

Leibniz Supercomputing Centre – site update

Salvatore Cielo, LRZ

LRZ in a nutshell



LRZ as IT Service Provider

Daily digitalisation affecting every aspect of our lives, many research, teaching, and administrative processes at universities nowadays require a myriad of IT services. LRZ supports these processes in numerous ways, ranging from communications infrastructure (such as email and web services) to e-learning platforms, from enablement of breakthrough scientific findings through computational simulations to archiving of result datasets. The Munich Universities, Ludwig-Maximilians-Universität München (LMU) and Technical University of Munich (TUM) both have access to these services directly from LRZ or to use as their IT service provider. Other Bavarian universities also have access to LRZ's services.

Consulting and Support

LRZ offers clients a wide range of training and individual consulting, covering all aspects of IT relevant to research and academia. It negotiates state-wide educational rates for software licenses and provides professional antivirus software free of charge for all of its clients.

Information security and data protection have always been a core competency of LRZ, both in its guiding principles and in its daily operations.

Through the partnership initiative *IT²*, the LRZ offers domain-specific, customized services and close cooperation for computer-aided scientific endeavours.



Exterior view of the LRZ building
at the Technical University of Munich (TUM)



LRZ as Supercomputing Center

The LRZ has been operating world-class supercomputers for decades.

The current supercomputer, the SuperMUC-NG, is no. 6 of the most powerful computers in the world with a peak performance of 36.6 Petaflops (almost 30 quadrillion operations per second). With 718 Terabytes main memory, 50 Petabytes external data storage, and a high-speed interconnect, the SuperMUC-NG provides research information technology for researchers in the fields of e.g. physics, chemistry, life sciences, geography, climate research, and engineering. Throughout the entire computing process, the LRZ focuses closely on supporting our users so they can take optimal advantage of all the resources we have to offer. Last but certainly not least, SuperMUC-NG's innovative water-water cooling system makes it one of the most energy-efficient supercomputers worldwide.

Centralized IT Systems at LRZ

LRZ operates systems for which local operations would be technically infeasible or economically inefficient. In addition to multiple servers for email, video and streaming services, for instance, LRZ also offers its clients a range of central systems including data storage, automatically executed nightly tape systems storing tens of thousands of Terabytes of backup and archiving data in millions of files.

LRZ operates not only supercomputers, it also runs Linux clusters and virtual machines for a wide variety of scientific requirements, including High Performance Computing, Cloud Computing, and Big Data.



SuperMUC-NG supercomputer
at the Technical University of Munich (TUM)

LRZ in a nutshell



Munich Research Network
(Munich Research Network, MNRN)

Full coverage - from Munich to the top of the alpine mountain Zugspitze and even to the peak of the Zugspitze, Germany's highest mountain - 1,300 network components, 3,000 VPN access points, and over 100,000 connected devices. The Munich Research Network (MNRN) operated by LRZ for universities, colleges, Max-Planck Institutes, and various other scientific research facilities is remarkably capable. The various VPN facilities and the 3G/4G are connected via a backbone network with up to 100 Gbit/s and to the Internet with more than 24 Gbit/s.

Within the MNRN scientific network, 20 Petabytes of data are transferred every month. Of those 20 Petabytes, approximately 2 Petabytes are sent or received over the Internet.

Energy Efficient Operations - Green IT

Water-water cooling, energy aware supercomputing, reuse of waste heat by deployment of absorption chillers, energy monitoring - these are just a few of the measures undertaken by LRZ to keep the energy usage for IT and supercomputing as low as possible. Proactive network and active research ranging from hardware improvements over energy efficient algorithms to optimizing facilities management, are all hallmarks of the commitment of LRZ to Green IT. Furthermore, 100% of the electricity it uses comes from renewable energy sources.

The 100th anniversary of the
Munich Research Network
Munich Research Network



Research and Development at LRZ
Research and Development at LRZ
Research and Development at LRZ
Research and Development at LRZ

Research and Development at LRZ

These approaches to the analysis of large volumes of data (Big Data), reducing energy usage of large IT systems, improving data security, or supporting a transition to a green world all present new challenges for computer science. By connecting research and development with practical operational experience, LRZ plays a key role in pushing the envelope to meet these challenges. By developing state-of-the-art IT services, the LRZ supports scientific excellence along with its partners in countless regional, national, and European research projects in a wide variety of fields including astrophysics, climate research, medical technology, nanotechnology, architecture, and mobility.

Virtual Reality and Visualization Center

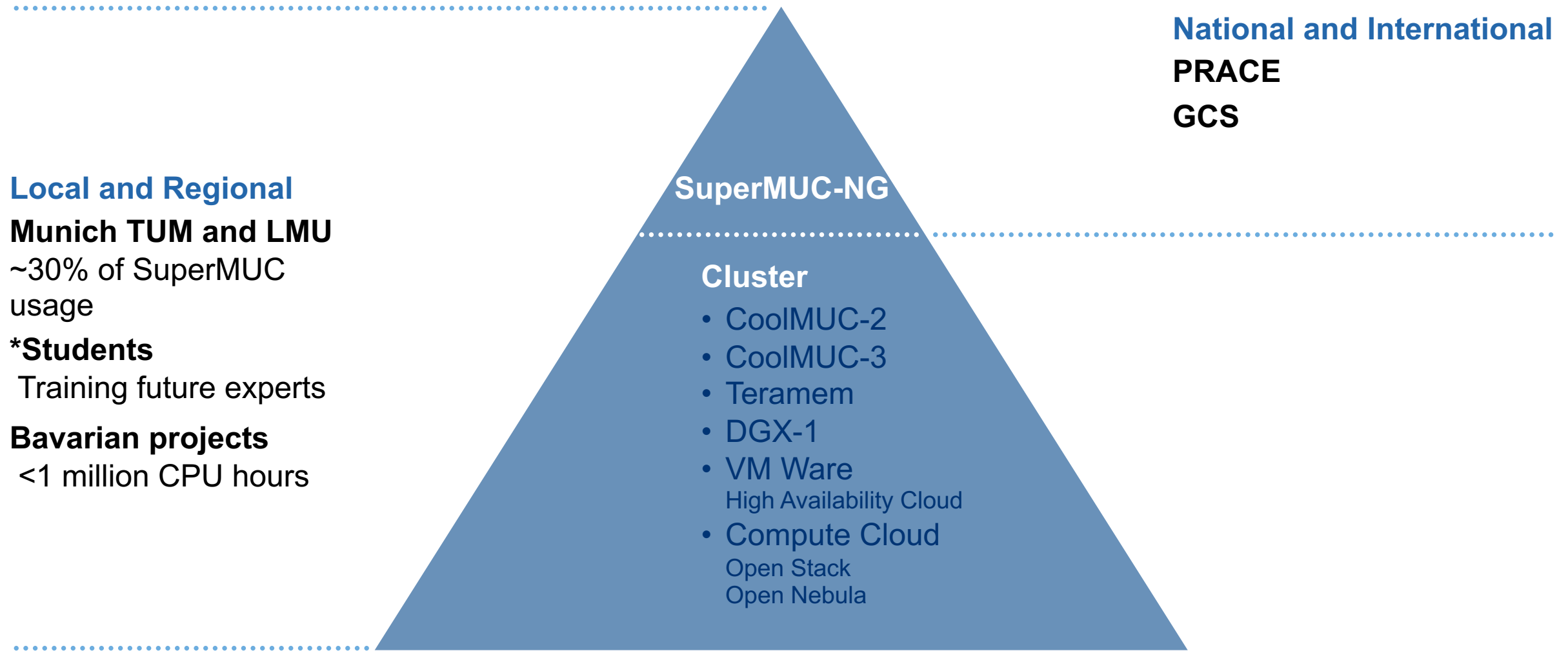
The Virtual Reality and Visualization Center (VRC) at LRZ offers custom technologies to visualize scientific data. This allows for a more rapid advancement and significant enrichment of scientific knowledge. The study of potentials is understood that data and beyond new innovations in data is greatly improved by the three dimensional, high-resolution data projection on the Projection Wall, by the use of the flat-panel projection installation, and by the interactive navigation panels in the VRC leading to breakthroughs in understanding and interpreting results. In addition to being used in the natural sciences and in technology, simulation results in humanities and social science research are also visualized using the VRC, for instance in the form of art and multimedia, archeology, and psychology.

Support for the
Munich Research Network





LRZ Systems and Access



System Overview

SuperMUC-NG (Next Generation)



Specs

- Peak Performance: 26.7 Pflop/s
- 719 Tbyte main memory and
- 70 Pbyte disk storage
- 6,480 Lenovo ThinkSystem nodes with Intel Xeon processors (Skylake)
- 311,040 compute cores
- Intel Omni-Path interconnects
- Direct hot water cooled + Adsorption coolers (47 C)

HPC + Cloud

- Usage of own and individual virtual machines (integrated cloud)
- Pre- and post-processing with user's individual software
- Integrated development, ability to use familiar software and tools
- Remote visualization and integration to V2C

SuperMUC-NG (Next Generation)



#9

in the world
Overall performance
(as of June 2019)



#1

in the world
Data-intensive applications
SSSP benchmark

#5

in the world
Data-intensive applications
BFS benchmark



#1

System in the EU



HPCwire Award
for Energy Efficiency

200 research fields

7.6 Billions

Compute hours utilized



5.6 Millions

Computing jobs performed



750

Research projects supported



1,995

Researchers as users



Highlights

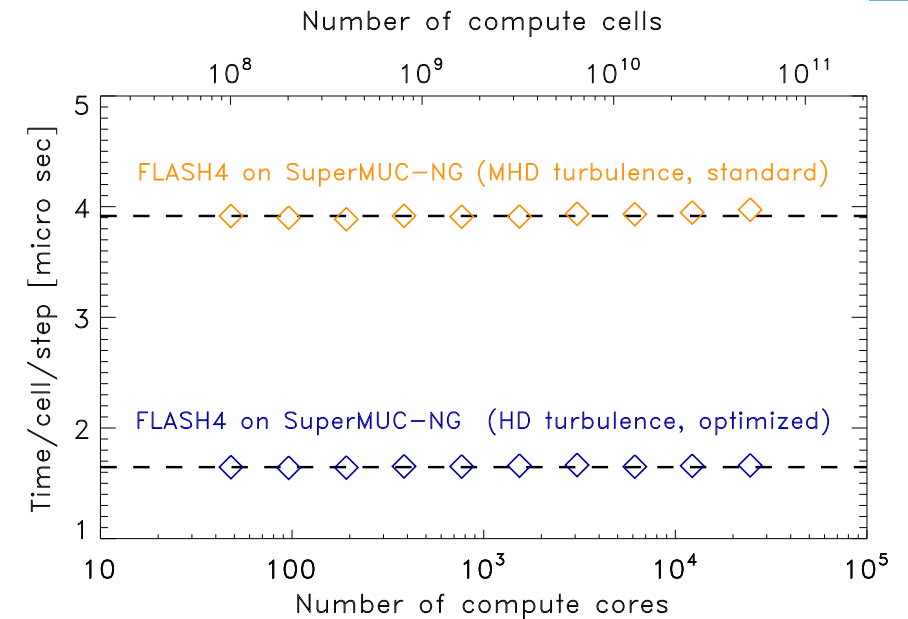
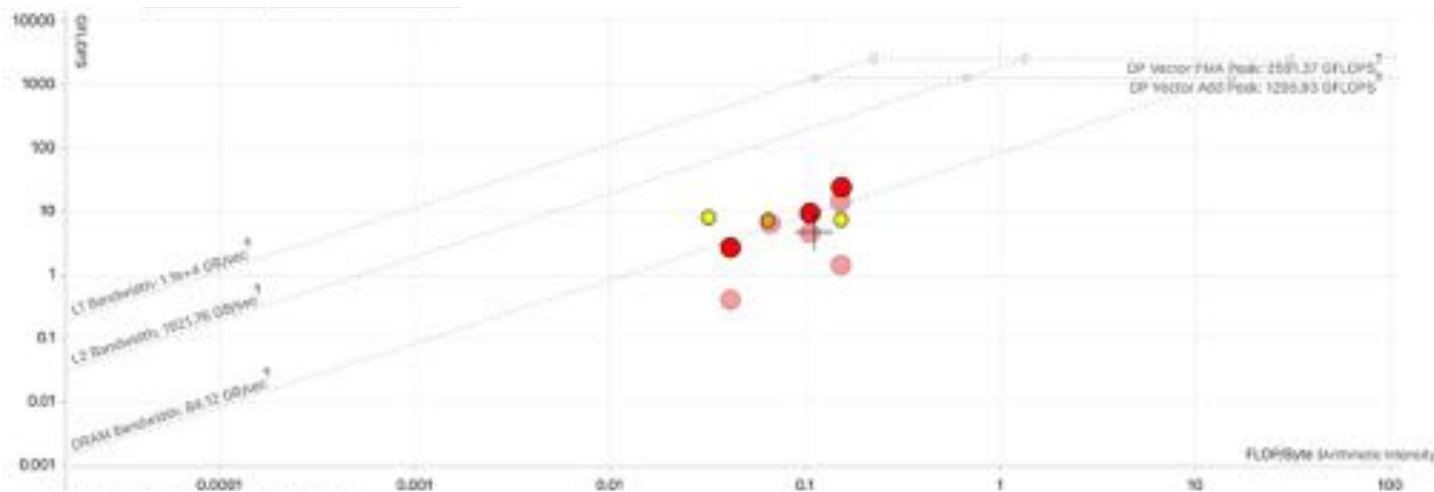
Highlights from HPC and APPLICATION labs

Work on AI in HPC environments

- See ~~David's~~ ~~Walter's~~ Sofia's talk of yesterday, „Deploying AI Frameworks on Secure HPC Systems with Containers“

Code profiling and optimization

- 2nd and 3rd level support (LRZ and GCS)
- Extreme-scaling activities



▲ Scaling of **FLASH** code in large turbulent simulation (user: Prof. C. Federrath)

◀ Roofline analysis of **ECHO** GR-MHD code (user M. Bugli) with **Intel Advisor**

What do the *first image of a black hole* and HPC have in common?

Image reduction:
PBytes of data

Theoretical modeling:
comparison with
simulations is necessary

ECHO-3DHPC has been
part of the comparison
project of general relativity
simulation codes (Porth et
al. 2019, arXiv: 1904.04923)
to validate the observational
results

Both ECHO and BHAC
(Black Hole Accretion Code;
Porth et al.) have been
optimized in collaboration
with LRZ

The use of both SuperMUC
and Hazel Hen (HLRS
Stuttgart) is acknowledged
in the EHT papers

(credits: EHT Collaboration 2019)

VisIt + OSPRay on HPC systems

finalist at SC19 SciViz



VisIt

- Data processing and visualization tool
- GUI or **batch-cli** mode (for HPC)
- Broad range of supported data format, used **across all science** and beyond
- Parallel rendering up to ~**1k** of cores

Advantages of SDV

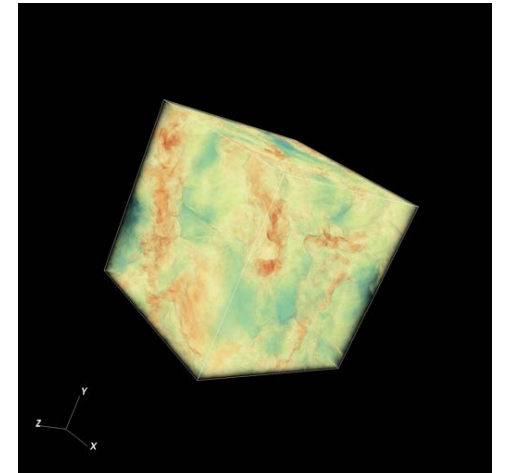
- Analysis and visualization on **same place**
- **Full-HPC** capabilities

OSPRay

- Improves parallelism and performance
- Hybrid **MPI-TBB** parallelism
- Aftereffects “for free”

SciViz at SC19 ►

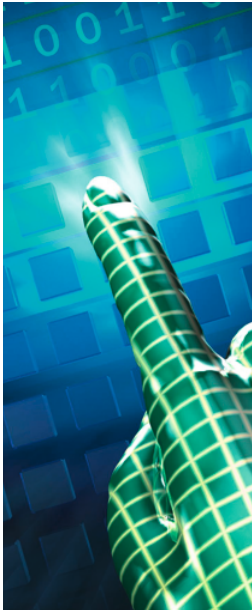
- FLASH dataset
- $(10k)^3$ grids → **40 TB**
- **Volume** + Streamlines
- Intel **HPC DevCon**



You can count on us!



STORAGE SERVICES



GREEN IT



RESEARCH & DEVELOPMENT



VIRTUAL REALITY

LRZ supports ground-breaking research and education throughout a wide range of scientific disciplines by offering highly available, secure and energy-efficient services based on cutting-edge IT technology. Today it is one of the foremost European computing centres in the area of scientific research by academic communities.



Leibniz Supercomputing Centre

Leibniz Supercomputing Centre (Leibniz-Rechenzentrum, LRZ) of the Bavarian Academy of Sciences and Humanities is the IT service provider for all Munich universities as well as a growing number of research organisations throughout Bavaria. In addition to this regional focus, LRZ also plays an important role as one of the members of the Gauss Centre for Supercomputing (GCS), delivering top-tier HPC services on the national and European level. LRZ was founded in 1982. Its facilities are located on the Research Campus in Garching.