Services at HLRS

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High-Performance Computing-Center Stuttgart (HLRS)
www.hlrs.de

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Service Areas

- HPC Systems → Thomas Beisel
  - **High end systems → federal center**
  - **Clusters and development systems → for Uni. Stuttgart**
- Numerical Methods & Libraries → Uwe Küster
  - **Compilers & Processors**
- Parallel Computing → Rolf Rabenseifner
  - **Training**
  - **Application Services**
    - in Chemistry, Fluid Dynamics, Physics, Structural Mechanics
- Applications, Models and Tools → Rainer Keller
  - **Parallel Programming Models (MPI, OpenMP)**
  - **Profiling & Debugging Libraries/Tools**
- Visualization → Uwe Wössner
  - **COVISE, Video & Conferencing Service**
- Support of Federal Projects → Heinz Pöhlmann
- Teraflop Workbench → Thomas Bönisch
  - **Optimization / Porting Support**

HPC Systems → Thomas Beisel

- High end systems → federal center
- Clusters and development systems → for Uni. Stuttgart

- Co-operation with NEC
- Vectorization Support
- Special needs in system management, e.g., jobs on 64 or 72 nodes
- Consulting in disk/data management
- Annual **Workshop on Scalable Global Parallel File Systems**

The team:

HLRS:
Thomas Beisel
Bernd Krischok **Dieter Raith**
Peter Haas **Rolf Supper**

http://www.hlrs.de/hw-access/platforms/
http://www.hlrs.de/news-events/events/

Numerical Methods & Libraries → Uwe Küster

- Compilers
- Processors

- Benchmarking of compilers and processors
- Vectorization & optimization support for numerical methods
- Numerical libraries

The team:

HLRS:
Uwe Küster
Denis Altmann **Peter Lammers**
Tünde Erdei **Nina Shokina**
Elke Krumrück **Manuela Wossough**

http://www.hlrs.de/organization/num/

Parallel Computing → Rolf Rabenseifner

- Training
  - Parallelization Consulting
- Application Services / Consulting
  - in Chemistry, Fluid Dynamics, Physics, Structural Mechanics

- …

The team:

HLRS:

Rolf Rabenseifner	→ **Training, Consulting**
Panagiotis Adamidis	→ **Parallelization Consulting**
Martin Bernreuter	→ **Structural Mechanics / CAE**
Norbert Ibold	→ **Physics**
Heinz Pöhlmann	→ **Chemistry, federal projects**
Martin Winter	→ **CFD**

http://www.hlrs.de/organization/par/
http://www.hlrs.de/news-events/events/

Application Software Packages at HLRS

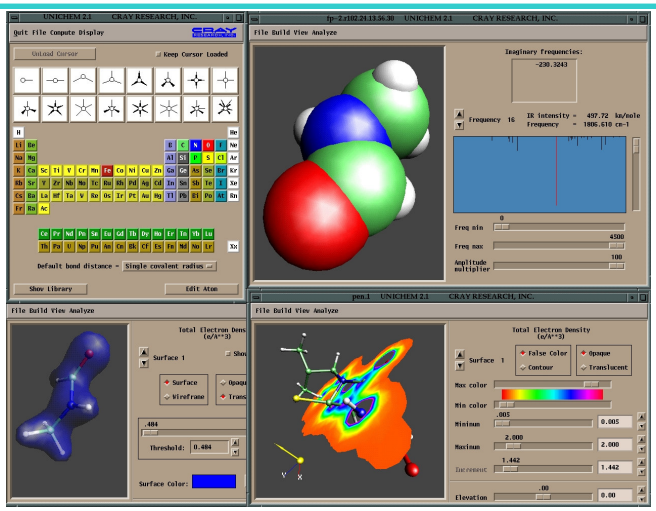
Computational Chemistry
- GAMESS-US, GAUSSIAN, MOLPRO, MOPAC 6, TURBOMOLE

Computational Fluid Dynamics
- CFX, FASTEST-3D, FIDAP, FIRE, FLUENT, POLYFLOW, StarHPC

Structure Mechanics
- ABAQUS, HyperMesh, LS-DYNA3D, PERMAS

Due to the wide range of methods and procedures available in every software package, each individual problem case has to be considered separately to select and to use suitable software package(s).

Computational Chemistry – Pre- and Postprocessing



Application Software Packages at HLRS

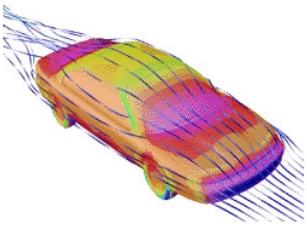
	NEC SX-8	Cray Opteron Cluster	NEC Xeon EM64T Cluster	HP zx6000 ia64-Cluster	Volvox
Computational Chemistry					
GAMESS-US	available				
GAUSSIAN94	available				
GAUSSIAN98	available				
MOLPRO96	available				
MOLPRO98	available				
MOLPRO2000	available				
MOLPRO2002	available				
MOPAC 6	available				
TURBOMOLE					
Fluid Dynamics					
CFX		available	available	available	available
FIDAP		available	available	available	available
FIRE		available	available		available
GAMBIT		available	available		available
GRIDGEN		available	available		available
ICEM-CFD		available	available		available
FLUXEXPERT					available
FLUENT		available	available	available	available
PLOYFLOW		available	available		
STAR-HPC		available	available	available	available
SWIFT		available	available		available

Status
Sep. 11, 2006

Actual version → http://www.hlrs.de/organization/aw/services/awpakete.html

Computational Fluid Dynamics

Wide range of application areas



- Automotive aerodynamics
- Airflow around aircraft wings
- Combustion
- Flow in melts
- Heat exchanger tubes (heating and cooling)
- Flow around turbine blades

Application Software Packages at HLRS

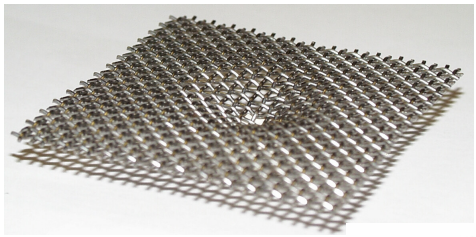
	NEC SX-8	Cray Opteron Cluster	NEC Xeon EM64T Cluster	HP zx6000 ia64-Cluster	Volvox
Structure Mechanics					
ABAQUS		available		available	available
ANSYS				available	
HyperMesh					
LS-DYNA3D	available	available			
PERMAS				available	

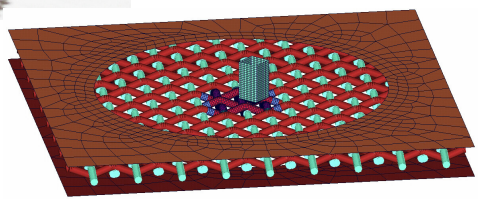
Status
Sep. 11, 2006

Actual version → http://www.hlrs.de/organization/aw/services/awpakete.html

Structure Mechanics - Example: Impact on a fencing mask

mask (wire fabric) must resist penetration by a broken blade



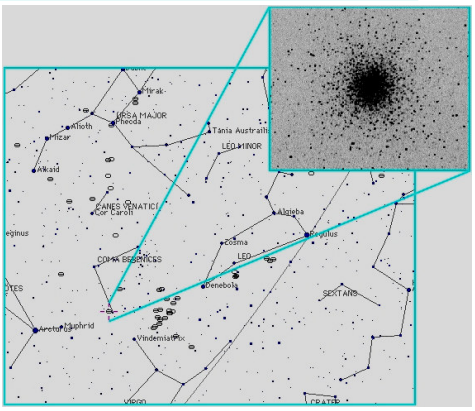


Computational Physics

Areas of application

- Solid-state physics
- Astrophysics
- quantum physics
- high energy physics

- mainly using in-house codes
  - only a few program packages available



Applications, Models and Tools → Rainer Keller

- Parallel Programming Models (MPI, OpenMP)
- Profiling & Debugging Libraries/Tools

- Parallel Debuggers and Correctness Tools:
  - **DDT, Totalview, Valgrind, Marmot, Thread Checker**
- Performance Libraries & Analysis Tools:
  - **OPT, Trace Collector, Trace Analyzer, Vtune, Thread Profiler, MKL, Paraver**
- Annual HLRS Metacomputing and Grid Workshop

The team:

HLRS:
Rainer Keller
Bettina Krammer **Katharina Benkert**
Alexander Schulz **Sabine Roller**
Sven Stork **Sunil Reddy Tiyyagura**

http://www.hlrs.de/organization/amt/

Visualization → Uwe Wössner

- COVISE
- Video Service
- Conferencing Service
- Virtual Environmental Lab
- Augmented Reality

- see also [30] *Virtual reality based visualization* [**talk and demo in the Cave**]

The team:

HLRS:
Uwe Wössner
Martin Becker **Mario Baalcke**
Michael Braitmaier **Florian Niebling**
Blasius Czink **Jutta Sauer**
Andreas Kopecki **Uwe Zimmat**

http://www.hlrs.de/organization/vis/

Support of Federal Projects → Heinz Pöhlmann

- Review Process for project proposals → Steering Committee
- Each federal project on NEC SX-8 has a **dedicated advisor**
- Annual **Result and Review Workshop** at HLRS

The team:

HLRS:
Heinz Pöhlmann
Martin Bernreuther
Thomas Bönisch
Natalia Currle-Linde
Norbert Ibold
Rainer Keller
Uwe Küster
Peter Lammers
Isabel Loebich
Rolf Rabenseifner
Martin Winter

http://www.hlrs.de/userprojects/
http://www.hlrs.de/news-events/events/

Teraflop Workbench → Thomas Bönisch

- Optimization / Porting Support

- Make **new** science and engineering possible with **Teraflops sustained performance**
- Assess and demonstrate system capabilities for industry-relevant applications
- **Cooperation** project between HLRS and NEC.
- Annual **Teraflop Workshop** at HLRS

The team:

HLRS:
Thomas Bönisch
Katharina Benkert
Peter Lammers
Sunil Reddy Tiyyagura

NEC:
Martin Galle
Stefan Borowski
Stefan Haberhauer
Fredrik Svensson

http://www.teraflop-workbench.de/
http://www.hlrs.de/news-events/events/

Research

- HLRS active in many EU, federal, and states research projects

Groups:

- Distributed Systems → Stefan Wesner et al.
  - **e.g., AKOGRIMO, NextGrid, …**
- Applications, Models & Tools → Rainer Keller et al.
  - **e.g., HPC Europa, Open MPI, InGrid, …**
- Visualization → Uwe Wössner et al.
  - **e.g., COVISE, CoSpaces, …**
- Project & User Management, Accounting → Thomas Bönisch et al.
  - **e.g., DEISA**

Summary / Questions?

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  - **Optimization / Porting Support**

Appendix

Application Support at HLRS

- More than 15 years experience in consulting and user support
- Support in problem solving in the area of computer simulation for science and engineering
- Support service for federal research projects and local university
- Content and area-specific consulting by staff members with scientific background
- Selection, licensing, installation, maintenance and tests of relevant application software packages
  - on supercomputers
  - on workstations (for pre- and postprocessing)

Application Support at HLRS

- Main scientific areas include
  - Chemistry
  - Physics
  - Computational Fluid Dynamics
  - Structure Mechanics
- All staff members have a scientific background and degree
- All staff members are skilled in high performance computing
- *Scientists talking to scientists*

Application Support at HLRS

- Comprehensive application support
- Extensive consulting and problem analysis
- Develop problem solving strategies
- User support in creating models, in selection of software and software usage
- User support in generating input data sets, working in pre- and postprocessing and interpreting results
- Support in optimization of user program codes
- Close cooperations if desired

Application Support at HLRS

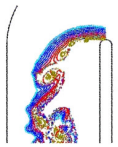
- Selection of appropriate software packages

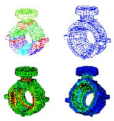
- Close coordination with actual user demand
- Software must be suitable and optimized for supercomputers
- Optimal usage of supercomputer resources
- Use of vectorised and/or parallelised program versions
- Central installation and maintenance allow efficient usage of latest software versions
- License conditions are intensively negotiated with software vendors to provide favourable conditions for the users

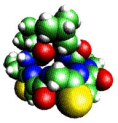
Application Support at HLRS

- Aims of scientific and technical computer simulations

- Improvement and optimization of equipment
- Significant reduction of development time and costs
- Avoid or reduce test series and prototype development
- Solution of complex problems in basic research







Computational Chemistry

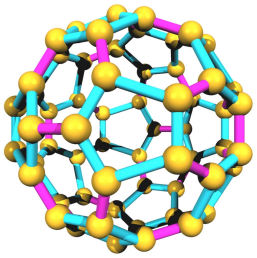
Determination of molecular properties - 3 main methods

- Molecular mechanics and dynamics using force fields
  100.000 - 1.000.000 atoms, computational effort ~ N^2,
  classical mechanics, empirical potential functions
- Semiempirical methods
  1.000 - 10.000 atoms, computational effort ~ N^3,
  quantum mechanics, approximated Schrödinger equation,
  integral calculations using additional empirical data
- ab initio methods
  100 - 500 atoms, computational effort ~ N^4,
  quantum mechanics, exact Schrödinger equation,
  integral calculations without any empirical data,
  systematic improvement of approximations

(N = number of degrees of freedom)

Computational Chemistry

Areas of application



- Polymers and new materials
- Catalysis and surface chemistry
- Drug design
- Protein design and structure determination
- Electronic properties and excited states
- Exploration of structure-activity relationships
- Chemical reactions (e.g.: intermolecular rearrangements)

Software packages used

- GAMESS-US, GAUSSIAN, MOLPRO, MOPAC 6, TURBOMOLE

Computational Physics

Example: Astrophysics

- Stellar dynamics of a globular cluster
- A system of about 100.000 – 1 million stars orbiting around each other
- Classical experiments cannot be performed, only accessible by numerical simulations
- Needs about 100 GFlop for 100.000 stars
  and 100 TFlop for 1 million stars
- Timescale 1 million years
- Massive parallel code implemented in MPI
- Limited to about 50.000 stars using 512 PE's on the CRAY T3E

Computational Fluid Dynamics

- Numerical simulation based on Navier-Stokes equations
- Finite volume, finite element, finite difference and spectral methods
- Laminar and turbulent models
- Thermodynamics including heat transportation in fluid and solid phase
- Heat radiation
- Chemical reactions
- Multi phase flow
- Acoustics
- Electromagnetic field influences

Software packages used

- CFX, FASTEST-3D, FIDAP, FIRE, FLUENT, POLYFLOW, StarHPC

Structure Mechanics

Finite element analysis

Areas of application

- Forming engineering
- Deformations and strains in materials
- Crash analysis
- Fracture analysis
- Equipment engineering
- Automotive engineering
- Heat engineering
- Thermohydraulics

Software packages used

- ABAQUS, HyperMesh, LS-DYNA3D, PERMAS