High-Performance Computing in an Industrial Setting

Dr. José Gracia
High Performance Computing Center (HLRS)
University of Stuttgart
Outline

• HLRS in a nutshell

• industrial setting and offering

• a show-case: RECOM Services
Who am I?

- studied Physics at Heidelberg Univ.
- PhD in Theoretical Astrophysics (numerical simulation)
- 6 years Postdoc in Greece and Ireland

HPC from a user perspective
- joined HLRS in 2009

HPC from a research perspective
- lead parallel programming and tools group

HPC from a service provider perspective
HIGH-PERFORMANCE COMPUTING CENTER STUTTGART (HLRS)
High Performance Computing Center Stuttgart (HLRS)

Höchstleistungsrechenzentrum Stuttgart

• Central service unit / facility of the University of Stuttgart (tier-2)
• One of three national HPC centres (JSC, LRZ; tier-1)
• Hosting member of PRACE (tier-0)

  Provides computing resources to academic users

• Stakeholder in public-private joint-venture HWW

  Provides computing resources to industrial users
The Mission of Supercomputing
# History of HLRS

<table>
<thead>
<tr>
<th>University Level</th>
<th>Federal Center and PPP for Industrial Usage</th>
<th>Growing Science &amp; Education</th>
<th>European Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>• 1960 High Performance Computing</td>
<td>- 1995 First NEC System</td>
<td>• 1999 NSF/USA Award</td>
<td>- 2007 Co-Founder of Gauss Center for Supercomputer</td>
</tr>
<tr>
<td>• 1982 First German Cray System</td>
<td>- 1995 Foundation of HWW for co-operation with industry</td>
<td>• 1999 Initiated European Grid pilot project</td>
<td>- 2011 ITEA Award for project ParMA</td>
</tr>
<tr>
<td>• 1986 Co-Financing of a Cray by Porsche</td>
<td></td>
<td>• 2003 Winner of HPC Challenge at SC’03</td>
<td>- 2011 First PFLOP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• 2004 First TFLOP</td>
<td>- 2012 European provider for PRACE</td>
</tr>
</tbody>
</table>
Current flagship system - Hermit

Cray XE6 system:

- Peak Performance \( \sim 1 \text{PFLOP/s} \)
- 38 racks with 96 nodes each
- 3552 compute nodes
- Each compute node has 2 sockets with AMD Interlagos @ 16 cores each
  total of 113,664 cores
- 2.7PB storage capacity @ \( \sim \) 150GB/s IO bandwidth
- Additional nodes for external access, pre- & post-processing, remote visualization, etc.
- \( \sim \)2MW power consumption
HLRS as an research institution

- Broad experience in collaborative research projects on national, European and international level

- Funding per year:
  - 3,9 M€ state funding
  - 5,0 M€ project funding

- Staff:
  - ~ 25 permanent staff
  - ~ 70 project staff (PhD, Postdocs)
  - ~ 30 research assistants
Research topics

• Exascale Computing:
  – Programming models
  – Programming tools
  – Fault-tolerance
  – Energy efficiency

• Computational science:
  – Molecular Dynamics
  – Optimization
  – Medical Engineering
  – Visualization

• (Big) Data Management
• Cloud Computing
Why use supercomputers?

- Reality
- Physics
- Math.
- Programming
- Simulation
The Region of Stuttgart as a partner

**BOSCH**
- Turnover: 51.4 Mrd. €
- Staff: 300,000

**KÄRCHER**
- Turnover: 1,526 Mrd. €
- Staff: 7,452

**DAIMLER**
- Turnover: 97.7 Mrd. €
- Staff: 260,100

**STIHL**
- Turnover: 2.4 Mrd. €
- Staff: 11,310

**MAHLE**
- Turnover: 5.3 Mrd. €
- Staff: 47,500

**Porsche**
- Turnover: 7.79 Mrd. €
- Staff: 12,722
Our vehicles to work with industry

- public-private joint venture hww
- Cluster of Excellence “Simulation Technology”
- Automotive Simulation Centre Stuttgart (ASCS)
- public research project with industrial participation
Public-Private Partnership

• Stakeholders:
  – HLRS/Universität Stuttgart (18.75%)
  – T-Systems & T-Systems sfr (40%)
  – Porsche AG (10%)
  – State of Baden-Württemberg (12.5%)
  – Karlsruhe Institute of Technology (18.75%)

• Purpose:
  – provision of parallel computing resources
  – cloud-services for HPC
HLRS industrial customers in 2013
Industrial usage

CPU/Core hours sold

- 140,000,000
- 120,000,000
- 100,000,000
- 80,000,000
- 60,000,000
- 40,000,000
- 20,000,000
- 0

Cluster of Excellence “Simulation Technology”

- German Initiative of Excellence
- 10 year project (2007 – 2017)
- 60 Mio € Funding by DFG
- 7 Specific Research Fields
- More than 100 Researchers
- Industrial Collaboration
SUSTAINABLE SIMULATION CONCEPT FOR AUTOMOTIVE INDUSTRY
Members of ASCS

Automotive OEM
- Daimler
- Porsche
- Opel

Hardware vendors
- Cray
- NEC

Research
- University of Stuttgart
- FKFS
- Fraunhofer Gesellschaft
- Karlsruhe Institute für Technologie

Software vendors
- Siemens Industry Software GmbH
- SFE GmbH
- Mentor Graphics Deutschland GmbH
- INTES GmbH
- ESI Group
- Engineous Software GmbH
- DYNAmore GmbH
- Dassault Systemes Simulia GmbH
- CD-dapco
- Altair Engineering GmbH
Industrial HPC strategy of state of Baden-Württemberg

coordination and SME support

solution centers

computing resources

Research and service centers

June 2014
Academic and industrial training 2015

- New Education & Training Center
  - 300m² education space
  - 40 m² office space
  - Special equipment for HPC training

- New training concepts
  - Extension of existing training activities
    (25 courses / 600 participants)
  - European training center
  - Cooperation with the local industry (ca. 200 – 300)
INDUSTRIAL SHOW CASE: RECOM SERVICES GMBH
RECOM Services GmbH – business area:

Optimisation of combustion of fossil fuels for large electric power plants through numerical simulations on supercomputers
Schematics of a combustion furnace

Fire Side

Fuel Gas:
NOx, CO, SOx, Unburnt carbon, Particulate/Ash, CO₂

Overfire Air
Fuel & Air

Heat Transfer

Water-/Steamside

Steam

Water

67 m

12 m
Simulating real processes in virtual reality

Visualisation of simulation result

3D combustion model
code: RECOM-AIOLOD

Simulation on supercomputers:
NEC-SX9 at HLRS

De optimisation of the furnace yields:
- Reduction of emission
- Increase of availability on efficiency of power plant
- Reduction of CO2 emission

June 2014
RECOM-AIOLOS: Performance

- Linear
- ParMA Optimized - Hybrid 4MPIx2OpenMP
- ParMA Optimized - Pure MPI
- Original Application - Pure MPI

Performance increase of 49%
Initial solution

Oxygen [vol.-%, tr.]

Char [kg/kg]

CO [vol.-%, tr.]
Optimal solucion

Oxygen [vol.-%, tr.]

Char [kg/kg]

CO [vol.-%, tr.]
Economic results

• Increase of the efficiency of the power plant:
  – savings in fuel cost: 125,000 € per year
  – reduction of CO2 emission: 16,000 t per year

• RECOM has acquired large-volume industrial contracts to conduct similar optimisations -> new business area
  – Thermal treatment of sewage sludge
    (Eisenmann, Holzgerlingen, Germany)
  – Integration of a carbon-capture-and-storage plant with a gas-fired power station
    (Fichtner, Stuttgart, Germany)
  – Energy transfer in large heat-exchangers
    (Martin, Munich, Germany)
OTHER EXAMPLES OF INDUSTRIAL USAGE
Molecular Dynamics

Institute of Thermodynamics and Thermo Process Engineering
University of Stuttgart

Immersive Protein Visualization
Medical Engineering
Augmented reality in manufacturing (Automotive ind.)
Conclusions

• HLRS maintains tight relations to industry on regional and national level

• A significant fraction of the usage of HLRS systems is due to industry through a public-private joint venture (hww)
  – industrial users have access to the latest supercomputing systems at very economic cost
  – the generated income benefits our users from academia and other public bodies
Thank you for your attention!

Questions: gracia@hlrs.de