

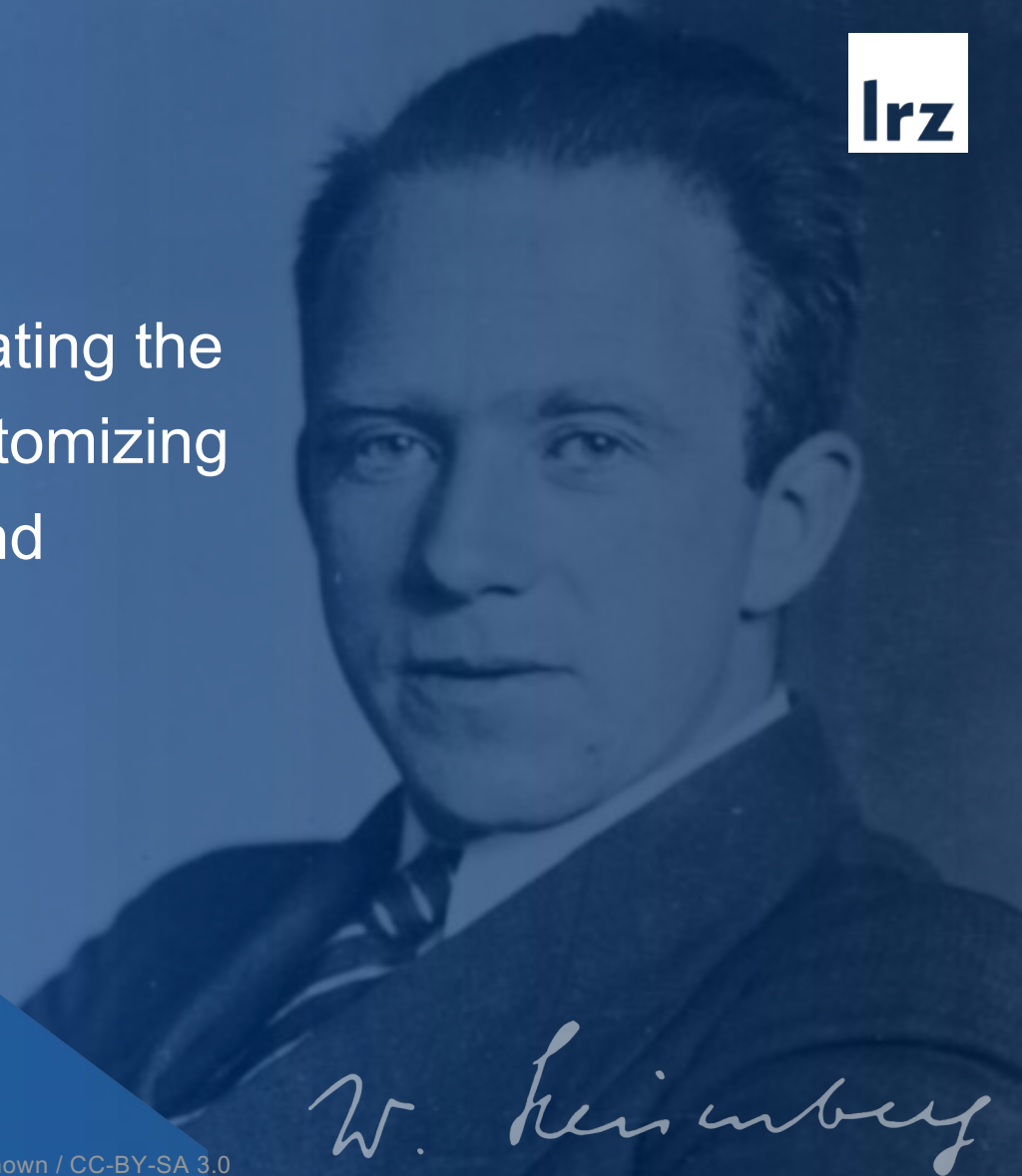
Site Update: Leibniz Supercomputing Centre

HPC User Forum | September 2021 | Laura Schulz, Head of Strategic Development

”

There is a fundamental error in separating the parts from the whole, the mistake of atomizing what should not be atomized. Unity and complementarity constitute reality.”

Werner Heisenberg



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



Bayerische
Akademie der Wissenschaften



Since 1962

260 Employees

Board of LMU and TUM university professors

IT Service Backbone for the Advancement of Research Science

LRZ as IT Center of Excellence Munich Universities TUM & LMU



110,000 students
30,000 employees
8,500 scientists

3 billion € budget
31 Nobel laureates

Over 10,000 publications (2017)

.....

Headquarters of:

Fraunhofer Society
Max Planck Institutes
Helmholtz Association





Bavaria

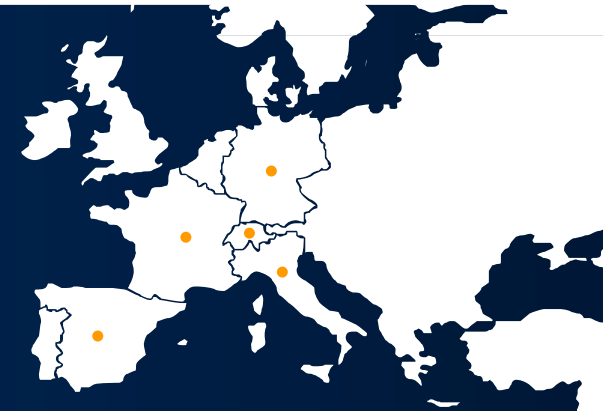
Bavarian universities
Fraunhofer Society
Max Planck Institutes
Helmholtz Association
DLR Oberpfaffenhofen
(Earth Observation Center)
State Institutions
(z.B. Bavarian State Library)



Germany

Gauss Centre for Supercomputing (GCS)
Association of German Tier 0
Supercomputing Centers

LRZ | Garching, München | SuperMUC-NG
HLRS | Stuttgart | Hazel Hen
JSC | Jülich | JUWELS



Europe

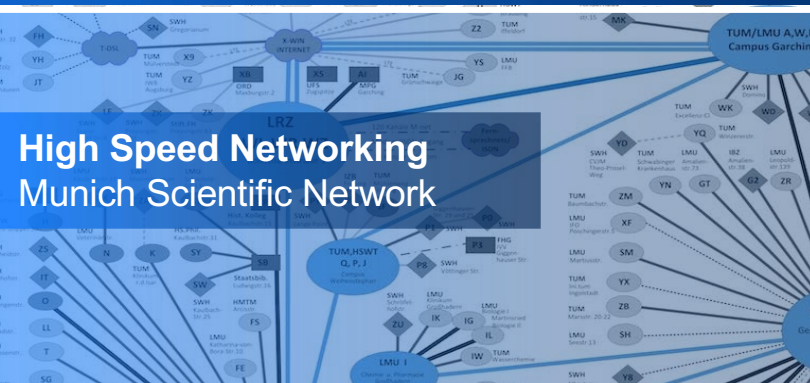
EuroHPC and PRACE
Tier-0 Infrastructure
Base members:

GCS (Germany: LRZ, HLRS, JSC)
BSC (Spain)
CSCS (Switzerland)
CINECA (Italy)
GENCI (France)

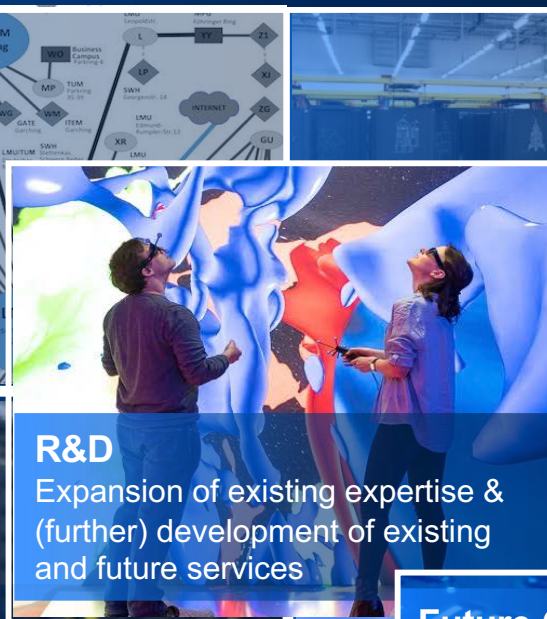
PARTS OF THE WHOLE

LRZ as IT and Computing Center of Excellence

Services and Capability Development for Innovative Science



High Speed Networking
Munich Scientific Network



R&D
Expansion of existing expertise &
(further) development of existing
and future services



High Performance Computing
SuperMUC-NG, LRZ Linux Cluster



Big Data Center
Digital Archive of the Bavarian State Library

Future Computing
Technology exploration of future
architectures (AI, BD, QC)
in partnership with university chairs
(TUM, LMU, FAU, UR)

**Virtual Reality and
Visualisation**
V2C (CAVE, Powerwall)



E-Mail



Network



Storage



Cloud



Cluster



HPC



Training

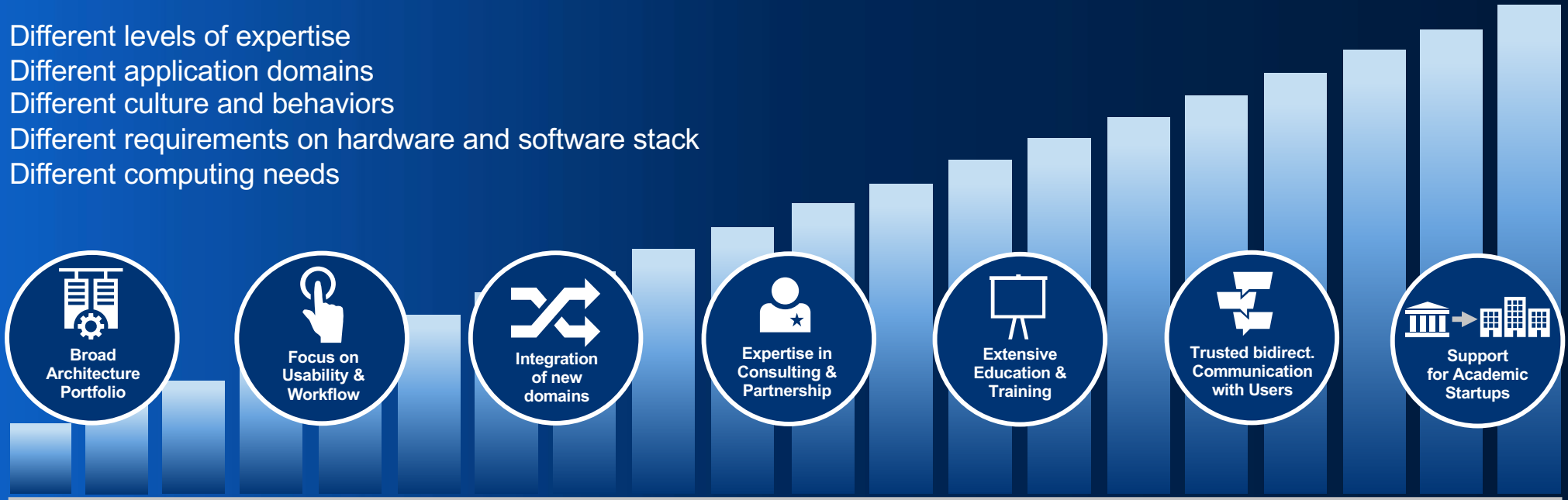


Consulting

From Long-Tail to Power-Users

A Broad Range of Users

Different levels of expertise
Different application domains
Different culture and behaviors
Different requirements on hardware and software stack
Different computing needs



Current and Coming Capabilities in the HPC Ecosystem



HPC / ModSim

AI & Machine Learning



Quantum Computing

Big Data / HPDA

User Segments: Expertise, Behaviors, Needs, Expectations



Clickers



Librarians



Directives



Power Users



Bare Metals

How do we support
innovative science
for each?



Domain Diversity

Hardware Diversity

Capability Diversity

User Diversity

Workflow Diversity

Software Diversity

PARTS OF THE WHOLE

Service Portfolio

Resource Portfolio

Decisions for Acquisitions and Capability R&D Investments

Application-Driven Co-Design as a Service to Science

Understanding

Workloads
Better

Influencing

Vendor
Designs

Advancing

Software
Co-Design



Quantum Computing Community Outreach, Tech Assessment & Scouting The Bavarian Quantum Computing eXchange (BQCX)

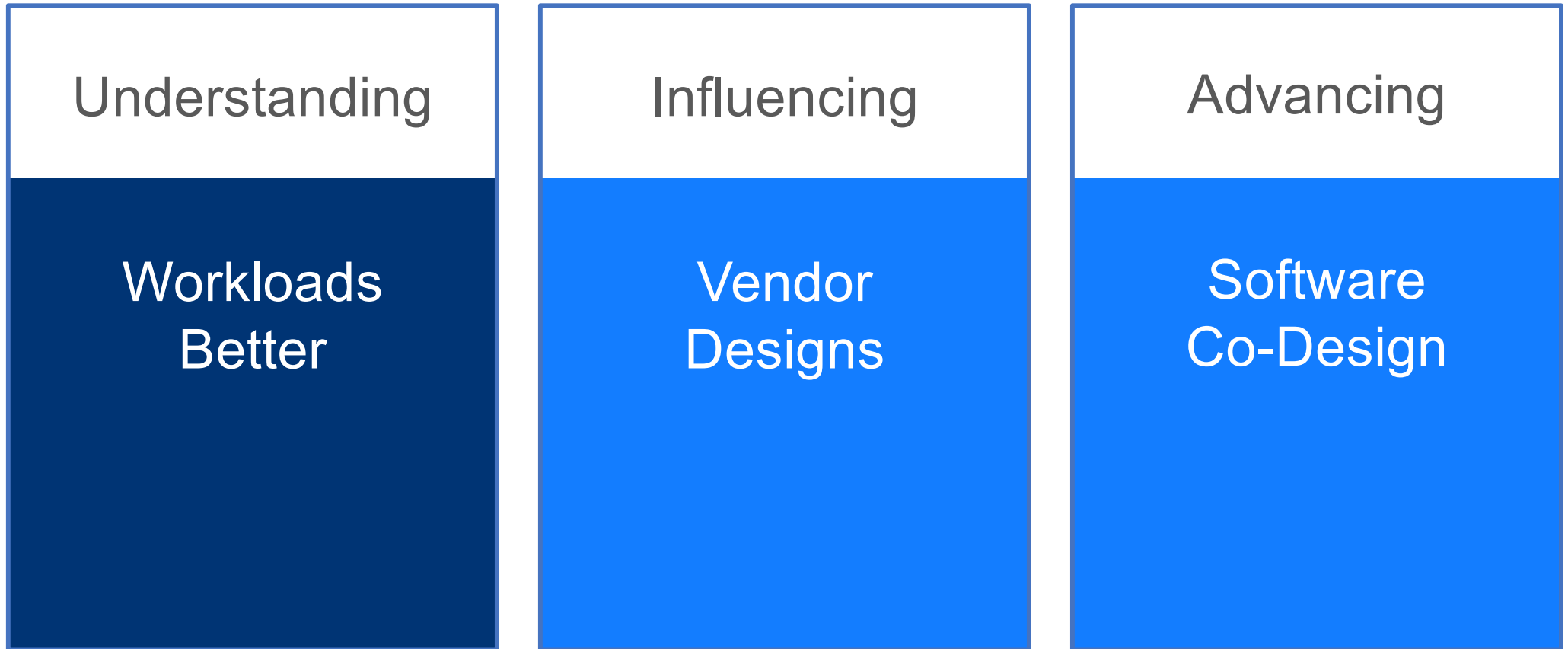


Founded in July 2019

- Bringing together and understanding the community and needs
- Monthly forum for presentations of field experts for awareness and networking
- Tech scouting and assessment

quantum.lrz.de

Application-Driven Co-Design as a Service to Science



LRZ “SuperMUC-NG”

Top500 (July, 2021): #15

Lenovo Intel (2019)

311,040 cores Intel Xeon Skylake

26.9 PetaFlops Peak

19.48 PetaFlops Linpack*

719 TeraByte Hauptspeicher

70 PetaByte Disk

TIME FOR THE NEXT PHASE

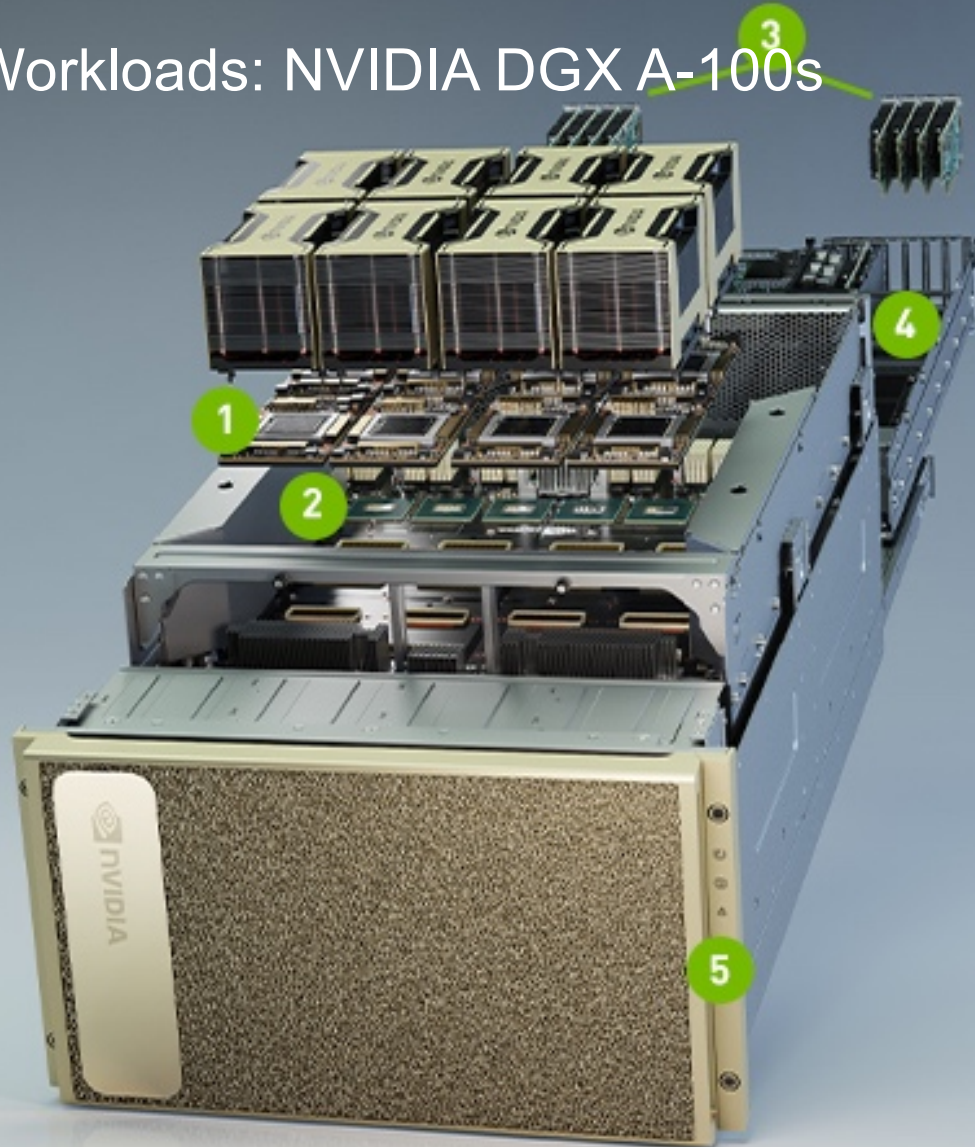
SuperMUC-NG Phase 2

Intel Xeon Scalable processors
“Sapphire Rapids” CPUs
“Ponte Vecchio” GPUs
DAOS storage system
Intel Optane persistent memory

Lenovo's SD650-I v3 platform

Coming Spring 2022

ML/AI Workloads: NVIDIA DGX A-100s



System for MCML

Munich Center for
Machine Learning

NVIDIA DGX-a100

HPC/AI

40 AI Petaflop/s

SSD Storage

HDR Infiniband

ExaMUC

2024 +/-

Integration Approach



Paper:

On the Inevitability of Integrated HPC Systems and How they will Change HPC System Operations

<https://www.isc.lrz.de/fileadmin/ISC/Download/heart-hpc.pdf>

HARDWARE:

Co-Design Approach as Innovation Procurement to Address:

Power Limits

Specialization

Diverse Workloads

Data Movement

SOFTWARE:

Development of production-ready software stack enabling low- energy, high-performance exascale systems

REGALE

Goal: Holistic resource management for performance, power, energy & throughput for efficient applications

DEEP-SEA

Dynamical Exascale Entry Platform (DEEP) –
Software Exascale Architecture (SEA)
Goal: Development of a comprehensive base software stack

Bavarian

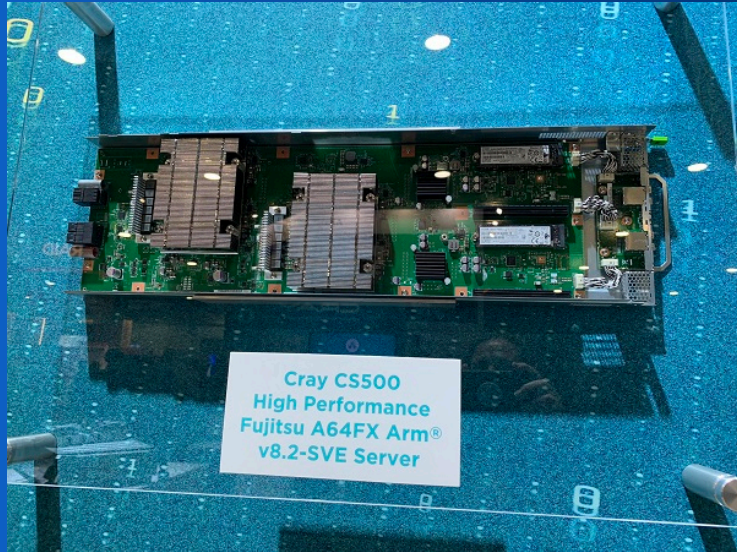
Energy

Architecture

Software

Testbed





HPCWire photo

One component: HPE Cray CS500

Diverse Portfolio of
CPUs, GPUs, FPGAs and ASICs

Internal Evaluation of hardware and software

Decision Assistance for Procurements
and Resource Portfolio Design

Academic comparative studies

University BEAST labs

Contact:

Dr. Josef Weidendorfer,
Head of Future Computing

Energy Needs for an Exascale Class System

Heterogeneous system with various accelerator types



Programmability

Programming models from different vendors / communities (i.e. MPI, OpenMP, Spark and Tensorflow, etc.)



Usability for End User

Researchers want to do their science, not deal with workflow friction.





Enabling QC Integration in HPC Ecosystem

A key research field for LRZ

Understand how to integrate QC into an HPC ecosystem towards Exascale

- QPUs as a new class of accelerator
- Integration as challenge for hardware, software stack, programming models

Community Outreach and Alignment

- Think tanks
- IEEE Quantum Week Workshop (WIHPQC21): <https://www.hpcqc.org/>
- White paper in the works



Enabling QC Integration in HPC Ecosystem



Part of larger MQV Strategy towards a holistic QC approach

- Three different QC platforms under one umbrella
- Unified system software stack
- Data centre-ready platforms with user support strategy

LRZ works as part of MQV on integrating HPC-QC software environments

- Compilers, runtimes, tools
- Secure multi-user environments
- External resource management and access

Four focus areas (LRZ with CS at TUM and LMU)

- Programming Environments
- Quantum OS and Runtime
- Quantum Control Microarchitecture and Firmware
- Integration with HPC and Cloud Systems



Munich Quantum Valley (MQV)



Opening of the LRZ Quantum Integration Centre (QIC)

March 17, 2021

Quantum Computing
Services

Quantum Computing -
HPC Integration R&D

Four directions for resources, research and services

On-premise quantum systems

- DaQC project
- Lab space and cryostat procurement
- Future research directions

Practical QC Services

- Remote access
- User workflow optimization

Applied
R&D

High-performance Quantum Computing

- Atos QLM system at LRZ
- Software simulators on our HPC systems

Quantum User Community and Education

- The Bavarian Quantum Computing eXchange (BQCX)
- Course Portfolio

SUPERCOMPUTING CENTRE

Co-Design & Integration in HPC

TECHNOLOGY

USERS &
APPLICATIONS



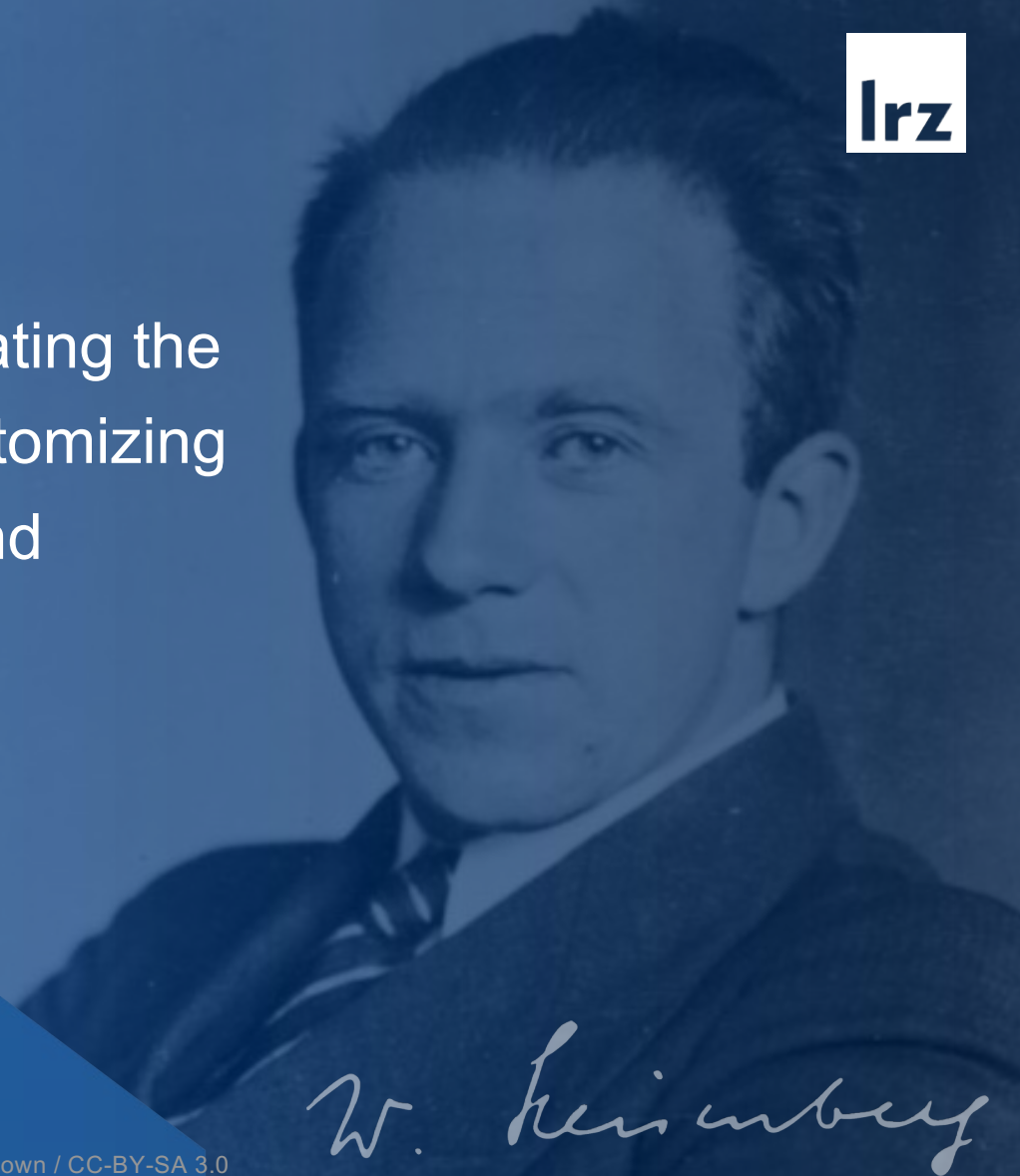
Broad Portfolio

Constant Feedback

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Werner Heisenberg





Laura Schulz

Head of Strategic Development & Partnerships
Leibniz Supercomputing Centre
schulz@lrz.de

Resources



Press Release SuperMUC-NG Phase 2:

https://www.lrz.de/presse/ereignisse/2021-05-04-SuperMUC-NG-Phase-2_ENG/

Munich Software Stack:

https://www.lrz.de/presse/ereignisse/2021-06-07-MunichSoftwareStack_eng/

Bavarian Energy, Architecture and Software Testbed (BEAST):

https://www.lrz.de/presse/ereignisse/2020-11-06_BEAST/

https://www.lrz.de/presse/ereignisse/2021-01-10-BEAST-JWeidendorfer_en/

AMD Corona Donation:

https://www.lrz.de/presse/ereignisse/2020-10-05_AMD-Covid-19_ENG_/

HPE Cray CS500:

https://www.lrz.de/presse/ereignisse/2020-06-23_LRZ-to-deploy-HPE_s-Cray-CS500-system-to-bring-innovative-architecture-to-the-science-of-its-users/

Opening of LRZ Quantum Integration Centre:

<https://www.lrz.de/presse/ereignisse/2021-03-17-LRZ-opens-Quantum-Integration-Centre/>

Munich Quantum Valley:

<https://www.lrz.de/presse/ereignisse/2021-01-12-Munich-Quantum-Valley-eng/>

Bavarian Quantum Computing eXchange:

https://www.lrz.de/presse/ereignisse/2020-06-05_BQCX-brings-researchers-together/

<https://www.lrz.de/presse/ereignisse/2019-11-20-LRZ-embraces-quantum-computing/>