the view points were extended by invited talks, given by speakers from AustrianGrid and Microsoft, summarizing their experiences in European Industrial Grids. While in the year before, the focus was on authentication, it was an authorization now. The overlap with AAI and VO management was pointed out, as well as firewalls in a more or less anonymous environment.

7.3.12 6th HLRS/HHW WORKSHOP ON SCALABLE GLOBAL PARALLEL FILE SYSTEMS, HNF EUROPE SPRING MEETING 2007 AND OPENFABRICS
April 16–18, 2007, Stuttgart, Germany
Representatives from science and industry interested in high performance storage solutions did meet at HLRS during April 16–18, 2007, for the Sixth Annual Workshop on Scalable Global Parallel File Systems. Under the motto of “Moving the World: Global and Individual”, this year’s three-day event tried to leverage contributions coming from three major research and development areas: federation of OSD-based file systems for use in European HPC Grid projects, an all-optical communication and switching infrastructure being able to transport 100-Gbit/s serial signals within the framework of the German Gauss Alliance, as well as standardization efforts performed by the OpenFabrics Alliance on the InfiniBand architecture. More than 150 participants did follow a total of 45 presentations that have been on the workshop agenda.
Dr. Peter Braam, founder and CEO of Cluster
HPC Grid Projects, an all-optical communication and switching infrastructure being able to transport 100-Gbit/s serial signals within the framework of the German Gauss Alliance, as well as standardization efforts performed by the OpenFabrics Alliance on the InfiniBand architecture. More than 150 participants did follow a total of 45 presentations that have been on the workshop agenda.

7.3.13 16TH CCSE WORKSHOP ON HIGH PERFORMANCE COMPUTING ON VECTOR-BASED ARCHITECTURES - RECENT ACHIEVEMENTS AND FUTURE DIRECTIONS
April 23, 2007, Japan Atomic Energy Agency, Tokyo, Japan
In co-operation with the Japan Atomic Energy Agency, a German-Japanese workshop on recent achievements and future directions in vector based architectures and their applications was held. Participants from both countries discussed developments and requirements from simulation point of view as well as technology developments.

7.3.14 1st HLRS PARALLEL TOOLS WORKSHOP
July 09–10, 2007, Stuttgart, Germany
HLRS organized and hosted the 1st Parallel Tools Workshop with contribution of tool developers from various institutions. The major aim of this workshop was to bring together the tool developer community and the professional user base. The concept of combining talks with live-demos, practicals and hands-on-sessions proved to be successful: the workshop attracted 65 participants, mostly from German Universities, research institutions and industry, and altogether 10 participants from the UK, France and the US. The sessions were split into topical areas currently of interest: from single processor performance optimization, to parallel debugging and various tools for performance analysis and optimization, as well as advanced programming models and integrated development environments for parallel applications. To enable the participants to get first-hand experience, each tool was made available on a cluster at HLRS, with a single command for setup using Oscar module-files. This allowed easy access to the wide range of tools. Attracting 67 participants, the workshop was highly successful. For the following year, the workshop will be held in 2008 again, together with workshop proceedings published in Springer.
7.3.15 3rd RUSSIAN-GERMAN ADVANCED RESEARCH WORKSHOP ON COMPUTATIONAL SCIENCE AND HIGH PERFORMANCE COMPUTING
July 23-27, 2007, Novosibirsk, Russia
Together with the Institute for Computational Technologies (ICT) in Academgorodok near Novosibirsk, HLRS organized the third Russian-German workshop in Academgorodok in July 2007. About 30 scientists from Siberia and Germany discussed on a variety of different subjects like High Performance Computing, electromagnetic simulation, fuel cells, oceanography and meteorology, simulation of tsunamis, modelling turbulence, simulation of optical fibres, of blood flow, aero acoustics, interval arithmetic and computational grid environments. This workshop was one of a series of events organized in getting closer to the science of the former soviet republic countries. See also the URL http://www.grc-hpc.de/. In the same framework, HLRS and ICT organize also the yearly Russian-German School on Parallel Programming using High Performance Computation Systems and the exchange of scientists.

7.3.16 PROBLEMS IN PARALLEL MODELING AND SIMULATION
September 10-15, 2007, Sevastopol, Russia
The High Performance Computing Center Stuttgart (HLRS) participated in an international research seminar on Problems in parallel modeling and simulation. The seminar was held in Sevastopol between September 10-15, 2007. Other participants along with members of HLRS were the Fakultät für Rechentechnik und Informatik (FRTI), Laboratorium für Echtzeitsysteme (EZESIS) GmbH, Technopark DonNTU UNITECH GmbH at Nationale Technische Universität Donzeich (Ukraine), as well as Nationale Wissenschaftskademie der Ukraine, Instut für Simulationsprobleme in Energetik, Kyiv.

7.3.17 D-GRID INDUSTRIAL GRIDS WORKSHOP
October 25, 2007, Stuttgart, Germany
In the second call for the German Grid initiative D-Grid, focus was layed on community projects with industrial participation. To cover the expectations and requirements especially of the industrial partners, the first Industrial Grids Meeting took place on October 25, 2007 in Leinfelden-Echterdingen (Stuttgart). Organized by the projects InGrid, AeroGrid, PartnerGrid, and ProGrid, representatives of all D-Grid projects with a strong stake in industry, especially the more than 40 industrial partners were invited and discussed a broad palette of topics that ranged over scientific, technical, commercial, financial as well as organizational working areas for the industrial Grid users. Important requirements were to improve usability, integration into the existing IT infrastructures and the possibilities for long-term usage. Another focal point was the integration of users into the Grid structure, comprising the management of roles and rights as well as service provision of legally binding business processes and the availability of service level agreements.

7.3.18 7th HLRS-NEC TERAFLOP WORKSHOP
November 21-22, 2007, Tohoku University, Sendai, Japan
The 7th Teraflop Workshop brought together scientists, application developers, international experts and hardware designers from different continents to discuss the current state and the future of supercomputing. Sessions on Emerging HPC Technologies, Computational Physics & Engineering, Future Architectures, Computational Fluid Dynamics/Climate, and Coupled Systems gave insight into new developments in supercomputing facilities and applications.
7.4 CONFERENCE SHOWS

7.4.1 CEBIT 2006 BW INTERNATIONAL
March 09-15, 2006, Hannover, Germany
From March 09-15 HLRS was exhibiting in the Baden-Württemberg International booth at Cebit which is the world’s largest trade fair showcasing digital IT and telecommunications solutions for home and work environments targeting user groups from industry, the wholesale/retail sector, skilled trades, banks, the services sector, government agencies, science and all users passionate about technology. The presentation on the booth included information brochures and leaflets about HLRS and its ongoing projects as well as live demonstration of visualization of scientific simulation results. Interactive remote simulations were also displayed. The presentation hardware consisted of a standard desktop PC with high-end graphics hardware and a 19” TFT display.

7.4.2 CEBIT 2006 FUTURE TALK, DAY OF SUPERCOMPUTING
March 11, 2006, Hannover, Germany
During CEBIT 2006 HLRS also organized and participated in the “Day of Supercomputing” series of presentations during the “Future Talk” event at Cebit. The talks gave insight into German supercomputing centers. These presentations were aimed at an open audience. Topics included engineering simulations, weather forecasts, biological simulations, astronomical simulations and many more. The HLRS provided a mobile video conferencing equipment. It has been used to establish live video-conferencing connections to the different supercomputing centers, to give short presentations and insights the particular supercomputing center, explaining and showing the available supercomputers.

7.4.3 D-GRID BOOTH AT GRID VILLAGE, ISC DRESDEN
June 27-30, 2006, Dresden, Germany
HLRS represented the community project InGrid at the D-Grid booth, Grid Village at ISC Dresden.
The German e-science initiative d-grid was exhibiting at the International Supercomputer Conference in Dresden. HLRS represented the community project InGrid at the D-Grid booth, Grid Village at ISC Dresden.
The booth attracted a lot of interest specifically from international visitors who wanted to get more information about German Grid computing.

7.4.4 INTERNATIONAL SUPERCOMPUTER CONFERENCE 2006
June 27-30, 2006, Dresden, Germany
As every year HLRS was presenting its research activities at the ISC in Dresden. HLRS presented a prototype of its driving simulator as well as immersive visualization of simulation results on a stereoscopic projection equipped with a stereo projector by Digital Image and an optical tracking system by ART. HLRS was also present at the Microsoft booth showing its results of the collaboration with Microsoft in the field of High Performance Computing and visualization. On the HP Booth, HLRS presented COVISE on a tiled display driven by an HP SVA cluster.

7.4.5 LONG NIGHT OF SCIENCES
July 07, 2006, Stuttgart, Germany
As usual, HLRS took part in the university’s open day. HLRS opened the CAVE and the computer room of the SX-8. In our little Computer History Exhibition, visitors could see Computing machines from 1632 to 2006. In the CAVE, visitors could go on a virtual ride with our Porsche driving simulator. Datasets of different university institutes and companies have been presented. They represented various application areas like Mechanical engineering, aerospace, biology, medicine, architecture and art.

7.4.6 CAVE INAUGURATION
October 10, 2006, Stuttgart, Germany
During the year, the HLRS CAVE, our immersive visualization environment, has been refurbished by replacing the four old CRT projectors with eight modern ProjectionDesign F1+ DLP SXGA+ beakers. To achieve this, we had to modify those projectors in order to upgrade them with an optical lens shift. The two projectors for each wall of the CAVE are used to project an active stereo picture. This means that the projectors need to be synchronized. This is achieved by the use of electronics provided by Digital Image.
The refurbishment of the HLRS CAVE has been celebrated with a barbecue party. Lots of in-house and external guests enjoyed the festivities.

7.4.7 WOMEN & GIRLS TECHNOLOGY DAY
October 14, 2006, Stuttgart, Germany
HLRS was presenting its research activities at the Women & Girls Technology Day. HLRS had a booth at which poster and demonstrations on Virtual Reality visualization were shown. HLRS presented its work on a 3D immersive backprojection and informed the participants about the versatile possibilities in the field of scientific computing. The aim of the workshop was to encourage women and girls to chose technical professions.

7.4.8 SUPERCOMPUTING CONFERENCE 2006
November 11-17, 2006, Tampa, FL
Since 10 years, the HLRS is presenting its on-going projects and research on a booth at the Supercomputing Conference. This year’s highlight was a dark blue Porsche Cayman S with which we presented a 20 million
cell airflow simulation using Augmented Reality methods. The HLRS had a permanent stand on the Microsoft booth showcasing remote execution of graphical applications and AR-Visualization. Talks have been given on several partner booths, such as the NEC and MS-booth. Together with the CalIT², Collaborative Visualization of Proteins has been demonstrated between two installations on the Supercomputing show floor and the CalIT² home site in San Diego. The Presentation hardware was a 4x5 tiled display on a joint SDSC, NCRR booth and a 3x5 MAC-Mini tiled display the CalIT² booth. Another highlight was an interactive collaborative simulation carried out on compute nodes distributed over numerous booths such as SUN, Voltaire, HLRS and Cisco. The parallel simulation code Fenfloss was using OpenMPI over an Infiniband interconnect between the different booths. The collaborative Visualization was carried out using COVISE. The Visualization group was also giving a talk at SC-Global, presenting the seamless integration of COVISE in the AccessGrid conferencing environment. The presentation hardware consisted of an active stereo back-projection with a Cube3D by Digital Image and an optical tracking system by ART. Augmented Reality visualization of CFD results was demonstrated with a 1/18 model of a Porsche Cayman S. COVISE was also presented on a SONY SRX-R110, worlds first 4K Digital Cinema Projector using LCOS technology. It was driven by two systems with Quadro FX 4500G boards. Prof. Resch represented the HLRS by giving a talk with the title “VR in an HPC Framework - Being Inside the Simulation”.

7.4.10 SYMPOSIUM ON RAPID PRODUCT DEVELOPMENT
March 07, 2007, Stuttgart, Germany
Finalizing the SFB 374, the HLRS presented its work on rapid prototyping and simulation steering at the Symposium on Rapid Product Development organized by the SFB research consortium. It was shown how online simulations steered by novel interaction paradigms can speed up the product development cycle. At a physical prototype of a car middle console an online airflow simulation of the air vents was shown that could be steered by changing the direction of the vent outlet using a real interactor.

7.4.12 6TH FKFS CONFERENCE, PROGRESS IN VEHICLE AERODYNAMICS AND THERMAL MANAGEMENT
October 09-10, 2007, Stuttgart, Germany
The HLRS was presenting Virtual Reality visualization of simulation results in the new three wall projection environment at the FKFS. The projection environment consists of three passive stereo backprojection walls without a floor projection. An optical tracking system by ART is used for head tracking as well as interaction with the visualization. The projectors are driven by a six node graphics cluster with Nvidia Quadro FX 4500G boards and Gigabit Ethernet interconnect. In the model size wind tunnel, we presented an Augmented Reality visualization of airflow during the ongoing wind tunnel experiment.
For the first time the smoke wand was equipped with a marker in order to track its position which allowed to recomputed the particle paths through the simulated dataset in real time and compare the stream lines with the physical smoke traces.

7.4.13 SUPERCOMPUTING CONFERENCE 2007
November 12-17, 2007, Reno, NV
The HLRS presented ongoing projects and research on its booth at the Supercomputing Conference, which was held in Reno, Nevada this year. At the HLRS booth presentations were given on HLRS projects such as Microsoft TCI (Technical Computing Initiative), CoSpaces, HPC-Europa, and others. On our rear projection wall we showed recent datasets in Virtual Reality. To show the collaborative aspect of our visualization software COVISE we connected the booth to our CAVE in Stuttgart and to the VR lab of the University of Cologne and worked on datasets together with our colleagues back home.

However, the main attraction on the HLRS booth was a Mercedes GL, which was used to show Augmented Reality Visualization of the airflow around and inside the car. Visitors could have a look at spinning air particles and streamlines directly on the real car. Inside the car, the temperature distribution in the cabin, which is influenced by the air conditioning, could be examined. Other COVISE installations were running at the booths of Calit² and NCHC. In a funny Austin Powers ceremony at the Microsoft booth, HLRS representatives received a prize for our contribution in the MS HPC Institutes project.

Prof. Michael Resch was one of four invited plenary speakers who could present his work. In his talk, he explained the concept of HLRS with a focus on our manifold co-operations with industry and science.

Rolf Rabenseifner and Rainer Keller were involved in the tutorial programme where they talked about Hybrid MPI and OpenMP Parallel Programming.

7.4.14 COVISE USER MEETING
November 22, 2007, Castle Hohenheim, Germany
The HLRS presented latest research results on Virtual and Augmented Reality in the exhibition area of this years COVISE User Meeting in the historic premises of Schloss Hohenheim. The driving simulator was set up in front of a mobile passive stereo back projection system. This allowed the participants to experience a fast joyride but also to see the latest development in the research version of COVISE.
7.5 PUBLICATIONS

7.5.1 BOOKS


This book presents the state-of-the-art in simulation on supercomputers. Leading researchers present results achieved on systems of the Stuttgart High Performance Computing Center (HLRS) for the year 2007. The reports cover all fields of computational science and engineering, ranging from CFD and computational physics and chemistry to computer science, with a special emphasis on industrially relevant applications. Presenting results for both vector-based and microprocessor-based systems, the book makes it possible to compare the performance levels and usability of various architectures. As the HLRS operates the largest NEC SX-8 vector system in the world, this book gives an excellent insight into the potential of such systems. The book further covers the main methods in High Performance Computing. Its outstanding results in achieving the highest performance for production codes are of particular interest for both scientists and engineers. The book comes with a wealth of color illustrations and tables.


This book contains papers presented at the 5th Teraflop Workshop, held in November 2006 at Tohoku University, Japan and the 6th Teraflop Workshop held in March 2007 at the Stuttgart High Performance Computing Center (HLRS) in Germany. It presents the state-of-the-art in High Performance Computing and simulation on modern supercomputer architectures. It covers trends in hardware and software development in general and specifically the future of vector-based systems and heterogeneous architectures. The application contributions cover computational fluid dynamics, fluid-structure interaction, physics, chemistry, astrophysics, and climate research. Innovative fields like reactive flow simulations and nano technology are presented. Furthermore, the use of supercomputers in the growing field of medical simulations is shown. All papers were chosen from presentations given at the 4th Teraflop Workbench Project Workshop held at the Höchstleistungsrechenzentrum Stuttgart (HLRS) in March 2006.


The book presents the state of the art in High Performance Computing and simulation on modern supercomputer architectures. It covers trends in high performance application software development in general and specifically for parallel vector architectures. The contributions cover among others the field of computational fluid dynamics, physics, chemistry, and meteorology. Innovative application fields like reactive flow simulations and nano technology are presented. Furthermore, the use of supercomputers in the growing field of medical simulations is shown. All papers were chosen from presentations given at the 4th Teraflop Workbench Project Workshop held at the Höchstleistungsrechenzentrum Stuttgart (HLRS) in March 2006.


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7.5.2 BOOK CHAPTERS

7.5.3 JOURNAL PAPERS

7.5.4 OTHER REFEREED PAPERS
- Assel, M., Krammer, B., Loehden, A., Management and Access of Biomedical Data in a Grid Environment. 6th Cracow Grid Workshop CGW’06, Krakau/Poland, October 15-18, 2006

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source Management, in 2006 International Conference on High Performance Compu-
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7.5.5 OTHER PAPERS


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7.5.6 TUTORIALS/REPORTS


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Resch, M., HPC in Science and Industry, 2 hours talk as part of Scuola Estiva di Calcolo Avanzato, Castel Gandolfo – Roma/Italy, September 06, 2007


14.7 TALKS


Assel, M., Similarities between Grid-enabled Medical and Engineering Applications, eHealth Conference, Berlin/Germany, April 18, 2007


Benkert, K., Vector Computers, Max-Planck Institute for Mathematics in the Sciences, Leipzig/Germany, January 10, 2006

Benkert, K., Vector Computing and the Teraflop Workbench Project, COSC 6374, Parallel Computation (graduate course), University of Houston/USA, April 16, 2007

Benkert, K., An Introduction to H-Matrices, Systems Seminar, Department of Computer Science, University of Houston/USA, April 25, 2007

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Bönisch, T., The Teraflop Workbench, NEC User Group XVIII General Meeting, University of Toronto/Canada, May 23, 2006

Bönisch, T., Infiniband@HLRS, OpenFabrics Conference, Paris/France, June 23, 2006

Bönisch, T., Hinter den Kulissen eines Höchstleistungsrechenzentrums, Invited Talk, IDG Computerwoche Initiative Datacenter up-to-date, Frankfurt am Main/Germany, April 24, 2007

Heek, R., Operating Virtual Organizations using Bipartite Service Level Agreements, The 8th IEEE/ACM International Conference on Grid Computing (Grid 2007), Austin/USA, September 19-21, 2007


Jenz, D., Computational Steering, IGSSE Kickoff Meeting, Lindau/Germany, November 08, 2007

Keller, R., University College Cork/Ireland, MetaComputing Support with Open MPI, April 07, 2006

Keller, R., SC2006 Open MPI Demo and Research Interest, Talk at Sun Booth, November 14, 2006

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Keller, R., MPI in the Light of Multi-Core Architectures: Thread-Safety, Workshop, Sendai/Japan, November, 2007

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Koller, B., HLRS – The Virtual Engineering Collaboration Scenario in the BREIN European Project, 14th ISPE International Conference on Concurrent Engineering, Sao Jose dos Campos/Brazil, July 16-20, 2007

Krammer, B., Parallel Tools and Libraries at HLRS, 25. Treffen des ZKI AK Supercomputing, Cologne/Germany, March 30-31, 2006
Krammer, B., Itanium@HLRS, International Supercomputer Conference (ISC) 2006, Dresden/Germany, June 27-30, 2006

Krammer, B., Experiences with Infiniband-Clusters at HLRS, 26. Treffen des ZKI AK Supercomputing, Munich/Germany, October 19-20, 2006

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Küster, U., Fischer, R., Notes on Vectorization, NEC Users Group, Toronto/Canada, May 23, 2006

Küster, U., Vector Processing on Future High Performance Architectures, 5th Teraflop Workshop at Tohoku University, Sendai/Japan, November 20-21, 2006


Lammers, P., HLRS–NEC Teraflop Workbench Initiative, Supercomputing 2006, November 11-17, 2006


Lammers, P., Efficient Implementations of Simple Lattice-Boltzmann Kernels, Probleme Paralleler Simulationstechnik, Sevastopol/Kyiv, Ukraine, September 13, 2007


Rabenseifner, R., Performance Evaluation with the HPCC Benchmarks as a Guide on the Way to PetaFlop/s Systems, IWR-Colloquium, Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg/Germany, June 29, 2006

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Rabenseifner, R., Hybrid MPI and OpenMP Parallel Programming, guest lecture at University of Heidelberg/Germany, in Thomas Ludwig’s lecture on Cluster-Computing, July 20, 2007

Resch, M., Computer Environment, Clusters, Supercomputers, Storage, Visualization, 5th EUROMOTOR Short Course, Stuttgart/Germany, March 21-22, 2006

Resch, M., The Future of Grid in Europe, National Center for High Performance Computing (NCHC), Hsinchu/Taiwan, April 12, 2006


Resch, M., Performance and Industry, invited talk, IDC HPC User Forum, European Meeting, Zürich/Switzerland, June 02, 2006

Resch, M., Integrating HPC Simulation into Industrial and Scientific Workflows, invited talk, 2nd Erlangen International High-End-Computing Symposium, Erlangen/Germany, June 22, 2006

Resch, M., Compute Services für die digitale Fabrik, Workshop: Digitale Fabrik – vom Modell zur Simulation, Virtual Dimension Center (VDC) Fellbach/Germany, July 13, 2006

Resch, M., High Performance Computing for Science and Industry, Polytechnical University of St. Petersburg/Russia, July 31, 2006

Resch, M., Productive HPC for Scientific Applications, Scuola Estiva di Calcolo Avanzato (e-IRG), Heidelberg/Germany, April 19-20, 2007

Resch, M., The Teraflop Workbench – an Overview, 5th Teraflop Workshop, Sendai/Japan, November 20, 2006

Resch, M., VR in an HPC Framework – Being Inside the Simulation, 3rd Intuition International Workshop, Keynote, Fellbach/Germany, November 30 - December 01, 2006

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Resch, M., Collaboration with Industry – from HPC to Grids, Open Workshop on e-Infrastructures of the e-Infrastructure Reflection Group (e-IRG), Heidelberg/Germany, April 19-20, 2007

Resch, M., Challenges in HPC, 16th CCSE Workshop on High Performance Computing on Vector-based Architectures – Recent Achievements and Future Directions, Tokyo/Japan, April 23, 2007


Resch, M., Industrial Use of a Cray Supercomputer, Cray Technical Workshop, Helsinki/Finland, June 05, 2007


Resch, M., Koller, B., Service Level Agreement in BREIN, BoF SLAs for Grid Resource and Service Management, ISC 2007, Dresden/Germany, June 27, 2007


Resch, M., Zukünftige Architekturen für HPC, Ukrainian-German Workshop on Simulation on Supercomputers, Sevastopol/Ukraine, September 11, 2007

Resch, M., High Performance Computing in Germany and Europe – some Remarks, 27th IDC HPC User Forum, Stuttgart/Germany, October 01, 2007

Resch, M., HPC in Academia and Industry - Synergies at Work, Invited Plenary Speaker, SC’07, Reno/USA, November 15, 2007

Resch, M., The Teraflop Workbench – an Overview, 5th Teraflop Workshop, Sendai/Japan, November 20, 2006

Resch, M., HPC in Academia and Industry, Tohoku University, Sendai/Japan, November 21, 2007

Resch, M., HPC in Europe, NCHC, Hsinchu/Taiwan, November 23, 2007

Resch, M., VR in an HPC Framework – Being Inside the Simulation, 3rd Intuition International Workshop, Keynote, Fellbach/Germany, November 30 – December 01, 2006

Roller, S., Keller, R., Garby, M., Gabriel E., World Congress on Computational Mechanics, Minisymposium on Parallel Scientific Applications in Heterogeneous Grid Environments, http://www.hlrs.de/people/krammer/, 2006

Roller, S., Multi-scale Numerics in Low Mach Number Aeroacoustics: High-order Schemes, Heterogeneous Domain Decomposition, and Asymptotic Approaches, invited talk in Minisymposium Multiscale Aspects of Wave Propagation, 7th World Congress on Computational Mechanics (WCCM), Los Angeles/USA, July 16-22, 2006

Roller, S., Prototype Examples for Grid Applications in CFD, 7th World Congress on Computational Mechanics (WCCM), Los Angeles/USA, July 16-22, 2006

Roller, S., The InGrid Project, 9th Metacomputing and Grid Workshop, Stuttgart/Germany, July 27, 2006

Roller, S., Low Mach Number Aeroacoustics: Modeling and Direct Simulation (Poster), Multiscale Modeling and Applications, Cargese/France, August 07-11, 2006

Roller, S., Wesner, S., BEinGrid Business Experiments in Grid, Unicore Summit 2006 at EuroPar Dresden/Germany, August 30-31, 2006

Roller, S., Klimach, H. and Munz, C.-D., A block structured Low Mach Number MPV Scheme for Heterogeneous Domain Decomposition, ECCOMAS CFD 2006, Egmond aan Zee/The Netherlands, September 05-08, 2006

Roller, S., InGrid – Innovative Grid-Entwicklungen für ingenieurwissenschaftliche Anwendungen, invited talk, RWTH Aachen/Germany, September 27, 2006


Roller, S., Resch, M., Galle, M., Bez, W., The HLRS – NEC Teraflop Workbench, NEC Users Group Conference, Cetraro/Italy, May 23, 2007

Roller, S., Nachhaltigkeit aus Sicht von InGrid, D-Grid Nachhaltigkeitworkshop, Berlin/Germany, June 11, 2007

Roller, S., Multi-Scale Simulation of Aeroacoustic Applications - Approaches and Experiences, Forschungszentrum Karlsruhe/Germany (FZK), IKET, June 29, 2007

Roller, S., Hybrid Coupling of Multi-Scale Problems in Computational Aeroacoustics, 9th US National Congress on Computational Mechanics (USNCCM), San Francisco/USA, July 23, 2007

Roller, S., Security Workshop at D-Grid All-Hands-Meeting, Göttingen/Germany, September 12, 2007

Roller, S., Geschäftsmodelle aus Sicht von InGrid, D-Grid Nachhaltigkeitworkshop, Berlin/Germany, October 09, 2007


\begin{itemize}
  \item Tiyyagura, S., Linear Iterative Solver for NEC Parallel Vector Systems, 4th Teraflop Workshop, Stuttgart/Germany, March 30-31, 2006
  \item Tiyyagura, S., Küster, U., Borowski, S., Performance Improvement of Sparse Matrix Vector Product on Vector Machines, ICCS’06, University of Reading/UK, May 28-31, 2006
  \item Tiyyagura, S., Küster, U., Block-based Approach to Solving Linear Systems, 5th Teraflop Workshop, Tohoku University, Sendai/Japan, November 20-21, 2006
  \item Tiyyagura, S., Küster, U., BLIS – Vectorized Sparse Linear Solver, NEC SX-8 Usage and Programming, Stuttgart/Germany, March 29, 2007
  \item Tiyyagura, S., Fluid Structure Interaction on High Performance Computers in the Teraflop Workbench Initiative, 6th HLRS Workshop on Scalable Global Parallel File Systems and HNF Europe Spring Meeting 2007, Stuttgart/Germany, April 16-18, 2007
  \item Tiyyagura, S., Küster, U., Solving Sparse Linear Systems on Modern Processors, Probleme Paralleler Simulationstechnik, Sevastopol/Ukraine, September 13, 2007
\end{itemize}

75.8 PROFESSIONAL ACTIVITIES

\begin{itemize}
  \item Program committee member for the HIPHERION workshop at Cluster2006, Barcelona, 2006
  \item Program committee member EuroPVM/MPI, 2007
  \item Member of the Program Committee for the 4th International Conference on Autonomic and Trusted Computing (ATC-07), Hong Kong/China, July 11-13, 2007
  \item Member of the Program Committee for the Workshop on Non Functional Properties and Service Level Agreements in Service Oriented Computing [NFPSLA-SOC 2007] co-located with The 9th International Conference on Service Oriented Computing (ICSOC 2007), Vienna/Austria, September 17, 2007
  \item Member of the Program Committee for the Usage of Service Level Agreements in Grids Workshop in conjunction with the 8th IEEE International Conference on Grid Computing [Grid 2007], Austin, Texas/USA, September 19, 2007
  \item Organizer of the Cluster OpenMP Workshop, May 19, 2006
  \item Organizer of the 9th MetaComputing and Grid Workshop, July 26-28, 2006
  \item Program committee member of EuroPVM/MPI [since 2002]
  \item Program committee member of the Cray User Group [since 2000]
  \item Program committee member of HIPHERION’06 [Workshop at IEEE Cluster Conference 2006]
  \item Program committee member of Special Session on Concurrent Programming Environment at ICHIT 2006
  \item Member of the HPC Challenge Benchmark Award Committee [since 2005] (award at Supercomputing Conference Series)
  \item Chairman of the Scientific Advisory Board of the Swiss Center for Scientific Computing (CSCS)
  \item Member of the Scientific Committee of the French HPC Project FAME 2
  \item Chairman of the NEC User Group [NUG]
  \item Member of the HPC Customer Advisory Board of Microsoft
  \item Reviewing for the European Commission
  \item Member of the Editorial Board of Computational Technologies
  \item Member of the steering committee of the German e-science initiative d-grid
  \item Chairman of the Technology and Business Council of T-Systems SFR
  \item Scientific Advisor of the Triangle Venture Capital Group
  \item Reviewing for DFG
  \item Reviewing for BMBF
  \item Deputy Dean of the School of Mechanical Engineering of the University of Stuttgart
  \item Member of the Board of the Center of Competence for HPC of the State of Baden-Württemberg [hkw-bw], Germany
  \item Member of the Board of the “Computer Science Network Stuttgart/Informatik Verband Stuttgart”
  \item Member of the Board of the Virtual Dimension Center Fellbach [VDC]
  \item Member of the Advisory Board of the "Dr. Karl and Elisabeth Eisele Foundation", Fellbach, Germany
  \item Member of the Board of Trustees of the Foundation “Environment and Damage Prevention” of the SparkassenVersicherung
\end{itemize}

\begin{itemize}
  \item Program committee member for Conference EuroPVM/MPI, Bonn, September 17-20, 2006
  \item Co-Chairman, 7th Teraflop Workshop, November 21-22, 2007, Tohoku University, Sendai, Japan
  \item Co-Chairman, Ukrainian – German Workshop on Simulation on Supercomputers, September 11-14, Sevastopol, Ukraine
  \item Co-Chairman, German-Russian Workshop on HPC, July 23-27, 2007, Akademgorodok, Russia
  \item Co-Chairman, 6th Teraflop Workshop, March 26-27 2007, HLRS, Stuttgart, Germany
  \item Chairman of the 1st Parallel Tools Workshop Organizer, Best Practice in High Performance Computing using High Performance Computing Systems, August 09-20, 2007, Novosibirsk, Russia
  \item Program Committee, 16th International Conference on Software Engineering and Data Engineering [SEDE-2007], July 09-11, 2007, Las Vegas, Nevada, USA
  \item Program Committee, ISC’2007, June 27-30, 2007, Dresden, Germany
  \item Program Committee, IASTED International Conference on Parallel and Distributed Computing and Networks [PDCCON2007], February 13-15, 2007, Innsbruck, Austria
  \item Chairman of the award committee for the ISC’2007 Award, Dresden, Germany
  \item Co-Chairman, 5th Teraflop Workshop, November 20-21 2006, Tohoku University, Sendai, Japan
  \item Workshop Organizer, Best Practice in HPC Procurements, Supercomputing 2006, November 12, 2006, Tampa, FL, USA
  \item Program Committee, 2nd European Workshop on High Performance Computing, September 25-27, 2006, Oxford, UK
  \item Program Committee, Computational and Informational Technologies in Science, Technique and Education, September 20-22, 2006, Pavlodar, Kazakhstan
\end{itemize}
Co-chairman, 3rd Russian-German School on Parallel Programming using High Performance Computation Systems, August 28-September 08, 2006, Novosibirsk, Russia

Co-Chairman, 9th HLRS Metacomputing and Grid Workshop, July 26-28, 2006, Stuttgart, Germany

Co-Chairman, 4th Teraflop Workshop, March 30-31 2006, HLRS, Stuttgart, Germany

Chairman of the award committee for the ISC’ 2006 Award, Dresden, Germany

Program Committee, ISC’2006, June 27-30, 2006, Dresden, Germany

Program Committee, 3rd International Summer School and Scientific Workshop on High Speed Hydrodynamics and Numerical Simulation, June 22-28, 2006, Kemerovo, Russia

Co-Chairman, 5th Workshop on Scalable Global Parallel File Systems, April 03-05, 2006, Stuttgart, Germany

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**SABINE ROLLER**
- Project Manager of InGrid
- Member of D-Grid Steering Board
- Program Committee of D-Grid Security Workshop
- Program Committee of Industrial Grids Meeting
- Project Manager of Teraflop Workbench
- Program Committee of 6th Teraflop Workshop
- Program Committee of 16th CCSE Workshop on High Performance Computing on Vector Based Architectures - Recent Achievements and Future Directions
- Program Committee of 7th Teraflop Workshop
- Reviewer for American Mathematical Society (AMS), Mathematical Reviews

**MICHAEL SCHLIEPHAKE**
- University of Co-operative Education Stuttgart, lecturer for “Distributed Systems”
- Program Committee member of GSEM06 (Grid Services Engineering and Management)
- Program Committee member of eChallenges 2006 and eChallenges 2007
- Program Committee member of IST-Africa 2006 and 2007
- Program Committee member of GECON 2007 (Grid economics and Business Models)
- Program Committee member of Grid Workshop at IST-Mobile Summit 2006
- Program Committee member Unicore Summit 2006 and 2007
- Reviewer for Future Generation Computing Systems (FGCS)

**STEFAN WESNER**
- Program Committee member of GSEM06 (Grid Services Engineering and Management)
- Program Committee member of eChallenges 2006 and eChallenges 2007
- Program Committee member of IST-Africa 2006 and 2007
- Program Committee member of GECON 2007 (Grid economics and Business Models)
- Program Committee member of Grid Workshop at IST-Mobile Summit 2006
- Program Committee member Unicore Summit 2006 and 2007
- Reviewer for Future Generation Computing Systems (FGCS)
At HLRS are working 27 people as permanent staff, 47 as third party funded staff as well as 35 students on an international level. Guest scientists - for example from USA, Russia and India - are working here also in different projects.
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Dipl.-Inf. Kirill Dichev 60492
Dipl.-Inf. Valentín Himmler 87216
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Dipl.-Ing. Alexander Schulz 68039

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