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The year 2004 was marked by a number of changes at the Höchstleistungsrechenzentrum HLRS. These changes are seen in internal organization, systems operated, a new building and a new concept for collaboration with partners both regional and international.

At the system level HLRS started its migration path that led it towards a two-architecture concept. The first part of our next generation vector supercomputer was brought in early in 2004. The old SX-4 and SX-5 systems were dismantled and replaced by SX-6 systems that served as preparatory tools for the large SX-8 system to come in 2005. At the same time we were able to replace our old Cray T3E system by a cluster of AMD Opteron processor. It is these two lines (vector and cluster) that will form the back bone of our computing infrastructure.

HLRS has also extended its level of co-operation in 2004. It has further deepened its links inside Europe. This reports names 12 European projects in which HLRS is involved. The number reflects the international and collaborative research approach of our center. Furthermore HLRS has started negotiations about an integration of its resources in the DEISA infrastructure which forms the backbone of a European Supercomputing Infrastructure. These negotiations could be successfully finished in early 2005. As much as HLRS is part of an international community it also has strong regional ties. Collaboration in the center of simulation technology of the University of Stuttgart with Mathematicians, Computer Scientists, and Application Scientists has strengthened the scientific foundation of HLRS. Collaboration with the Universities of Karlsruhe and Heidelberg further highlights the potential of the technology region of Baden-Württemberg.
2 Organization

2.1 Structure

2.2 Staff

The year 2004 has seen an increase in staff numbers compared to the previous years. This is mainly due to an increase in external funding through projects. The head count on January 1st 2005 was as given:

<table>
<thead>
<tr>
<th>Category</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permanent</td>
<td>31</td>
</tr>
<tr>
<td>Third party funded staff</td>
<td>31</td>
</tr>
<tr>
<td>Research Ass. (Students)</td>
<td>25</td>
</tr>
<tr>
<td>Total</td>
<td>87</td>
</tr>
</tbody>
</table>

HLRS staff now totals 87 of which 3 are currently on parental leave. A breakdown of gender shows that percentage of female scientists has become relatively high. A general problem is that female PhD students tend to go on maternal leave and then break off their scientific career.

Guest Scientists

May 1st – July 15th
Prof. Barbara Chapman, Associate Professor at the Department of Computer Science, University of Houston, TX, USA. Prof. Chapman did work and lecturing in the field of OpenMP and compiler technology.

October 10th – November 20th
Dr. Haidong Li, Research Fellow, School of Engineering - University of Durham, UK. Li works on gas turbines and aero engines developments. In the framework of the HPC Europa Project, he developed a parallelization of his simulation software to use HPC systems.

July 8th – September 28th
Mrs. Olga Moldovanova, Fakultät für Rechentechnik und Informatik (FRTI), National Technical University Donetsk, Ukraine. Mrs. Moldovanova is working on simulation of mine ventilation systems.

July 15th – July 23rd
Dr. Andrea Cavalli, Department of Pharmaceutical Sciences, Bologna, Italy. HPC-Europa guest working on CPMD and Gaussian98 on NEC SX-6.

August 1st – September 5th
Mr. Horacio Gonzalez-Velez, School of Informatics, University of Edinburgh, UK. HPC-Europa guest working on the Edinburgh Skeletal package, eSkel using PACX-MPI.

October 11th – November 12th
Mrs. Sandra van der Graaf, Food and Bioprocess Engineering, Wageningen University, The Netherlands. HPC-Europa guest, working on parallellizing her Lattice-Boltzman.

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

This section describes changes in the configuration of systems that are available to the users of the HLRS. HLRS installs a new generation NEC supercomputer in 1H 2005. The number and size of PC-based Clusters has been increased.

3.1 NEC SX-8 576 M72

This is the latest generation of NEC’s vector system. HLRS builds a supercomputer by clustering NEC SX-8 nodes using NEC’s high performance crossbar interconnect. This system will deliver more than 4 TFLOPS sustained performance on a HLRS customers CFD application. System installation started in December 2004 and will be finished in June 2005. Production started with 36 nodes on March 23, 2005. The specification of the system is:

CPU: NEC SX-8, 2GHz
Number of CPUs: 8 per node, total of 576
Peak Performance: 12.7 TFLOPS
Memory: 9.2 TB
Interconnect: NEC IXS, 16 GB/s bidirectional
Disk Space: 160 TB

3.2 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.

CPU: NEC SX-6, 565 MHz
Number of CPUs: 8 per node, total of 40
Peak Performance: 361 GFLOPS
Memory: 512 GB
Interconnect: NEC IXS, 8 GB/s bidirectional
Disk Space: 160 TB

3.3 Cray Opteron Cluster

To reduce operational costs and increase performance and memory size for users of the Cray T3e MPP System the University of Stuttgart replaced it by an AMD Opteron based Cluster. The cluster is operational since 2Q 2004.

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

3.4 EM64T Platform

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

CPU: Intel Xeon EM64T, 3.2 GHz
Number of CPUs: 404
Peak Performance: 2.6 TFLOPS
Memory: 240 GB
Interconnect: Infiniband
Disk Space: 1 TB
The distribution of application fields in number of projects shows both the traditional strengths of HLRS and the type of architecture available in Stuttgart. The field of Computational Fluid Dynamics summarizes all activities that relate to flows. This includes climate research as well as blood flow simulation and traditional engineering CFD as is used in car and aerospace industries. These applications benefit from the vector supercomputer architectures. The second largest application field is physics together with solid state physics. These applications are typically found on the cluster like systems of HLRS.

4.2 Usage of the Systems

4.2.1 System Usage by Field

The strong role of CFD is emphasized again when looking at system usage. Almost 80% go to projects in this field. It is interesting to note that CFD is the strongest field both on vector based systems and on micro-processor based systems. The second strongest field on the cluster is solid state physics. The reader has to keep in mind, however, that both systems presented here are mainly transitional systems with the final supercomputer configuration being only available in 2005.
stand 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**

February 17 – 19, August 04 – 06, and November 29 – December 1 at ZHR 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 ZHR and NIC/ZAM in collaboration with HLRS.

March 8 – 12 at HLRS and September 13 – 17 in Kassel:
The focus is on iterative and parallel solvers, the parallel programming models MPI and OpenMP, and the parallel middleware PETSc. Thereby, different modern Krylov Subspace Methods (CG, GMRES, BiCGSTAB ...) as well as highly efficient preconditioning techniques are presented in the context of real life applications. Hands-on sessions will allow users to immediately test and understand the basic constructs of iterative solvers, the Message Passing Interface (MPI) and the shared memory directives of OpenMP. The workshop was organized by HLRS, IAG, and University of Kassel.

March 15 – 19 at HLRS:
The focus is on vectorization, optimization on new HLRS platforms, MPI-2 and MPI Performance Optimization, advanced topics in parallel programming with MPI, and advanced topics in shared memory parallelization with OpenMP. Hands-on sessions are included.

March 29 – April 2 at HLRS:
Numerical methods to solve the equations of Fluid Dynamics are presented. The main focus is on explicit Finite Volume schemes for the compressible Euler equations. Hands-on sessions will manifest the content of the lectures. Participants will learn to implement the algorithms, but also to apply given (black-box, commercial) software and to interpret the solutions correctly. Methods and problems of parallelization are discussed. This course is organized by HLRS, IAG, and University of Kassel, and is based on a computational practical awarded with the „Landeslehrpreis Baden-Württemberg 2003“ [held at University of Stuttgart, under auspices of the BMBF project NUSS, contract 08NM227].

October 11 – 15 at HLRS:
The focus was on programming models MPI and OpenMP, domain decomposition, parallelization with PETSc, and optimization. Hands-on sessions are included.

**4.3 Workshops**

<table>
<thead>
<tr>
<th>Date</th>
<th>Organizer</th>
<th>Location</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feb. 17-19, 2004</td>
<td>ZHR</td>
<td>Dresden</td>
<td>Parallel Programming</td>
</tr>
<tr>
<td>Mar. 8-12, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Iterative Linear Solver and Parallelization</td>
</tr>
<tr>
<td>Mar. 15-19, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Advanced Topics in High Performance Computing and Parallel Programming</td>
</tr>
<tr>
<td>Mar. 29-Apr. 2, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Introduction to Computational Fluid Dynamics</td>
</tr>
<tr>
<td>Aug. 4-6, 2004</td>
<td>ZHR</td>
<td>Dresden</td>
<td>Parallel Programming</td>
</tr>
<tr>
<td>Oct. 11-15, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Parallel Programming with MPI and OpenMP and Advanced Topics</td>
</tr>
<tr>
<td>Nov. 29-Dec. 1, 2004</td>
<td>NIC</td>
<td>Jülich</td>
<td>Parallel Programming</td>
</tr>
</tbody>
</table>

In these workshops 2004, more than 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.
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.

### 5.1 Lectures

<table>
<thead>
<tr>
<th>Lecturer</th>
<th>Title of Lecture</th>
<th>Semester</th>
<th>University</th>
</tr>
</thead>
<tbody>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (II)</td>
<td>SS 2004</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Mechanical Engineering</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (I)</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Mechanical Engineering</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (II)</td>
<td>SS 2004</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Automotive Engineering</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (I)</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Automotive Engineering</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (II)</td>
<td>SS 2004</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Technology Management</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td>Introduction to Computer Science (I)</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td></td>
<td>in Technology Management</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch,</td>
<td>Seminar on Computational Science and</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Peter Streiner</td>
<td>Engineering</td>
<td>SS 2004</td>
<td></td>
</tr>
<tr>
<td>Matthias Müller</td>
<td>C++ for Scientific Computing</td>
<td>SS 2004</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Claus-Dieter Muñz</td>
<td>Computer Practical on Numerical Fluid Mechanics</td>
<td>SS 2004</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>(IAG), Sabine Roller</td>
<td>Computer Practical on Numerical Gasdynamics</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>(IAG), Mark Ferch</td>
<td>Visualization of Technical and Scientific Data</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>(IAG), Sabine Roller</td>
<td>Microprocessors</td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Robert Piotter,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michael Resch</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uwe Wittmann</td>
<td></td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Peter Haas</td>
<td></td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
<tr>
<td>Uwe Küster</td>
<td></td>
<td>WS 2004/2005</td>
<td>Univ. of Stuttgart</td>
</tr>
</tbody>
</table>

### 5.2 100-online

Parallel Programming Workshop Online: The new courses at HLRS in 2004 (see Workshops) have been recorded with Lecturnity. The recording is available online in two formats [Lecturnity and RealMedia], see http://www.hlrs.de/organization/par/par_prog_ws/. A CD-version is in preparation.

### 5.3 PhD Thesis

Dipl.-Ing. Björn Sander, Numerische Untersuchung an einem abdominalen Aortenaneurysma [in German], Stuttgart, Germany, 2004. The thesis investigates abdominal aortic aneurysms. It describes numerical simulation of the flow of blood in such configurations as well as the movement of artery walls.
6 Research

6.1 Projects

This section covers in more detail the projects that were running or newly started in 2004. A complete list of currently running projects includes:

<table>
<thead>
<tr>
<th>Project</th>
<th>Funded by</th>
<th>Duration</th>
<th>Web page</th>
</tr>
</thead>
<tbody>
<tr>
<td>GeoHPC</td>
<td>Landesstiftung</td>
<td>01.09.2004 - 31.08.2006</td>
<td><a href="http://www.uni-tuebingen.de/zag/geoengineering/HPD/">http://www.uni-tuebingen.de/zag/geoengineering/HPD/</a></td>
</tr>
<tr>
<td>CrossGrid</td>
<td>European Commission</td>
<td>01.03.2002 - 30.04.2005</td>
<td><a href="http://www.crosgrid.org/">http://www.crosgrid.org/</a></td>
</tr>
<tr>
<td>Grid Application</td>
<td>DAAD</td>
<td>01.01.2003 - 31.12.2004</td>
<td></td>
</tr>
<tr>
<td>Infrastructure for General Bioinformatics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CoreGRID</td>
<td>European Commission</td>
<td>01.09.2004 - 31.08.2008</td>
<td><a href="http://www.coregrid.net/">http://www.coregrid.net/</a></td>
</tr>
<tr>
<td>Akogrimo</td>
<td>European Commission</td>
<td>01.07.2004 - 30.06.2007</td>
<td><a href="http://www.mobilegrids.org/">http://www.mobilegrids.org/</a></td>
</tr>
<tr>
<td>ELeGI</td>
<td>European Commission</td>
<td>01.02.2004 - 31.01.2008</td>
<td><a href="http://www.elegi.org/">http://www.elegi.org/</a></td>
</tr>
<tr>
<td>TrustCoM</td>
<td>European Commission</td>
<td></td>
<td><a href="http://www.eu-trustcom.com/">http://www.eu-trustcom.com/</a></td>
</tr>
</tbody>
</table>

6.1.1 National

6.1.1.1 GeoHPC

Abstract

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

Partners

Center for Applied GeoScience, University of Tübingen, HLRS

6.1.1.2 Lunar-probe

Abstract

The aim of this project is the simulation and design of an stationary 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. 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 Monte-Carlo (MC)-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.
6.1.2 International (European and Others)

6.1.2.1 HPC-Europa

Abstract

The HPC-Europa project is 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, accompanied by several networking and research activities.

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

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

Partners

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

6.1.2.2 GRIDSTART

Abstract

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

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

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

HLRS mainly contribute with its experience in the area of Problem Solving Environments; Tools and Grid Systems and will especially participate in design and further development of a Grid Application Management Tool.

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

6.1.2.3 Grid Application Infrastructure for General Bioinformatics

Abstract
The project will extend the Grid computing approach to the pre- and post-processing stage and also to the development phase of applications. It will thus not only allow to perform large scale computations, but also reduce the turn-around times for the complete scientific production cycle.

Applications include CT data modelling, protein folding and computational micro-array analysis.

Partners
The Partners in the project are HLRS and the National Center for High Performance Computing (NCHC), Taiwan.

6.1.2.4 CrossGrid

Abstract
CrossGrid is a European R&D project, which aims to develop, implement and exploit new Grid components for interactive compute and data intensive applications. Examples are simulation and visualization for surgical procedures, flooding crisis, distributed data analysis in high-energy physics, or air pollution combined with weather forecasting. The current CrossGrid testbed includes resources from 18 sites across 9 European countries.

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

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

6.1.2.6 GridCoord

Abstract
The GridCoord project aims at strengthening the co-operations amongst the European funding authorities and Grid projects in order to improve the coordination of the future activities in the field of Grid computing. Furthermore it plans to develop a roadmap for future Grid activities within the European Union and its associated states.

To reach its goals, GridCoord is organizing a series of workshops, each focusing on a specific interest and/or research group. The HLRS is organizing the GridCoord Industrial Workshop, a key event in this series, focusing on the requirements, plans
and current trends of European Industry. This includes software- and hardware vendors, service providers and end-users of various industrial fields.

**Partners**
The project consists of 13 partners, see http://www.cgridcoord.org/

### 6.1.2.7 LeGE-WG

**Abstract**
The Learning Grid of Excellence Working Group [LeGE-WG] aims to facilitate the establishment of a European Learning Grid Infrastructure by supporting the systematic exchange of information and by creating opportunities for close collaboration between the different actors in the formative process.

The Working Group operates on a 24 month basis and brings together actors with complementary interests in Grid computing and e-Learning from technology-oriented disciplines, pedagogy, government or regulating bodies and of course students. It will therefore provide an interdisciplinary consortium of experts and will promote close interaction between the communities associated with them, so as

- To achieve an in-depth understanding of the fundamental issues underpinning the application of GRID computing for e-Learning
- To cultivate the necessary common background for addressing the challenges associated with the establishment of a European Learning Grid Infrastructure
- To establish a solid baseline for full exploitation of the EU-US Co-operation Initiative on Science and Technology for e-Learning.

**Partners**
The consortium consists of 25 partners and is continuously extended. The organization of this large numbers is on a national node basis. The national nodes are Central Laboratory of the Research Councils [CLRC], Communication & Systemes - Systemes D’information [CS-SI], Dipartimento di Ingegneria dell’Informazione e Matematica Applicata [DIIMA], ZEUS Consulting S.A., SchlumbergerSema, HLRS, University of Graz, Kaunas University of Technology and EDAW (Principal Contractor).

### 6.1.2.8 GRASP

**Abstract**
The aim of GRASP project is to use Grid technology in order to realize current and future ASP business models that integrate distributed and heterogeneous resources. The main project objectives are:

- To design and implement a layered architecture for service provision using Grid technologies. To overcome weaknesses of current ASP solutions concerning resource management, security, definition of a service level agreement and pricing mechanism. For the realization of the services supplied by the Grid middleware, the consortium will use existing research results but, also study and evaluate the impact of COTS (such as the Microsoft .Net platform)
- To explore and evaluate three different business models that fully exploit the Grid technologies: a classical ASP [one-to-many model with one provider and many clients]; a many-to-many model where resource are heterogeneous and distributed and also the clients can make available their resource in order to receive an income); a federated model [where the provider is constituted by a federation of ASPs]
- To design three Grid-aware applications, developed using the GRASP architecture, in order to validate the effectiveness of the project results
- To define methodologies and techniques in order to make existing applications Grid-aware.

**Partners**
The GRASP consortium has been created with the aim to reach two objectives, both fundamental for the project to be successful. The first one is the implementation of an efficient infrastructure based on grid technologies. The second one is the integration of this infrastructure with an applicative level for execution of our business application and their provision to customers.

The partners are LogicDIS (GR), CRMPA (I), CCLRC (UK), SchlumbergerSema (ES), HLRS, and CS-SI (FR).

### 6.1.2.9 GeneSys

**Abstract**
The GeneSyS [Generic Systems Supervision] project’s mission is to enhance distributed systems and applications with a generic and standardized supervision solution and nurture its practical implementation and multi-sector exploitation as a key enabler for the competitiveness of European research and industry. The top-level objectives of the GeneSyS project are:

- To specify and develop an open, generic, modular and comprehensive supervision concept
- To integrate and validate this supervision structure within various industrial contexts
under the strategic objective of Grids for Complex Problem Solving with an overall budget of 11M€. The aim of the Akogrimo project is to architect and prototype a blueprint of a Next Generation Grids with exploits and closely co-operates with evolving Mobile Internet infrastructure based on IPv6. Accordingly, Akogrimo will bring together the market orientation and pervasiveness of mobile communication technology in everyday life with the promise of a dynamic concerted use of resources and services through a Grid infrastructure.

The main project objectives are:

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

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

Akogrimo Web page at: http://www.mobilegrids.org/

6.1.2.10 NextGRID

Abstract

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

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

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

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

Further information at: http://www.nextgrid.org/

6.1.2.11 Akogrimo

Abstract

The Akogrimo (Access to knowledge through the Grid in a mobile world) project is an Integrated Project in the sixth Framework Program of the European Commission under the strategic objective of Grids for Complex Problem Solving with an overall budget of 11M€. The aim of the Akogrimo project is to architect and prototype a blueprint of a Next Generation Grids with exploits and closely co-operates with evolving Mobile Internet infrastructure based on IPv6. Accordingly, Akogrimo will bring together the market orientation and pervasiveness of mobile communication technology in everyday life with the promise of a dynamic concerted use of resources and services through a Grid infrastructure.

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Akogrimo Web page at: http://www.mobilegrids.org/

6.1.2.12 TrustCoM

Abstract

The TrustCoM project is an integrated project funded by the European Commission in the sixth Framework Program.

The objective of TrustCoM [Trust and Contract Management] is to develop a framework which enables trustworthy business processing in dynamic virtual organizations [VOs]. Virtual Organizations are formed by various participants [companies, institutions, individuals, etc.] to supply services or produce goods co-operatively. The TrustCoM framework shall facilitate to securely share some resources [data, software, hardware] across organization boundaries, and to isolate others.
It will support the entire lifecycle of VO s, i.e. identification, formation, operation, and termination.

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

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

6.1.2.13 ELeGI

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

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

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

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

Partners
The Partners in this project are: RESIT, AtosOrigin, CCLRC, CEMSAC, CNRS, CRMPA, CRSA, CS SI, Microsoft EMIC, FAU Erlangen, FUNDP, HOU, KFU-Graz, UM2-Montpellier, University of Dundee, University of Southampton, UPPA, University of St. Andrews, and HLRS & Grid Middleware Assembly Workshop (PRAGMA 5), Hsinchu.

6.1.2.14 NATO Project

The NATO-funded project entitled Improving the Reliability of Computer Simulations to Predict Environmental Risks is a cooperation of the University of Houston, the University of Erlangen, the University of Stuttgart, and the Institute of Numerical Mathematics, Russia with Prof. Marc Garbey, University of Houston being the project leader. It focuses on the collaboration of the partners with regard to fault-tolerance of critical applications.

6.1.3 Industry

6.1.3.1 Teraflop Workbench

Abstract
The Teraflop Workbench will enable sustained Teraflop performance for a wide range of scientific and industrial applications. The Teraflop Workbench is a cooperation project between HLRS and NEC. The first 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. 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.

To show the application performance NEC and HLRS work together in selected projects with scientific and industrial developers and end users. Their codes come from areas like Computational Fluid Dynamics, Bioinformatics, Structural Mechanics, Chemistry, Physics, Combustion, Medical Applications and Nanotechnology.
6.2.2 New Co-operations established in 2004

- The HLRS is participating since September 2004 in the Open MPI effort, a joint collaboration between Los Alamos National Laboratories, Indiana University, the University of Tennessee, and some other institutions. In the frame of this co-operation, the HLRS has hosted a working meeting from September 13th to 17th, 2004.

6.3 Scientific Workshops

<table>
<thead>
<tr>
<th>Date</th>
<th>Organizer</th>
<th>Location</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>March 22-23, 2004</td>
<td>HLRS, hww</td>
<td>Stuttgart</td>
<td>3rd hww Workshop on Scalable Global Parallel File Systems</td>
</tr>
<tr>
<td>April 26-27, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Unicore User Workshop</td>
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<tr>
<td>April 27-28, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>4th International LeGe-WG Workshop</td>
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<tr>
<td>May 5, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Unicore User Workshop</td>
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<tr>
<td>May 6-7, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>1st Teraflop Workshop</td>
</tr>
<tr>
<td>July 5-7, 2004</td>
<td>HLRS, ICT</td>
<td>Novosibirsk, Russia</td>
<td>1st Russian-German School on Parallel Programming Using High Performance Computation Systems</td>
</tr>
<tr>
<td>September 13-17, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>OpenMPI Workshop</td>
</tr>
<tr>
<td>October 4-5, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>High Performance Computing in Science and Engineering – The 7th Results and Review Workshop of the HPC Center Stuttgart (HLRS)</td>
</tr>
<tr>
<td>December 9, 2004</td>
<td>HLRS</td>
<td>Stuttgart</td>
<td>Simulation and Virtual Reality for Small and Medium Size Companies</td>
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6.4 Conference Shows

- High Performance Networking Forum [HNF], March 19th, 2004, Hohenheim: VR presentation of a distributed online simulation over a 10-Gigabit/’s link
- WinHEC May 4th – 7th, 2004, Seattle, WA: Keynote presentation of online simulation steering in virtual environments with Bill Gates
- International Supercomputer Conference 2004 at Heidelberg, Germany, June 21st – 24th, 2004. HLRS booth together with the other national supercomputing centers [LRZ, NIC]
• nanoCAMP August 15th – 20th, 2004, Stuttgart: Tangible interface/Mixed
Reality presentation and workshop with German TV-Station 3-Sat
• Wissenschaftssommer September 25th – October 1st, 2004, Stuttgart: VR and AR presentation of research results
• Supercomputing Conference 2004 at Pittsburgh, PA, November 6th – 12th, 2004

6.5 Publications
6.5.1 Books

6.5.2 Journal Papers

6.5.3 Other Refereed Papers
6.5.4 Other Papers

3. Peggy Lindner, Rainer Keller, Matthias S. Müller, Michael M. Resch, DAMIEN - Project Successfully Completed, GRIDSTART Newsletter, Issue 6, pp. 9-11, April 2004

6.5.5 Tutorials


6.5.6 Talks

4. Stefan Wesner, Access to Knowledge through the Grid in a Mobile World, European Grid Technology Days 2004, September 2004
5. Stefan Wesner, Deploying Grids in a hybrid research-industrial environment, GGF10 Industry Track, September 2004
7. Andreas Kopecki, Uwe Wössner, Einsatz hybrider Prototypen in der Produktentwicklung, DaimlerChrysler CAE Forum, November 10th, Mühleningen
8. Andreas Kopecki, Uwe Wössner, Hybride Prototypen in kooperativen Umgebungen, Kooperation in virtuellen Umgebungen, June 28th, IAD Stuttgart
10. Michael M. Resch, The Role of Supercomputing Centres in Grids, NEC CCRLE 10th Anniversary Research Forum, Bonn, Germany, July 15th, 2004
12. Michael M. Resch, On the Status of Supercomputing in Germany, 10th ORAP Meeting, Paris, France, June 3rd, 2004
14. Michael M. Resch, Integrative Approaches in Supercomputing, ICA-Colloquium, University of Stuttgart, Stuttgart, Germany, May 17th, 2004
15. Michael M. Resch, NEC SX-Cluster and Cray Opteron Cluster, T-Systems HPCN Workshop, Braunschweig, Germany, March 22nd, 2004
17. Michael M. Resch and Matthias S. Müller, D-Grid – Auf dem Weg zur e-science in Deutschland, ZKI AK Supercomputing, Stuttgart, Germany, March 4th, 2004
6.5.7 Professional Activities

Thomas Bönisch
• Member of the program committee of the 14th Summer School on Computing Techniques in Physics, Trest Castle, Czech Republic, August 9th – 14th, 2004.

Edgar Gabriel
• Member of the program committee of the 10th International Workshop on High-Level Parallel Programming Models and Supportive Environments, to be held in conjunction with the IPDPS 2005, Denver, CO, April 4th – 8th, 2005
• Member of the program committee at the Second International Workshop on Programming Paradigms for Grids and Metacomputing Systems (PGaMS’05), Atlanta, GA, May 22nd – 25th, 2005
• Member of the program committee at the First International Workshop on Programming Paradigms for Grids and Metacomputing Systems (PPGaMS’04), Krakow, Poland, June 7th – 9th, 2004
• Member of the program committee of the International Conference on Computational Science 2005 (ICCS 2005), Atlanta, GA, May 22nd – 25th, 2005.

Matthias S. Müller
• Program committee member of HPC Asia 2004, 20th – 22nd, July 2004, Tokyo, Japan
• Member of the program committee of the 10th International Workshop on High-Level Parallel Programming Models and Supportive Environments, to be held in conjunction with the IPDPS 2005, Denver, CO, April 4th – 8th, 2005.

Rolf Rabenseifner
• Program committee member for EuroPVM/MP (since 2002)
• Program committee member of the Cray User Group (since 2000)
• Program committee member for PPGaMM Workshop at ICCS (since 2004)
• Program committee member of ParCo 2005 (Malaga, Spain)
• Program committee member of ISPA’05 (Nanjing, China).

Michael M. Resch
• Member of the Scientific Advisory Board of the Swiss Center for Scientific Computing (CSCS), Switzerland
• Director of the Center for Simulation Technology / Zentrum für Simulationstechnik (ZST) of the University of Stuttgart, Stuttgart, Germany
• Speaker of the Board of the Center of Competence for HPC of the State of Baden-Württemberg (hkz-bw), Germany
• Member of the steering committee of the German e-science initiative d-grid
• Reviewing for the European Commission
• Technical Papers Committee of Supercomputing 2004, Pittsburgh, PA, November 6th – 12th, 2004
• Technical program committee of the 1st international workshop on data processing and storage networking: towards Grid computing (DPSN04), Athens, Greece, May 14th, 2004
• Organizing committee of the European Workshop on High Performance Computing, Paris, France, September 19th – 22nd, 2004
• International Program Committee of the International Conference on Computational Technologies and Mathematical Modeling for Science, Engineering and Education in Alma Aty, Kazakhstan, October, 6th – 10th, 2004
• Chairman of the award committee for the ISC’2004 Award, Heidelberg, Germany, June 22nd – 25th, 2004
• Co-Organizer and program chair of the 7th HLRS Metacomputing Workshop, Stuttgart, Germany, April 26th – 27th, 2004
• Member of the program committee for PDCN’04, Innsbruck, Austria, February 17th – 19th, 2004.

Stefan Wesner
• Member of the Program committee of the Second International Conference on Trust Management 2004
• Program committee of Akogrimo workshop at Practical Aspects of Knowledge Management 2005.