Application Support at HLRS

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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

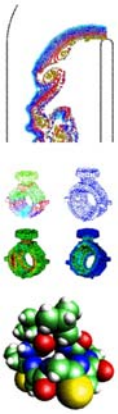
- Selection of appropriate software packages

- 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

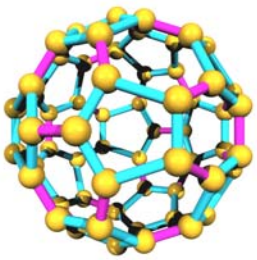
Determination of molecular properties - 3 main methods

- 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

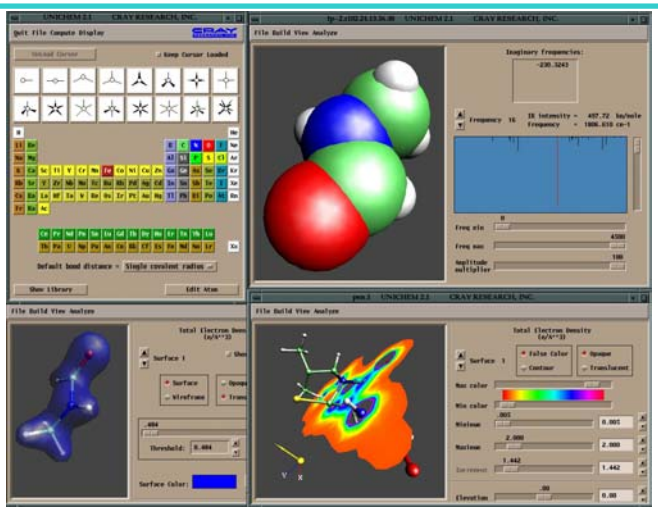


- Polymers and new materials
- Catalysis and surface chemistry
- Drug design
- Protein design and structure determination
- Electronic properties and excited states
- Exploration of structure-activity relationships
- Chemical reactions (e.g.: intermolecular rearrangements)

Software packages used

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

Computational Chemistry – Pre- and Postprocessing



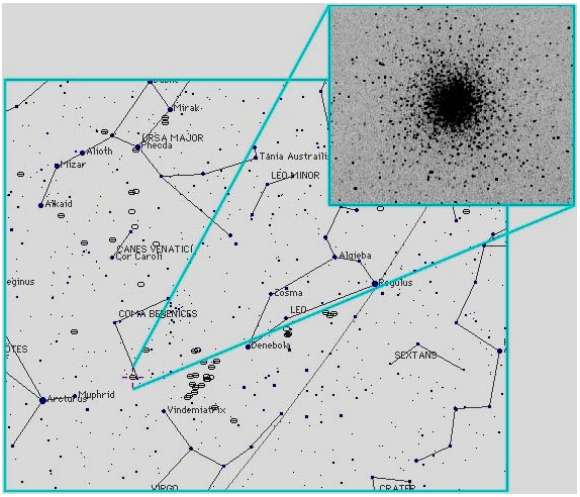
Computational Physics

Areas of application

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

- mainly using inhouse codes,
  only a few program packages available

Computational Physics – Example: Astrophysics



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

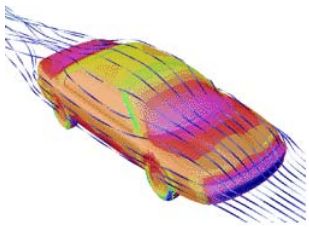
- Numerical simulation based on Navier-Stokes equations
- Finite volume, finite element, finite difference and spectral methods
- Laminar and turbulent models
- Thermodynamics including heat transportation in fluid and solid phase
- Heat radiation
- Chemical reactions
- Multi phase flow
- Acoustics
-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

Software packages used

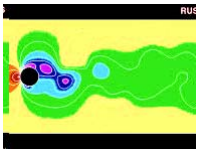
- CFX, FASTEST-3D, FIDAP, FIRE, FLUENT, POLYFLOW, StarHPC

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



Subsonic flow around cylinder, Re=2000,
Color coded pressure distribution, vortex development

Structure Mechanics

Finite element analysis

Areas of application

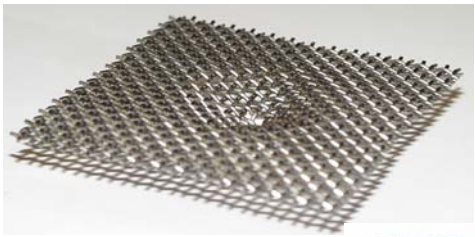
- Forming engineering
- Deformations and strains in materials
- Crash analysis
- Fracture analysis
- Equipment engineering
- Automotive engineering
- Heat engineering
- Thermohydraulics

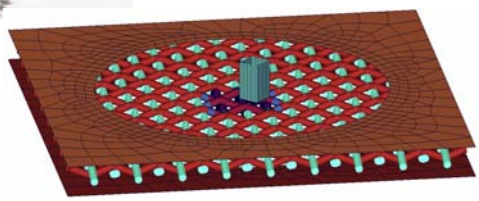
Software packages used

- ABAQUS, HyperMesh, LS-DYNA3D, PERMAS

Structure Mechanics - Example: Impact on a fencing mask

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





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).

Application Software Packages at HLRS

Application Software Packages on HLRS Computers

	NEC SX-4 NEC SX-5	CRAY T3E	HP-V2250	SGI ONYX-2
GAMESS-US	available	available		
GAUSSIAN94	available			
GAUSSIAN98	available	available		
MOLPRO96	available			
MOLPRO98	available			
MOPAC 6	available			
TURBOMOLE		available		
CFX	available			
FASTEST-3D	available			
FIDAP	available		available	
FIRE	available	available		
FLUENT	available	available	available	
POLYFLOW			available	
StarHPC	available	available		
ABAQUS	available		available	
HyperMesh				available
LS-DYNA3D	available	available		
PERMAS	available			