

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, ...)

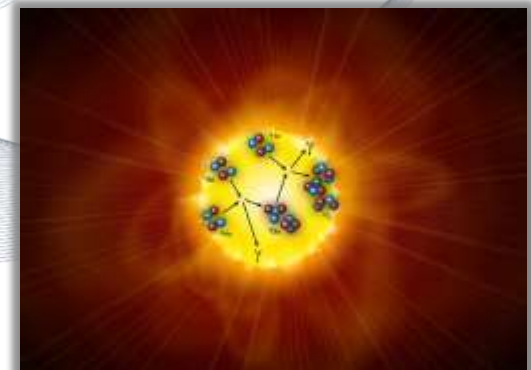
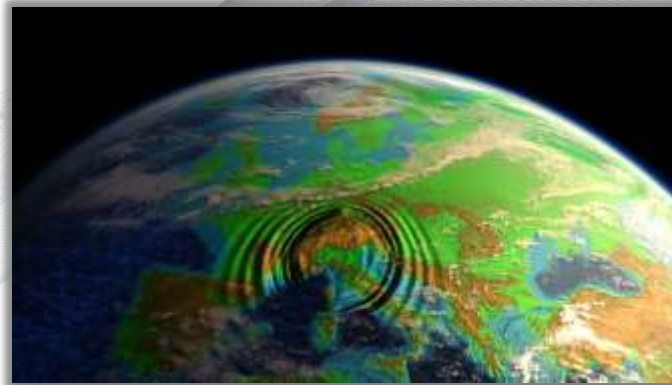
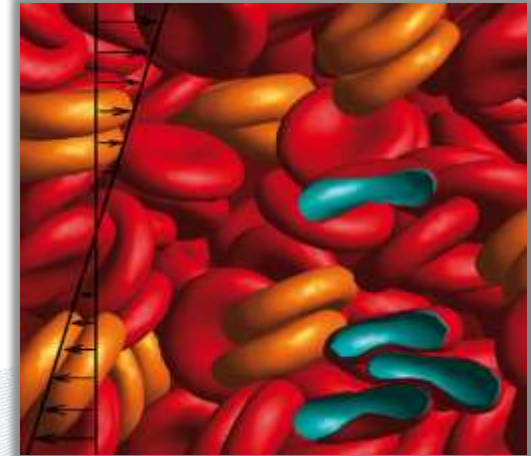
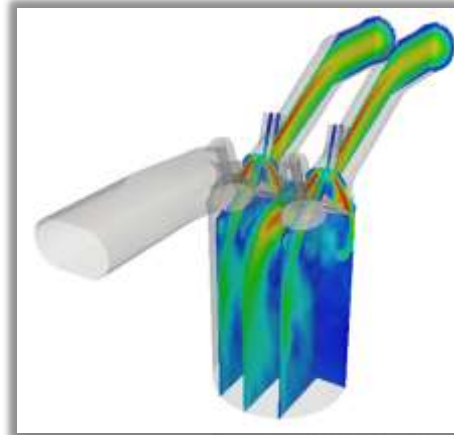
Integrated Life Cycle Management

- Application driven architecture variety
- permanent feed-back by user- and application requirements
- Three-fold round-robin type of Installation

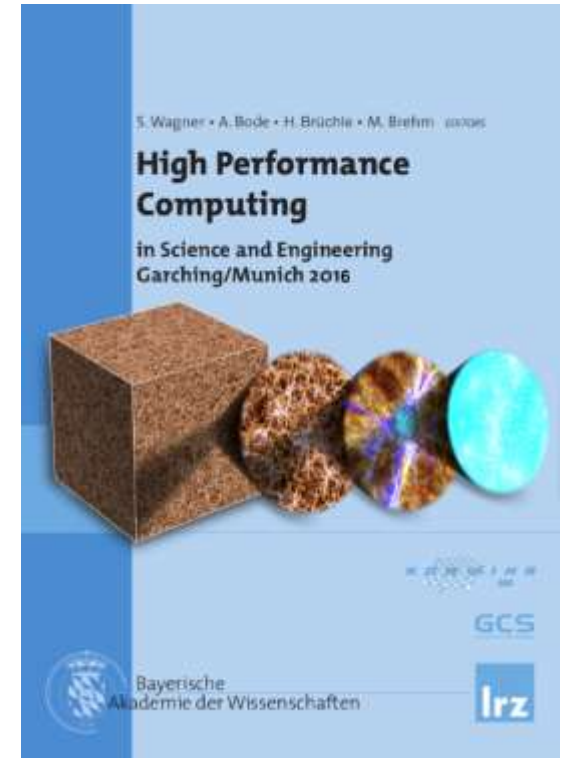
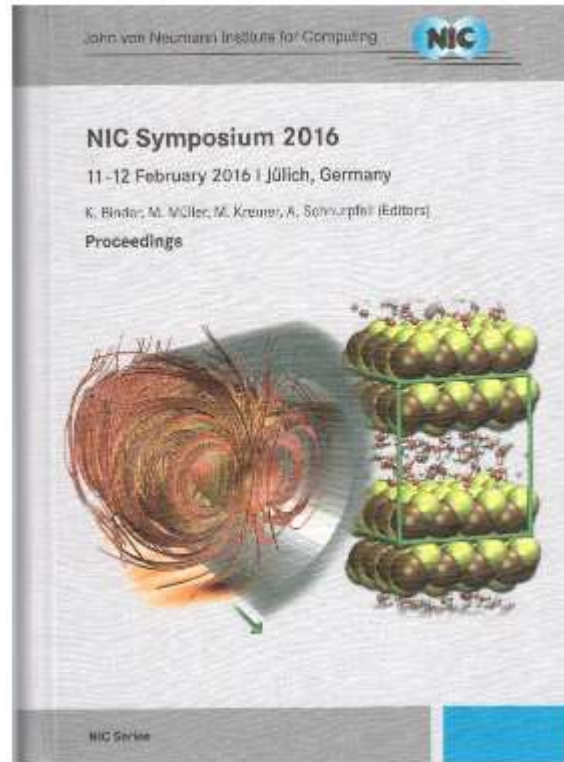
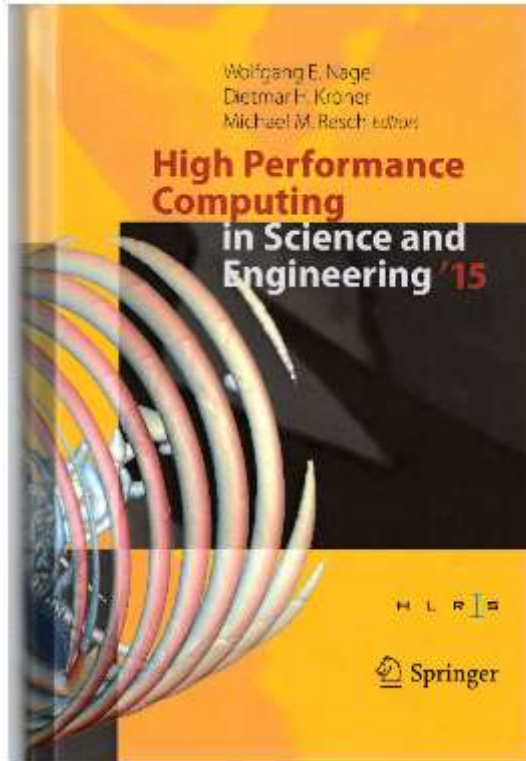
More than 400 active scientific projects:

Recent corresponding papers and publications in

- Astrophysics
- Chemistry
- Computational Fluidynamics
- 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)

→ Physical Review Letters 2016: <http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.116.172001>

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

→ Physical Review Letters 2015: <http://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.085305>

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/>

The screenshot shows the GCS website homepage with the following content:

- Navigation Menu:** HPC SERVICES | TRAINING & WORKSHOPS | PROJECTS | NEWS & EVENTS | ABOUT GCS
- Header:** GCS Gauss Centre for Supercomputing
- Search Bar:** A search input field with a 'Go' button.
- News Section:**
 - NEWS NEWS NEWS**
 - HLRS at CeBIT 2017 (Hall 6, Booth #B30)**

Feb. 24, 2017. Meet the High Performance Computing Center Stuttgart at CeBIT 2017 in Hannover (March 20-24) on the booth of Baden-Württemberg International/BWI in Hall 6 (Booth # B30). [More](#)
 - GCS at ISC'17 in Frankfurt**

The Gauss Centre for Supercomputing will participate in ISC'17 in Frankfurt/Main (June 18-22, 2017). Find GCS and its members HLRS, LRZ, and JSC at booth #B1310. [More](#)
 - Prestigious Award for Britta Nestler**

Dec. 9, 2016. Britta Nestler of KIT, user of GCS HPC systems, has been awarded with the prestigious Gotfried Wilhelm Leibniz Prize 2017. [More](#)
 - SCC 2016: One Week, 14 Teams, No Sleep...**

Dec. 8, 2016. GCS congratulates teams PivClub (TUM) and seqFALt (FAU) for a "job very well done" at SCC'16. [More](#)
- Service Section:**
 - Supercomputing at the Leading Edge A Key Technology for Science and Engineering**

The Gauss Centre for Supercomputing (GCS) provides the most powerful high-performance computing infrastructure in Europe to serve a broad range of research and industrial activities in various disciplines. GCS is the alliance of the three national supercomputing centres High Performance Computing Center Stuttgart (HLRS), Jülich Supercomputing Centre (JSC), and Leibniz Supercomputing Centre, Garching near Munich (LRZ).

 - About GCS
 - Projects
 - HPC Services and Computing Time**

GCS boosts computational science and engineering by offering a world-class computing and networking infrastructure. Each GCS centre hosts supercomputer systems well beyond the Teraflops performance mark, placing all three individual GCS institutions amongst the most powerful computing centres in the world. The system architectures implemented at the three GCS centres are complementary to ensure that a broad spectrum of applications can be accommodated. Furthermore, all three GCS centres feature state-of-the-art visualisation facilities and provide a wide range of tools and services for optimal user support. [More](#)

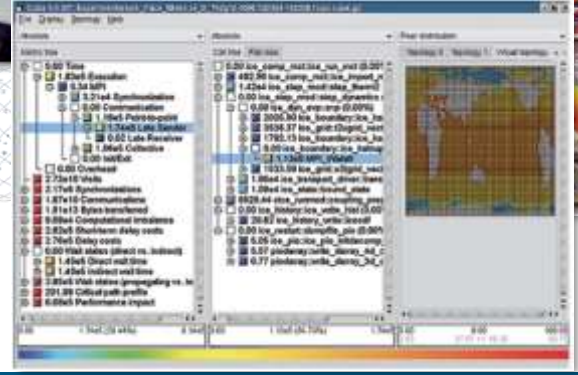
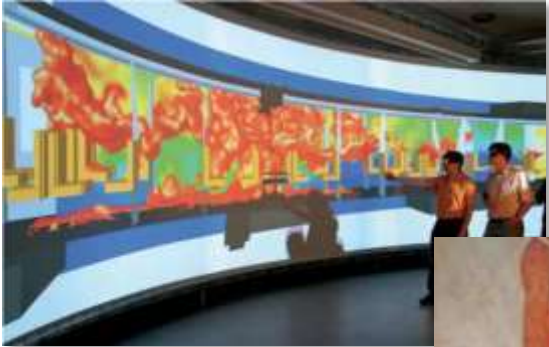
 - How to apply for computing time
 - HPC systems
 - Training courses**

GCS proudly provides first class training opportunities for German and international researchers and scientists. A large pool of highly qualified scientists as trainers with a training experience of well over 300 trainer-years ensures a superb quality of the comprehensive training program offered, which helps enable users of HPC infrastructures to maximize efficiency and research output on supercomputing systems. [More](#)
- Footer:** IMPRINT | CONTACT



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 screenshot shows the GCS website's 'Training & Workshops' page. At the top, there is a navigation bar with links for 'HPC SERVICES', 'TRAINING & WORKSHOPS', 'PROJECTS', 'NEWS & EVENTS', and 'ABOUT GCS'. Below this is the GCS logo and a search bar. The main content area is titled 'Training and Workshops' and is divided into three sections: 'Training courses', 'PATC - PRACE Advanced Training Centre', and 'Workshop and conferences'. Each section includes a brief description and a 'More' link. The 'Training courses' section mentions that GCS provides first-class training opportunities for German and international researchers. The 'PATC - PRACE Advanced Training Centre' section notes that GCS was nominated as a PRACE Advanced Training Centre in 2012. The 'Workshop and conferences' section states that GCS brings the national and international HPC user community together for mutual knowledge and expertise exchanges. Each text block is accompanied by a small photograph showing people working at computers or in a meeting.

HPC SERVICES | TRAINING & WORKSHOPS | PROJECTS | NEWS & EVENTS | ABOUT GCS

GCS

Gauss Centre for Supercomputing


GCS Home | Training & Workshops | Go

Training & Workshops

- Training courses
- PATC courses at GCS
- Workshops
- All dates


Training courses

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PATC - PRACE Advanced Training Centre

In 2012, GCS was nominated as a PRACE Advanced Training Centre (PATC). In this function, GCS offers part of its courses according to a transnational PATC curriculum. Additionally, GCS trainers participate in PRACE Seasonal Schools and run tutorials at international conferences. [More](#)



Workshop and conferences

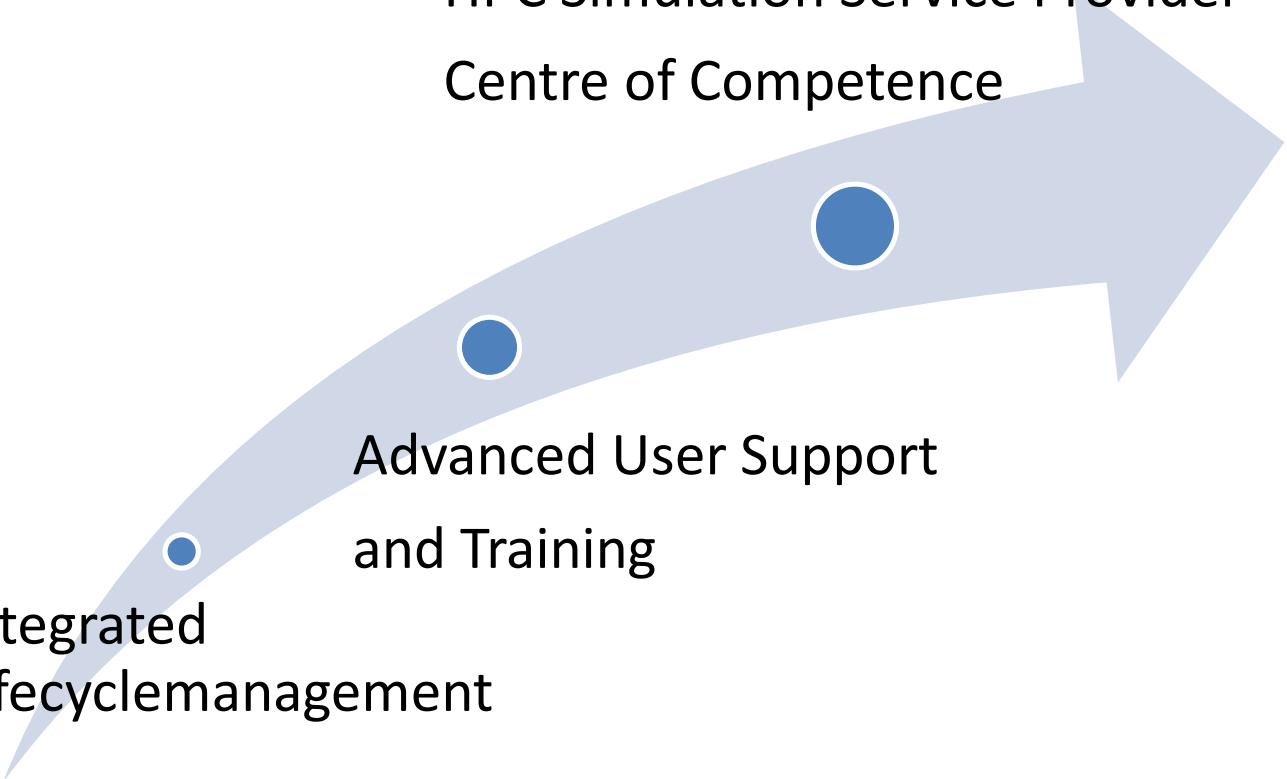
GCS brings the national and international HPC user community together for mutual knowledge and expertise exchanges on a regular basis. At recurring scientific workshops and seminars, researchers gain insight into their work and jointly discuss their results and findings as well as look at possible new solution approaches for the many challenges facing the HPC community. [More](#)





The Future of GCS

HPC Simulation Service Provider
Centre of Competence



Advanced User Support
and Training

Integrated
Lifecyclemanagement

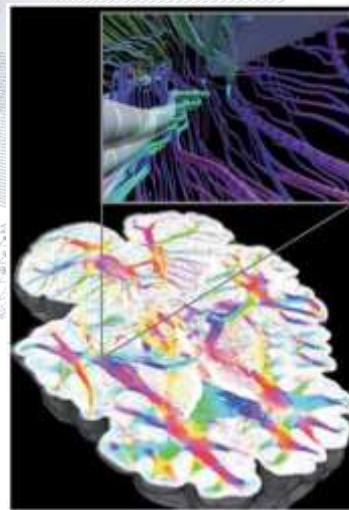
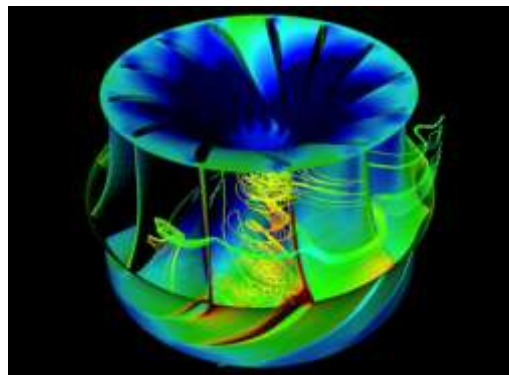
User- / Community Requirements

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!