The Leibniz Supercomputing Centre in the Landscape of High Performance Computing

Dieter Kranzlmüller

Munich Network Management Team
Ludwig-Maximilians-Universität München (LMU) &

Leibniz Supercomputing Centre (LRZ)
of the Bavarian Academy of Sciences and Humanities

High(est) Performance Computing in Germany

- Combination of the 3 German national supercomputing centers:
  - John von Neumann Institute for Computing (NIC), Jülich
  - High Performance Computing Center Stuttgart (HLRS)
  - Leibniz Supercomputing Centre (LRZ), Garching n. Munich

- Founded on 13. April 2007

- Hosting member of PRACE
  (Partnership for Advanced Computing in Europe)

Video: **SuperMUC rendered on SuperMUC by LRZ**

http://youtu.be/OIAS6iiqWrQ

SeisSol - Numerical Simulation of Seismic Wave Phenomena

Dr. Christian Pelties, Department of Earth and Environmental Sciences (LMU)
Prof. Michael Bader, Department of Informatics (TUM)

1,42 Petaflop/s on 147.456 Cores of SuperMUC
(44,5 % of Peak Performance)

http://www.uni-muenchen.de/informationen_fuer/presse/presseinformationen/2014/pelties_seisol.html

Picture: Alex Breuer (TUM) / Christian Pelties (LMU)

SuperMUC System @ LRZ

Phase 1 (IBM System x iDataPlex):

- 3.2 PFlops peak performance
- 9216 IBM iDataPlex dx360M4 nodes in 18 compute node islands
- 2 Intel Xeon E5-2680 processors and 32 GB of memory per compute node
- 147,456 compute cores
- Network Infiniband FDR10 (fat tree)

Phase 2 (Lenovo NeXtScale WCT):

- 3.6 PFlops peak performance
- 3072 Lenovo NeXtScale nx360M5 WCT nodes in 6 compute node islands
- 2 Intel Xeon E5-2697v3 processors and 64 GB of memory per compute node
- 86,016 compute cores
- Network Infiniband FDR14 (fat tree)

Common GPFS file systems with 10 PB and 5 PB usable storage size respectively
Common programming environment
Direct warm-water cooled system technology

- Running on all cores of SuperMUC Phase1+2

~100 target binding affinities
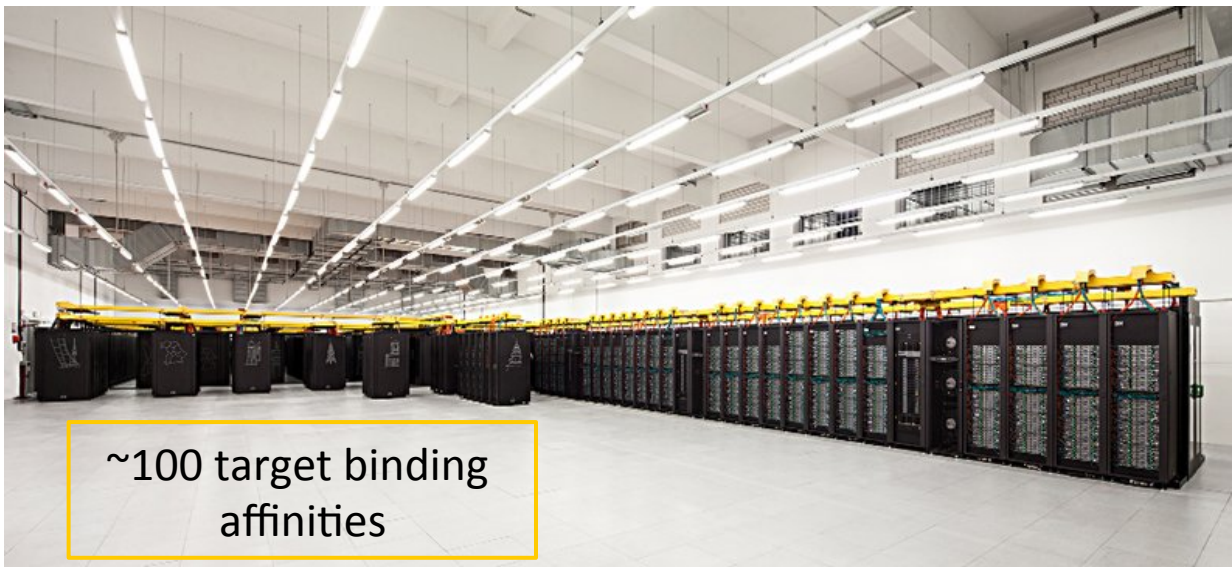
- Docking simulation of potentials drugs for breast cancer
- 37 hours total run time
- 241,672 cores
- 8.900.000 CPU hours
- 5 Terabytes of data produced

EU Projects COMPAT and MAPPER
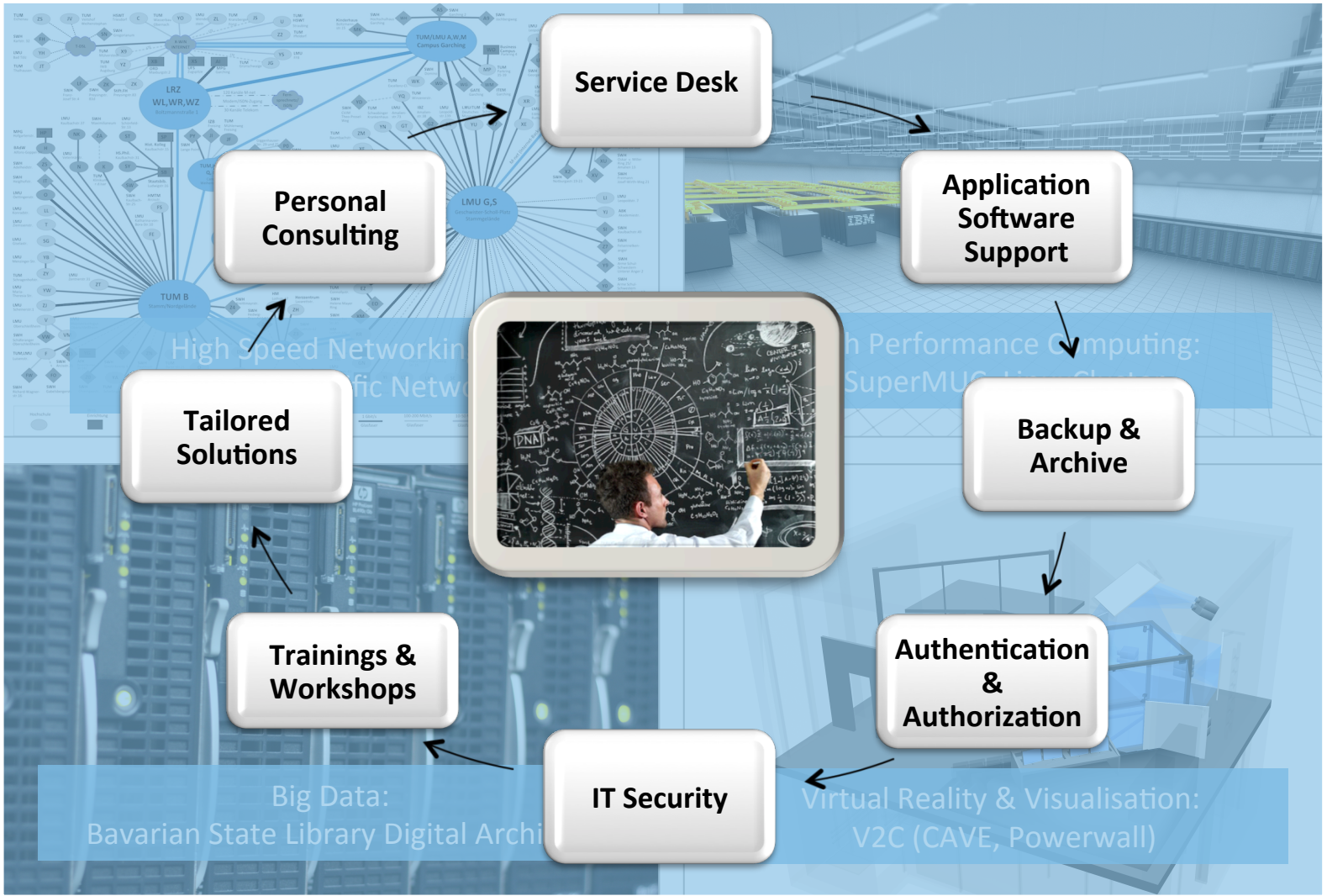http://www.compat-project.eu

With approx. 250 employees
for more than 100.000 students and
for more than 30.000 employees
including 8.500 scientists

- European Supercomputing Centre
- National Supercomputing Centre
- Regional Computer Centre for all Bavarian Universities
- Computer Centre for all Munich Universities

Photo: Ernst Graf

- Service Desk
- Personal Consulting
- Application Software Support
- Tailored Solutions
- Backup & Archive
- Trainings & Workshops
- Authentication & Authorization
- IT Security
- High Speed Networking: Scientific Network
- High Performance Computing: SuperMUC, Linux Cluster
- Big Data: Bavarian State Library Digital Archive
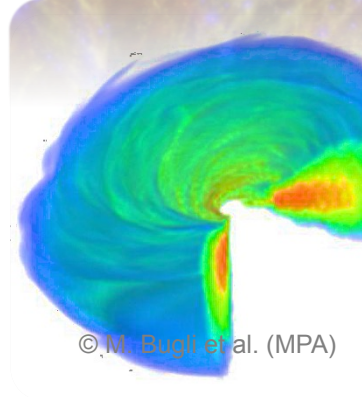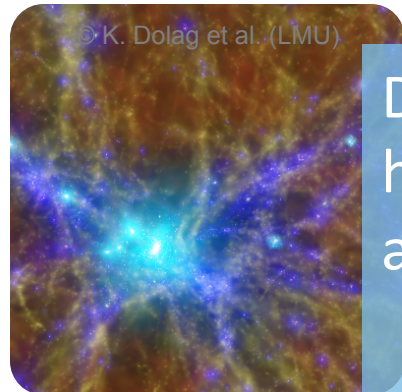- Virtual Reality & Visualisation: V2C (CAVE, Powerwall)

Members:
M. Allalen
F. Baruffa
C. Bernau
D. Brayford
G. Brietzke
H. Brüchle
M. Gerald
S. Hachinger
N. Hammer
L. Iapichino
F. Jamitzky
A. Karmakar
C. Navarrete
M. Ohlerich
A. Raganin
Y. Wang
V. Weinberg

Application specialists with domain expertise
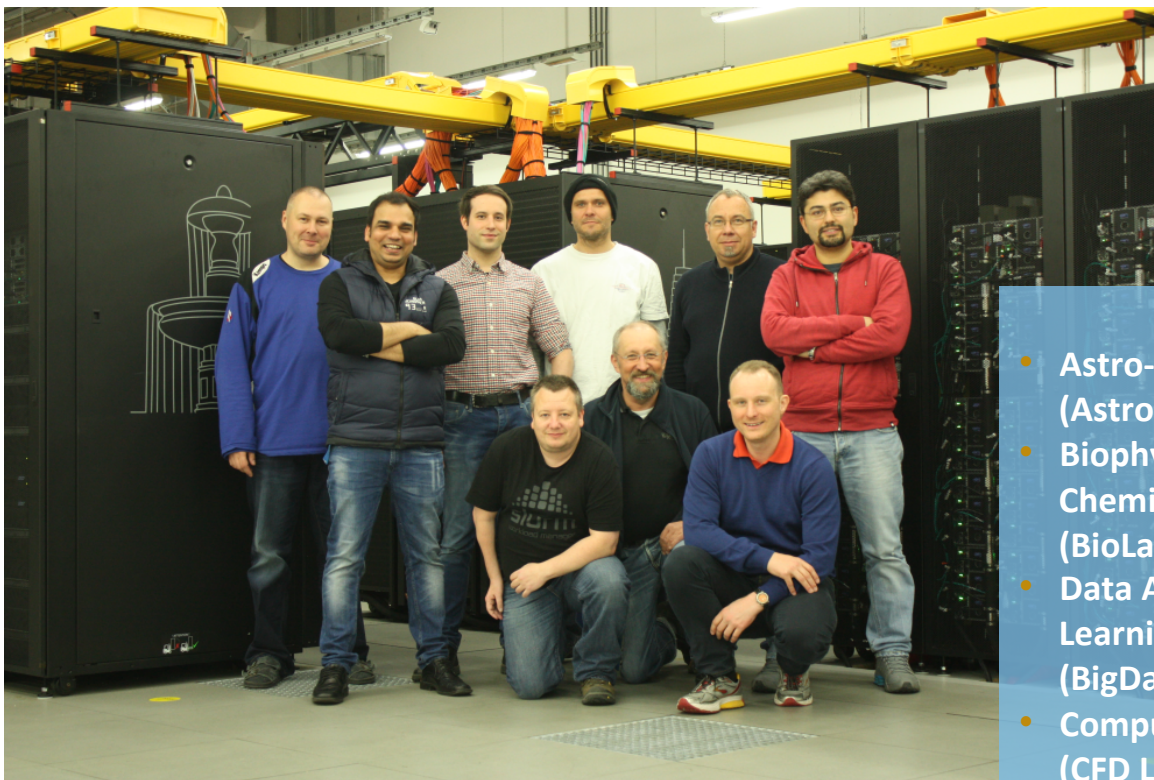
Domains:
- **Astro- and Plasma Physics (AstroLab)**
- **Biophysics and computational Chemistry (BioLab)**
- **Data Analytics and Machine Learning (BigDataLab)**
- **Computational Fluid Dynamics (CFD Lab)**
- **Geo Sciences (GeoLab)**

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Dedicated team to provide advanced high-level support to the Astrophysics and Plasma physics communities

- Efficient HPC utilization
- Scalable parallel algorithm design
- Application tuning and code modernization
- Long-lasting large-scale data management
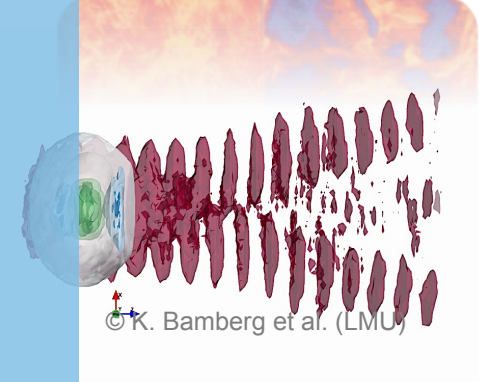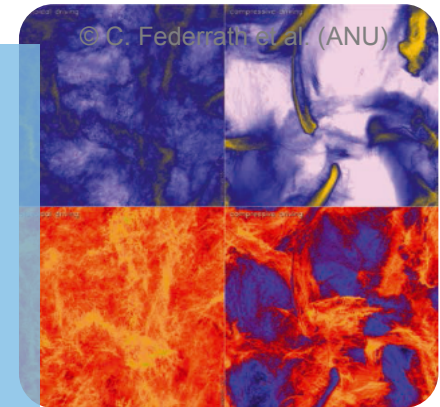
- ## High-Level Support
  - Advanced high-level support call (ADVISOR)

- ## Projects and Collaborations
  - Intel® Parallel Computing Center (IPCC)
  - Magneticum Project (Cluster Universe, LMU)
  - Hydro CLUES (LMU, AIP Potsdam)
  - Gadget algorithm improvements (PhD Project)
  - Largest Turbulence Simulation (ANU, Uni Heidelberg)
  - Plasma Wakefield Simulations (LMU/CERN)
  - C2PAP CosmoSim Web Portal (LMU, Cluster Universe)

- Work with simulation data of the universe to create different views for analysis (Zoom, Multi-Layers, Virtual Observatories)
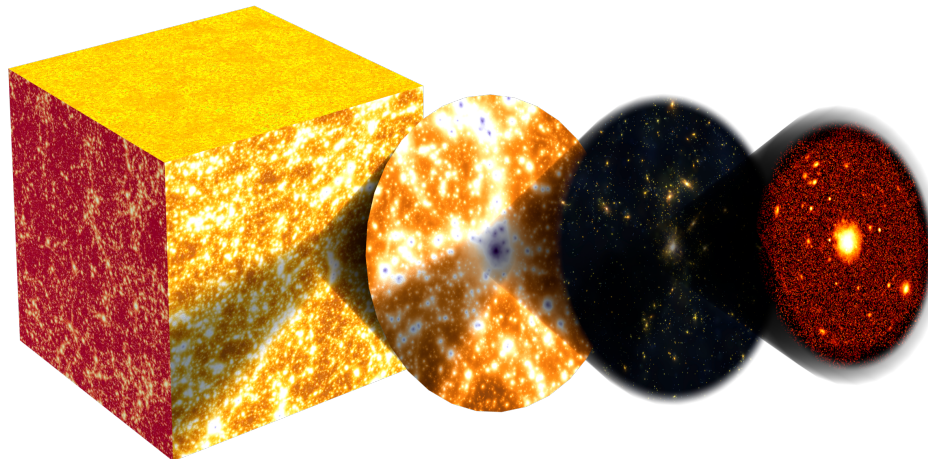
- Explore theoretical performance of future X-ray satellites (eROSITA, Athena)
- Perform realistic exploration of the potential of such experiments
- Evaluate ability to detect real galaxy clusters and groups across cosmic time
- Explore global and internal properties from current and future X-ray missions

- Large, underlying cosmological simulations allow users to select systems across a wide range of mass and dynamical states.

- **Individualized services** for selected scientific groups – **flagship role**
  - Dedicated point-of-contact
  - Individual support and guidance and targeted training & c...
  - Planning dependability for use case specific optimiz... ...uctures
  - Early access to latest IT infrastructure (hard- a... ...developments and specification of future requirements...
  - Access to IT competence network a... ...t CS and Math departments
- **Partner contribution**
  - Embedding IT experts i...
  - Joint research pro... ...g funding)
  - Scientific part... ...ual footing – joint publications
- **LRZ benef...**
  - U... ...g the (current and future) needs and requirements of the re... ...e scientific domain
  - Developing future services for all user groups
  - Thematic focusing: **Environmental Computing**

The LRZ Partnership Initiative Computational Science (piCS)
http://www.sciencedirect.com/science/article/pii/S1877050914003433

- Provide high-level IT infrastructure for Big Data and Data Science
- Develop future high-level Big Data services operated by LRZ

- Follows successful piCS model
  (Partnership Computational Sciences)

- Dedicated point of contact
- Initiates internal project through tiger-team – experts from all departments and groups at LRZ
- Initial workshop
    - Introduction of LRZ services
    - Extraction of user requirements for Big Data/Data Science Services
- Joint co-design of IT infrastructure and user application
- Individual support, guidance and training

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Dieter Kranzlmüller
kranzlmueller@lrz.de

Photo:Karl Behler