Gauss Centre for Supercomputing

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Managing Director

HPC User Forum 2017 / HLRS - Stuttgart
Gauss Centre for Supercomputing:

Leading Tier-0 HPC-Centre in Europe

- Alliance of the Three German Tier-0 Centres
  - Jülich Supercomputing Centre (JSC),
  - High Performance Computing Centre Stuttgart (HLRS),
  - Leibniz Rechenzentrum (LRZ), Garching

Key Facts

- To date in sum more than 20 Petaflops (continuously expanding)
- 400 people for Operation, HPC-research, Services, Training
- Extensive know-how in key scientific fields
Key Success factors of GCS

How to manage an alliance of geographically distributed centers?

Organization
  • association as a management holding
  • common governance and funding
  • open access for users to all GCS HPC-resources by common peer-review process

User Relationship Management
  • specialized user support, focusing on specific HPC topics
  • wide-range training concepts (PATC, Summerschool, Workshops, …)

Integrated Life Cycle Management
  • Application driven architecture variety
  • permanent feed-back by user- and application requirements
  • Three-fold round-robin type of Installation
More than 400 active scientific projects:

Recent corresponding papers and publications in

- Astrophysics
- Chemistry
- Computational Fluidodynamics
- Computer Science
- Earth and Environment
- High Energy Physics
- Material Science
- Life Science
- Solid State Physics
- Techniques and Tools
Scientific reports
Anwenderprojekte – wissenschaftliche Verwertung (Beispiele, S. 1)

Projekt: Kinetics and Thermodynamics of Conformational Changes Upon Protein Association Studied by Molecular Dynamics Simulations – published on GCS-Website: October 2016  
PI: Martin Zacharias, Lehrstuhl für Molekulardynamik, Physik-Department T38, TU München  
15 mio core hours on SuperMUC → Nature Comms. 7 (2016): http://www.nature.com/articles/ncomms10848

Projekt: Finite-Temperature Lanczos Simulations of Magnetic Molecules – (Website: September 2016)  
PI: Jürgen Schnack, Fakultät für Physik, Universität Bielefeld (Germany)  
8,8 mio core hours on SuperMUC → Nature Comms 4, (2014): http://www.nature.com/articles/ncomms6321

Projekt: In Silico Exploration of Prebiotic Peptide Synthesis by Ab Initio Metadynamics (Website: 09/2016)  
PI: Dominik Marx, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum  
320+ mio core Hours on JUQUEEN (GCS Large Scale Calls #8, #10, #12, #14)  
→ Nature Communications 5 (2013): http://www.nature.com/articles/ncomms6321

Projekt: 2+1+1 Lattice QCD Calculations With HEX Smeared Clover Fermions (Website: 10/2016)  
PI: Kalman Szabo, FZ Jülich, IAS, Jülich Supercomputing Centre  
69 mio core hours on JUQUEEN (GCS Large Scale Call 12)  

Projekt: Axion Cosmology and the Topological Susceptibility at Finite Temperature  
PI: Zoltan Fodor, Theoretische Physik, Bergische Universität Wuppertal)  
129 mio core hours on JUQUEEN (GCS Large Scale Calls #12 + #14)  
→ http://www.nature.com/nature/journal/v539/n7627/full/nature20115.html
Anwenderprojekte – wissenschaftliche Verwertung (Beispiele, S. 2)

Projekt: Dynamical Processes in Semiconductor Nanostructures (published on Website: Juni 2016)
PI: Gabriel Bester, University of Hamburg and the Hamburg Centre for Ultrafast Imaging (Germany)
14 m core hours on Hazel Hen of HLRS

Scientific and Computational Engineering

ANSYS, HLRS, and Cray Set New Supercomputing Record (HPC-Wire)
November 15, 2016 PITTSBURGH, Penn., Nov. 15

ANSYS (NASDAQ: ANSS), the High Performance Computing Center (HLRS) of the University of Stuttgart and Cray Inc. have set a new supercomputing world record by scaling ANSYS Fluent to over 172,000 computer cores on the HLRS supercomputer Hazel Hen, a Cray XC40 system – enabling organizations to create innovative and groundbreaking complete virtual prototypes of their products faster and more efficiently than ever. ANSYS, HLRS and Cray have pushed the boundaries of supercomputing by achieving a new supercomputing milestone by scaling ANSYS software to 172,032 cores on the Cray XC40 supercomputer, hosted at HLRS, running at 82 percent efficiency. This is nearly a 5x increase over the record set two years ago when Fluent was scaled to 36,000 cores.
239 Project Reports (22.11.2016)

Scientific Areas:
- Astrophysics: 35
- Elementary Particle Physics: 44
- Environment & Energy: 6
- Life Sciences: 27
- Materials Sciences & Chemistry: 33
- Computational and Scientific Engineering: 64

http://www.gauss-centre.eu/
HPC services

• Visualisation Facilities
• User Support
• Implementation Support
• Tool Development
• Training

All information available:
http://www.gauss-centre.eu/
Training Courses, Workshops

180 courses per year
2000 attendees

http://www.gauss-centre.eu/ gauss-centre/EN/Training/AllDates/_node.html
The Future of GCS

HPC Simulation Service Provider
Centre of Competence

Advanced User Support
and Training

Integrated
Lifecylemanagement
User- / Community Requirements

Applications
• Extreme Scaling
• Ensemble Simulations, Parameter Studies
• Memory Intense Extreme Computing
• Big Data / Analytics / Information retrieval
• Real Time Computing
• Machine Learning

Services
• providing specialized know-how and services for specific scientific fields
  • Multi-Method, Multi-Model, Multi-Scale Methods
  • Application Tuning
  • Data Management
Thank you!