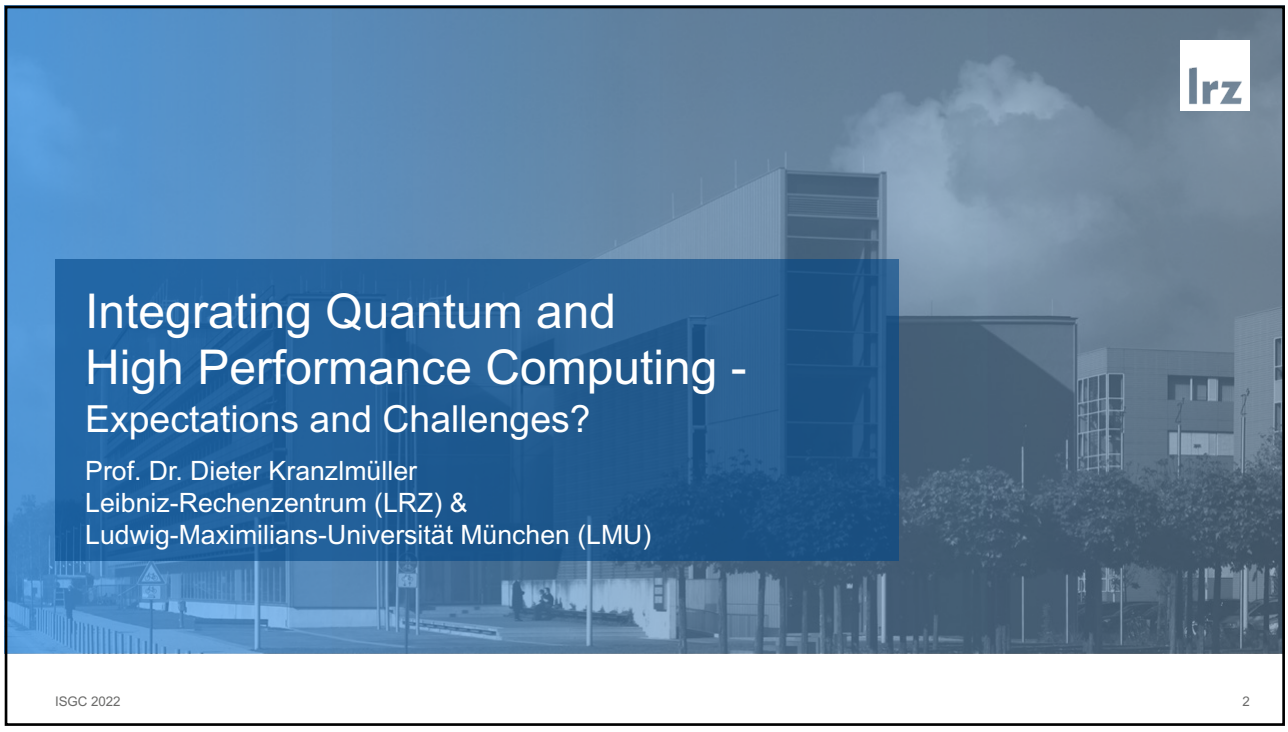
Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

1



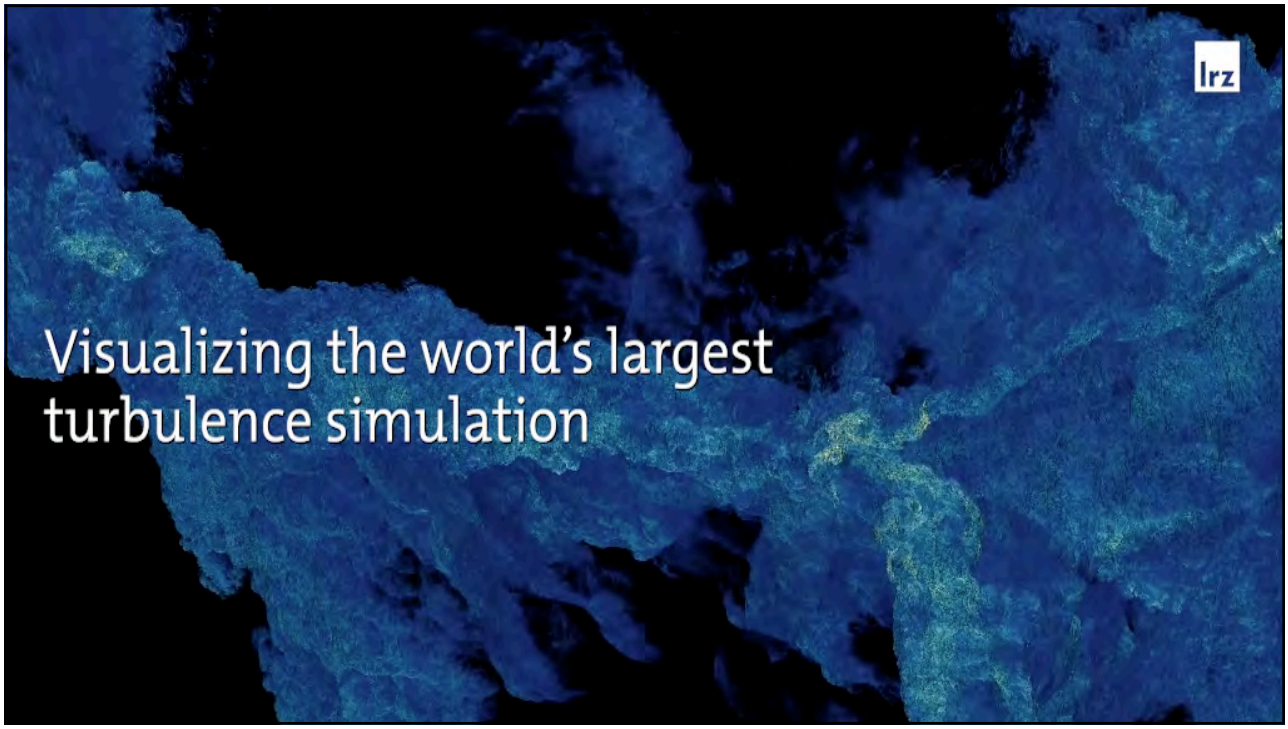
2


Picture: Ernst Gra
III (2006)
IV (2011)
II b (2011)
II a (2006)
I a (2006)
I b (2011)
Leibniz Supercomputing Centre (LRZ)
of the Bavarian Academy of Sciences and Humanities
3

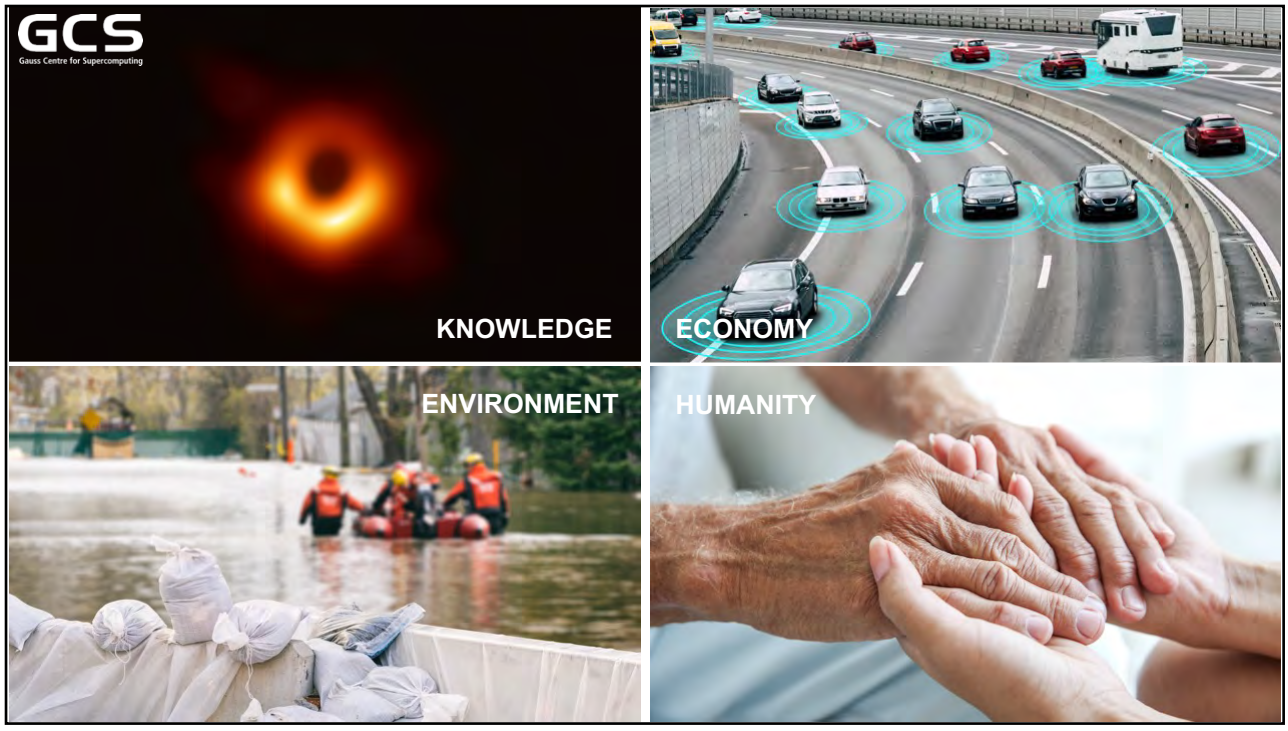
3


GCS
Gauss Centre for Supercomputing
lrz
ASTRO PHYSICS
SUPERMUC-NG
Source: F. Löchner for LRZ
ISGC 2022
4

4


lrz
Visualizing the world's largest
turbulence simulation

5


GCS
Gauss Centre for Supercomputing
KNOWLEDGE
ECONOMY
ENVIRONMENT
HUMANITY

6

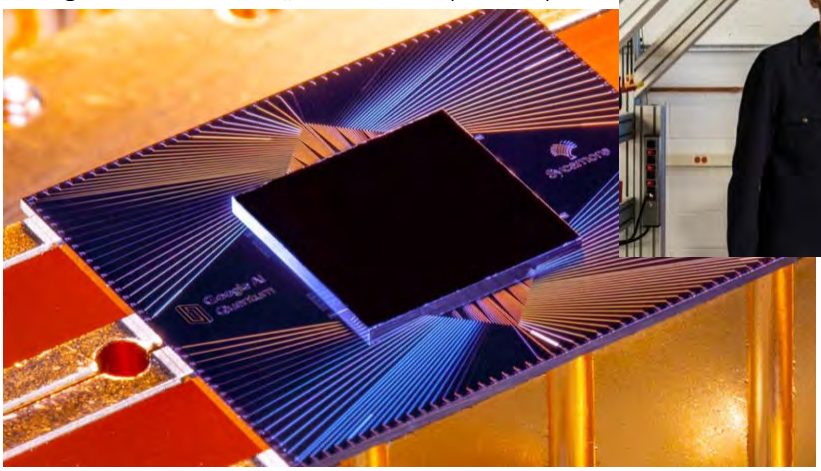

LRZ as IT Center of Excellence
Digital Infrastructure and Service for Innovative Science
lrz
High Speed Networking
Münchner Scientific Network
High Performance Computing
SuperMUC-NG, LRZ Linux Cluster
Research & Development
Expansion of existing expertise & (further) development of existing and future services
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
ISGC 2022
7

7


Where to go from here?
ISGC 2022
www.kitzbueheler-alpen.com/de/fieberbrunn/winter/skigebiet-skicircus-fieberbrunn.html
8

8

Google demonstrates „Quantum Supremacy“

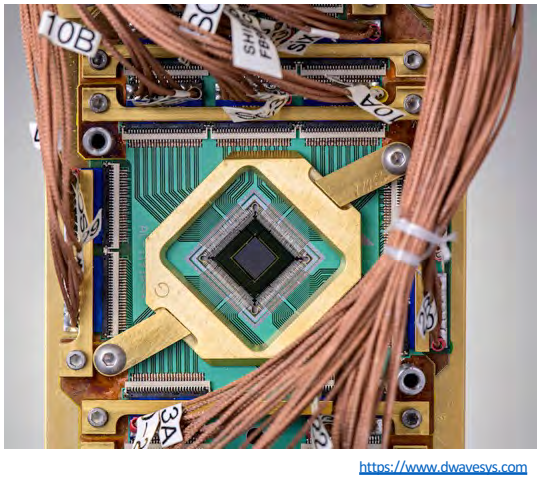


The Sycamore chip with 54 qubits showed that Quantum Supremacy is possible. (Source: Google)

https://www.handelsblatt.com/technik/forschung-innovation/computertechnik-google-verkuendet-durchbruch-beim-quantencomputer/25146366.html
https://www.heise.de/newsticker/meldung/Jetzt-auch-offiziell-Googles-Quantencomputer-zeigt-Quantum-Supremacy-4565771.html

9

Adiabatic Quantum Computers
D-Wave Systems

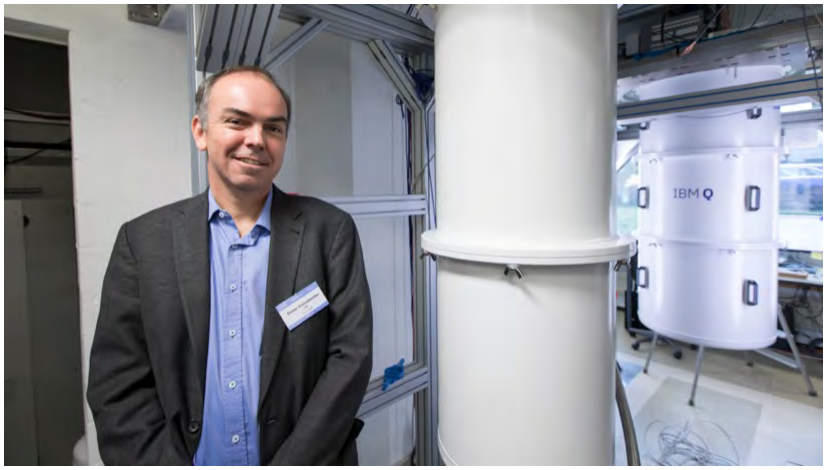


https://www.dwavesys.com

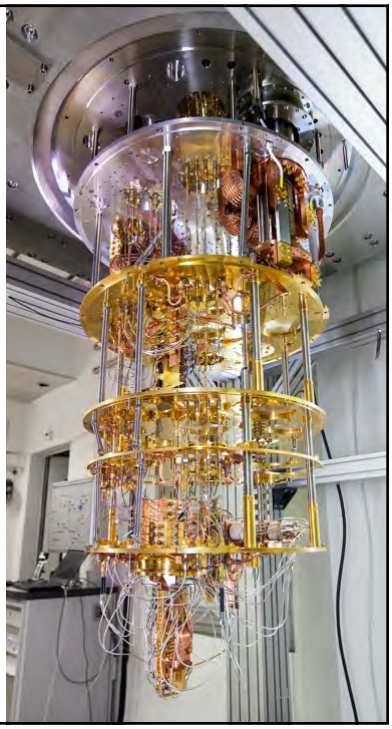
10

IBM Zurich Lab

IBM Q - Quantencomputer



By IBM Zurich Lab - https://live.staticflickr.com/4403/23518086798_a41771999f_o_d.jpg
https://en.wikipedia.org/w/index.php?curid=62790315



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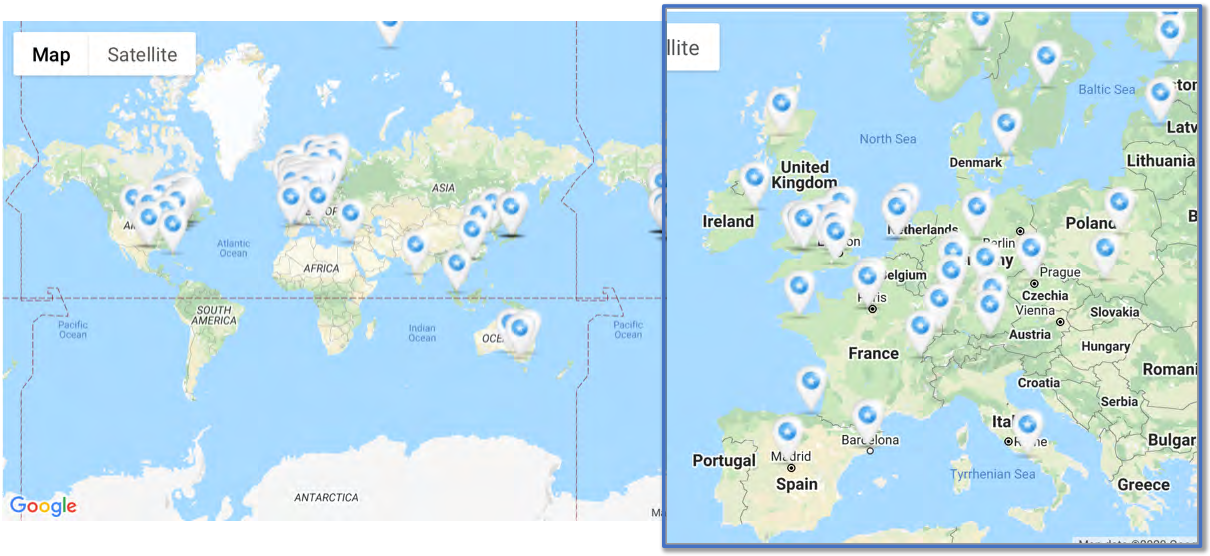
https://quantumzeitgeist.com/interactive-map-of-quantum-computing-companies-from-around-the-globe/

Quantum Computing Companies around the Globe



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The Origins of Quantum Mechanics

Werner Karl Heisenberg (5 Dez 1901 – 1 Feb 1976, geb. Würzburg, Bavaria)

- LMU Munich and University Göttingen
- 1932 Nobel Prize in Physics,
  „for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen.“
  The Nobel Prize in Physics 1932. NobelPrize.org. Nobel Prize Outreach AB 2022. Sat. 19 Mar 2022. https://www.nobelprize.org/prizes/physics/1932/summary/

By Bundesarchiv, Bild 183-R57262 / Unknown / CC-BY-SA 3.0, CC BY-SA 3.0 de https://commons.wikimedia.org/w/index.php?curid=5436254

Remark:

- 1933 Nobel Prize in Physics for Erwin Schrödinger and Paul Adrien Maurice Dirac "*for the discovery of new productive forms of atomic theory.*", (Advancement of quantum mechanics)
  The Nobel Prize in Physics 1933. NobelPrize.org. Nobel Prize Outreach AB 2022. Sat. 19 Mar 2022. https://www.nobelprize.org/prizes/physics/1933/summary/

From Quantum Mechanics to Quantum Computers

Richard Feynman (11. Mai 1918 – 15. Feb. 1988)

- Massachusetts Institute of Technology (MIT) and Princeton University, as well as Manhattan Project, Los Alamos
- 1965 Nobel Prize in Physics, together with Julian Seymour Schwinger und Sin-Itiro Tomonaga, *„for their fundamental work in quantum electrodynamics, with deep-ploughing consequences for the physics of elementary particles.“*
  The Nobel Prize in Physics 1965. NobelPrize.org. Nobel Prize Outreach AB 2022. Sat. 19 Mar 2022. https://www.nobelprize.org/prizes/physics/1965/summary/

http://www.nobelprize.org/nobel_prizes/physics/laureates/1965/feynman-bio.html

David Deutsch (born 18 Mai 1953 in Haifa)

- Since 2009 University Oxford
- 1998 Dirac Prize for his work on quantum computing, including how these machines could be realized using quantum gates.

https://www2.physics.ox.ac.uk/contacts/people/deutsch

Basics of Quantum Physics

How does a quantum computer work

A quantum computer is a processor whose function is based on the laws of **quantum mechanics**.

- **Superposition** of equal physical quantities, which do not interfere with each other.
- **Entanglement -** composite physical system which, considered as a whole, assumes a well-defined state without also being able to assign to each of the subsystems its own well-defined state.

https://de.wikipedia.org/wiki/Quantencomputer

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How does a Quantum Computer work

Superposition

Conventional Computer:

- 1 Bit: 0 or 1

https://de.wikipedia.org/wiki/Deutsche_Euromünzen
European Commission / Economic and Financial AffairsAffairs – http://ec.europa.eu/economy_finance/images/pimage8369.htm,
PD-Amtliches Werk, https://de.wikipedia.org/w/index.php?curid=7987242

Quantum Computer:

- 1 Qubit: 0 and 1 simultaneously

- Example: Schrödinger‘s Cat

https://media.giphy.com/media/LGveWkr2m3v7a/giphy.mp4

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How to use a Quantum Computer

Applications of Quantum Computers

Conventional Computer:

0000
0001
0002
0003
0004
0005
…

Max. 10.000 Steps

SuperMUC-NG:
26.900.000.000.000.000 Flop/s

Quantum Computer:

14 Qubits
2^{14} = 16385 States

➔ 1 Step

Speedup: 10.000

https://www.amazon.de/dp/B075392B4T/ref=pe_3044161_189395811_TE_SCE_dp_1

What to do with Quantum Computers

Quantum Algorithms – Grover & Shor

- 1996 Lov Grover: **Search in large databases**
  - Grover, Lov K.: A fast quantum mechanical algorithm for database search, Proceedings, 28th Annual ACM Symposium on the Theory of Computing, (May 1996) p. 212
- 1994 Peter Shor, **Factorization of large numbers**
  - Shor, Peter W.: Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer. In: SIAM Journal on Computing, 26/1997, S. 1484–1509, arxiv:quant-ph/9508027
- **Application example: Online Banking**:
  - HBCI – Home Banking Computer Interface
  - 768 Bit (1024-2048 Bit) RSA-Key pair for authentication
  - RSA – Rivest, Shamir, Adelman, asymmetric cryptographic method for encryption and digital signatures

https://en.wikipedia.org/wiki/Quantum_algorithm

Overview Quantum Algorithms

- **Algorithms based on the quantum Fourier transform**:
  Deutsch–Jozsa algorithm, Bernstein–Vazirani algorithm, Simon's algorithm, Quantum phase estimation algorithm. Shor's, Hidden subgroup problem, Boson sampling problem, Estimating Gauss sums, Fourier fishing and Fourier checking
- **Algorithms based on amplitude amplification**:
  Grover's algorithm, Quantum counting
- **Quantum Walks**:
  Element distinctness problem, Triangle-finding problem, Formula evaluation, Group commutativity
- **BQP-complete problems**:
  Computing knot invariants, Quantum simulation, Solving a linear systems of equations
- **Hybrid quantum/classical algorithms**:
  QAOA, Variational quantum eigensolver

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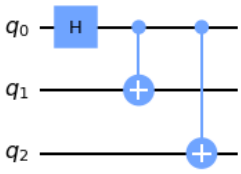
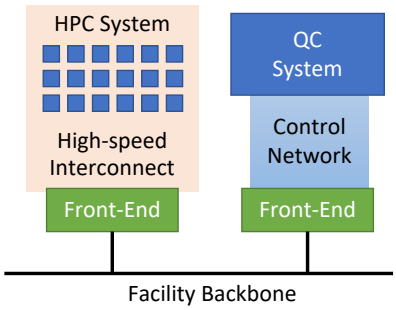
How to use a Quantum Computer in your HPC Data Center

Adding a Quantum Computer Module

- "*Once the technology is available, purchase it and place it in your data center and connect it to the network*"
- Programming with Quantum SDKs
  ➔ Building Circuits
- Examples:
  - Qiskit (IBM)
  - Cirq (Google)
  - …
- Job scheduler at Front End





https://qiskit.org/documentation/tutorials/circuits/1_getting_started_with_qiskit.html

Slide courtesy Martin Schulz

Trends in HPC

Power and Energy as Hard Constraints

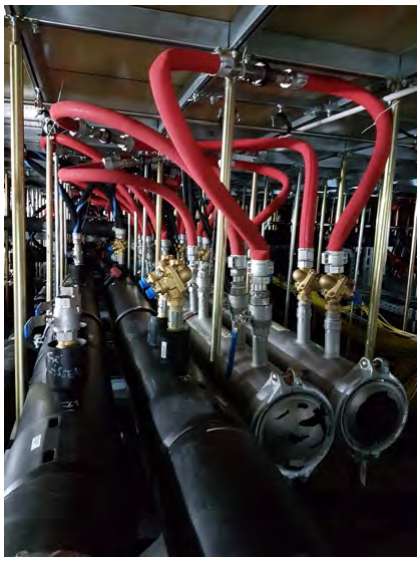
Power Limits

Cost are limiting

Power density is pushing limits

Societal pressure

SuperMUC-NG Cool Manager – 3000 l/h Water per Rack



Slide courtesy Martin Schulz

Trends in HPC

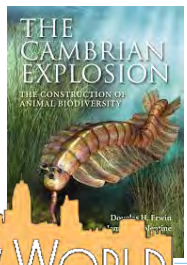
Cambrian Explosion of Architectures

Power Limits

Cost are limiting

Power density is pushing limits

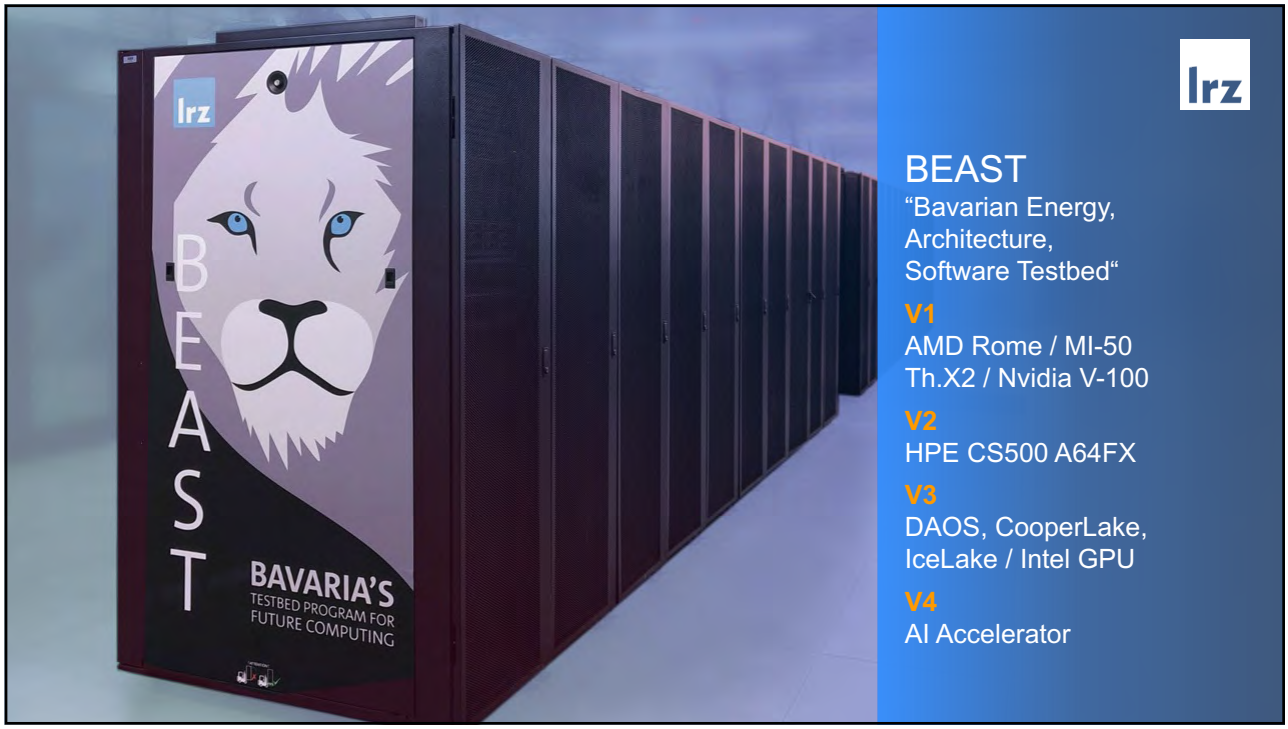
Societal pressure



Specialization

Driven by end of Dennard Scaling and Pending end of Moore's Law

Feature reduction is ending



lrz

BEAST

"Bavarian Energy, Architecture, Software Testbed"

V1
AMD Rome / MI-50
Th.X2 / Nvidia V-100

V2
HPE CS500 A64FX

V3
DAOS, CooperLake, IceLake / Intel GPU

V4
AI Accelerator

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Slide courtesy Martin Schulz

Trends in HPC

Cost of Data Movement is Becoming a Limiter

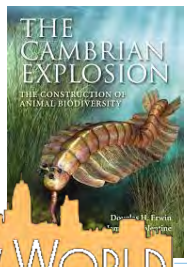
lrz

Power Limits

Cost are limiting

Power density is pushing limits

Societal pressure



BRAVE NEW WORLD

Specialization

Driven by end of Dennard Scaling and Pending end of Moore's Law

Feature reduction is ending

Data Movement = Cost

ISGC 2022 26

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Slide courtesy Martin Schulz

Trends in HPC

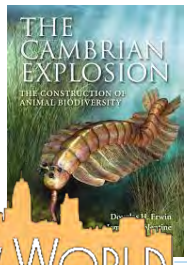
Workloads are Becoming More Complex and Diverse

Power Limits

Cost are limiting

Power density is pushing limits

Societal pressure

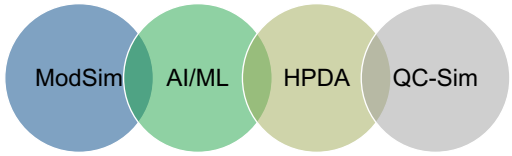


Specialization

Driven by end of Dennard Scaling and Pending end of Moore's Law

Feature reduction is ending

Data Movement = Cost



More Diverse Workloads

Slide courtesy Martin Schulz

Trends in HPC

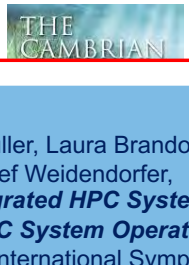
Consequences

Power Limits

Cost are limiti

Power density pushing limits

Societal press



Specialization

d

re's Law

ending

Martin Schulz, Dieter Kranzlmüller, Laura Brandon Schulz, Carsten Trinitis, Josef Weidendorfer, „***On the Inevitability of Integrated HPC Systems and How they will Change HPC System Operations***", HEART '21: Proceedings of the 11th International Symposium on Highly Efficient Accelerators and Reconfigurable Technologies, June 2021, Article No.: 2, Pages 1–6, https://doi.org/10.1145/3468044.3468046

The Integrated Supercomputing Architecture

Data Movement = Cost

QC-Sim

More Diverse Workloads

LRZ Integrated Supercomputing Architecture

The HPC Innovation/Integration Circle

HPC

Modeling & Simulation (M&S)
Natural World ▸ Hypothesis ▸
Equations ▸ Algorithms ▸
Computing ▸ Data ▸ Analysis

AI & Machine Learning

Data ▸ Algorithms
▸ Computing ▸ Pattern Recognition

Big Data

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LRZ Integrated Supercomputing Architecture

The HPC Innovation/Integration Circle

HPC

Modeling & Simulation (M&S)
Natural World ▸ Hypothesis ▸
Equations ▸ Algorithms ▸
Computing ▸ Data ▸ Analysis

AI & Machine Learning

Data ▸ Algorithms
▸ Computing ▸ Pattern Recognition

Quantum Computing

Big Data

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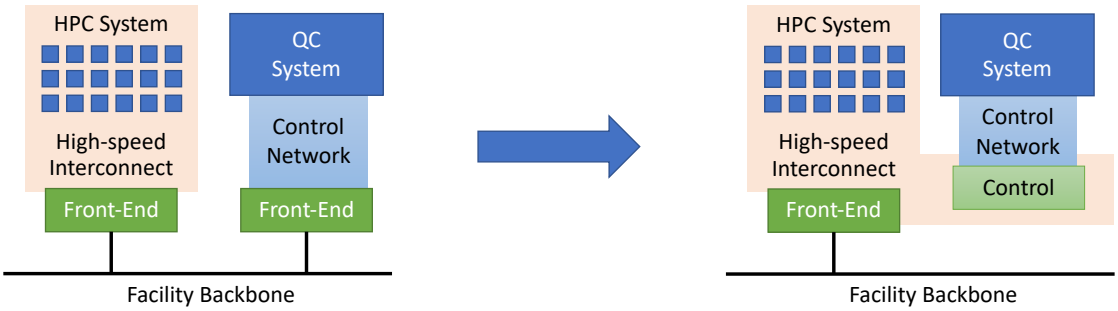
Utilizing the Ideas of the Integrated Supercomputing Architecture

From Independant Modules to an Integrated System



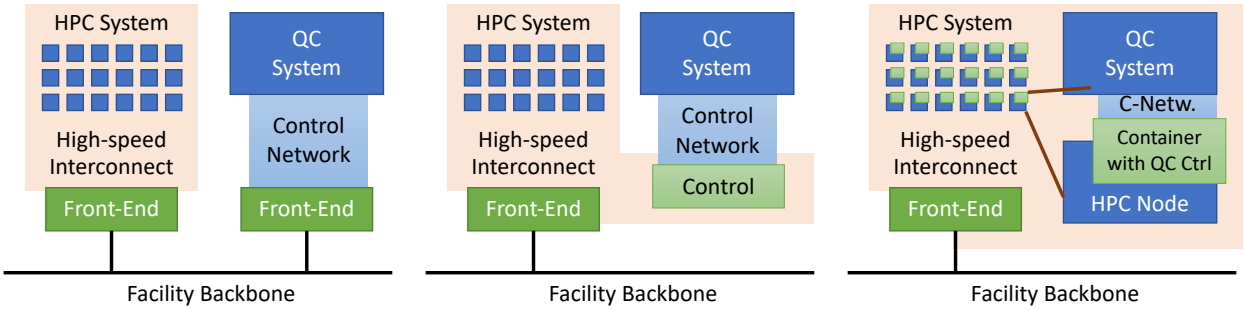
a) Segmentation into Modules

b) Physically Integrated

31

Full HPC-QC Integrated Architecture

Towards logically integrated Quantum Computers



a) Segmentation into Modules

b) Physically Integrated

c) Logically Integrated

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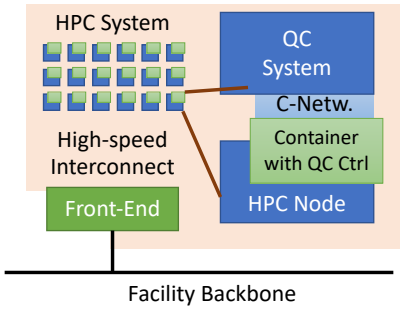
Full HPC-QC Integration

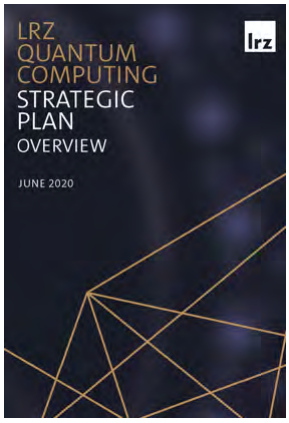
Utilizing the Integrated Quantum Computer

- Goal: **Use the QC as an accelerator for HPC**
- Approach: Call the QC from the HPC Code
  1. Through a dedicated library call
  2. Transparently inside OpenMP, MPI, or any math library
- To do:
  Add **Computer Science** methods and **Software Engineering** to the QCs coming from the physics labs



QC at LRZ

The LRZ Approach to Quantum Computing



As a User Facility and Service Provider
- Access provider and access manager
- Research consulting and support
- Academic education and training

As a Supercomputing Centre
- System hosting and operation
- **HPC-QC integration**
- Technologists training and certification

As part of the Bavarian Quantum Community
- Quantum ecosystem awareness through tech scouting
- User community analysis (surveys, focus/working groups)
- Community networking support

The LRZ Quantum Integration Centre addresses the needs highlighted in our strategic plan


lrz
QIC | QUANTUM
INTEGRATION CENTRE
Opening | QIC
LRZ Quantum Integration Centre | March 17, 2021
qic.lrz.de
ISGC 2022
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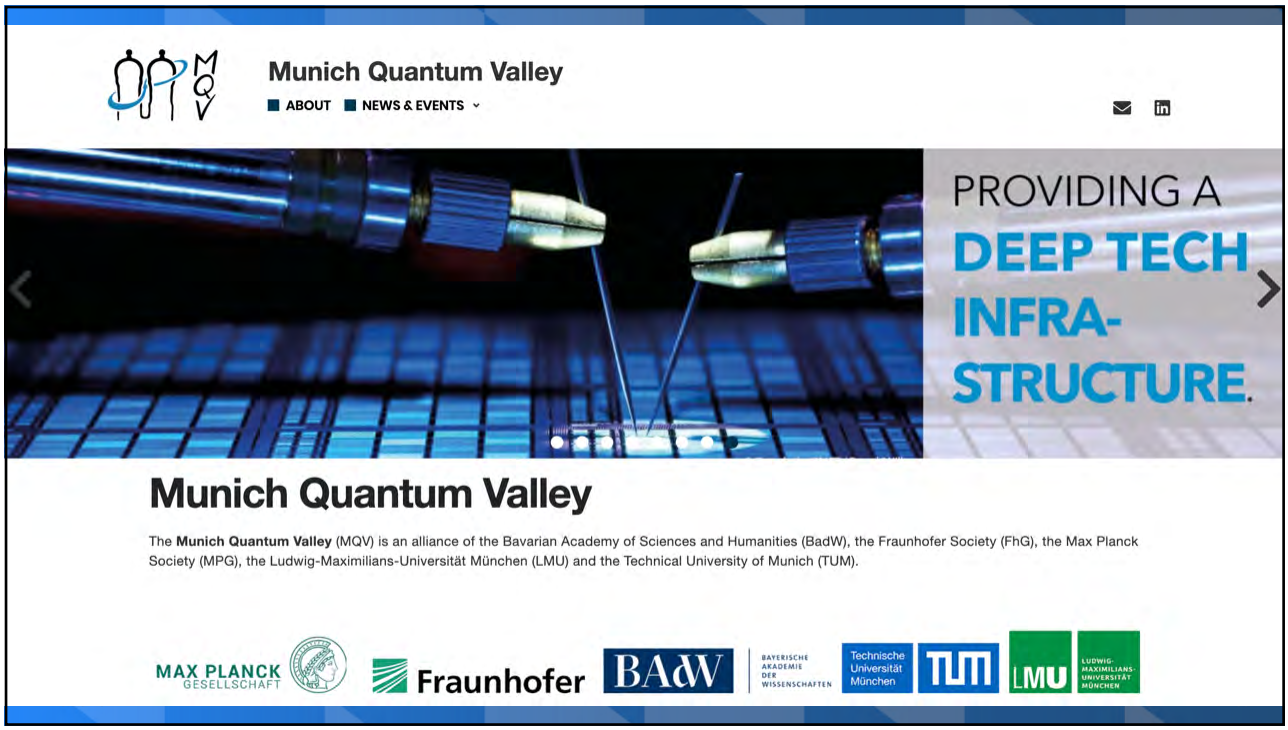
Munich Quantum Valley
ABOUT
NEWS & EVENTS
PROVIDING A
DEEP TECH
INFRA-
STRUCTURE.
Munich Quantum Valley
The Munich Quantum Valley (MQV) is an alliance of the Bavarian Academy of Sciences and Humanities (BadW), the Fraunhofer Society (FhG), the Max Planck Society (MPG), the Ludwig-Maximilians-Universität München (LMU) and the Technical University of Munich (TUM).
MAX PLANCK GESELLSCHAFT
Fraunhofer
BAdW
BAYERISCHE AKADEMIE DER WISSENSCHAFTEN
Technische Universität München
LMU
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

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The LRZ strategy in Quantum Computing

The LRZ strategy in Quantum Computing

On-premise quantum systems
- DAQC project
- R&D
- Hosting systems in the Munich Quantum Valley framework

Practical Quantum Computing services
- Quantum Technology portfolio
- Remote access
- User workflow optimisation

Applied research

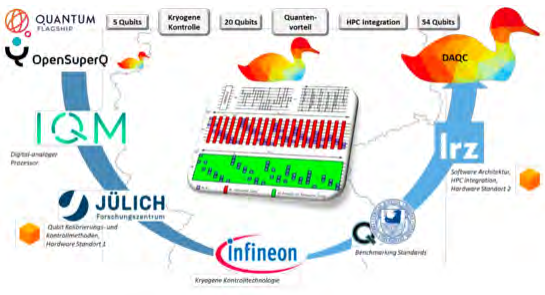
High-performance Quantum Computing
- The Atos QLM system at LRZ
- Software simulators on our HPC systems

Quantum user community and education
- The Bavarian Quantum Computing eXchange (BQCX)
- Alignment with the research community

On-premise quantum systems

Digital-Analogue Quantum Computer (DAQC)

BMBF-funded project, 02/2021-01/2025



- Development of a test system up to 54 qubits, potentially scalable to O(10^3)
- Integration into the HPC environment
- Procurement of a cryostat and setup of lab space in preparation

First German Quantum Computing Demonstrator

Q-Exa Project

- Project Runtime: 15.11.2021 - 14.11.2024
- Projekt Volume: 45,3 Mio. Euro (88,4 % funded by BMBF)
- Project Partners:
  - IQM Germany GmbH
  - Leibniz Supercomputing Centre (LRZ)
  - science + computing AG
  - HQS Quantum Simulations GmbH

- https://www.quantentechnologien.de/forschung/foerderung/quantencomputer-demonstrationsaufbauten/q-exa.html

Picture Courtesy of IQM

High-performance Quantum Computing

HPC simulation tools for Quantum Computing

- Current quantum hardware still too experimental to enable reliable tests for algorithm development
- Simulation as asset for researchers to prepare applications for upcoming architectures
- Constraints on algorithm complexity and memory footprint make it an HPC challenge

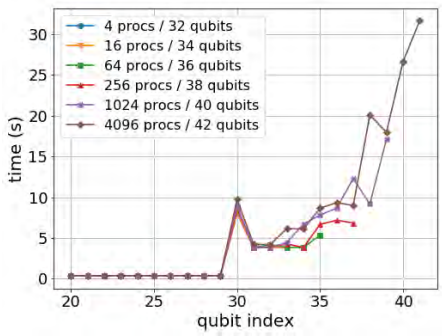
- Hardware simulators: Special-purpose systems optimised for running quantum algorithms
- Software simulators: Applications for executing quantum algorithms on high-end traditional HPC system
- Software emulators: Applications for studying the behaviours of quantum hardware on a traditional HPC system

High-performance Quantum Computing

HPC simulation tools for Quantum Computing

The Intel® Quantum Simulator (Intel-QS) is a simulator of quantum circuits on HPC systems

- First runs and scaling on SuperMUC-NG
- Optimization and development project: Collaboration between LRZ and Intel
- Tutorials at ISC19 (Intel booth) and HPCS19 on Intel-QS, more planned at LRZ



Weak scaling of Intel-QS up to 2000 nodes on SuperMUC-NG.
Guerreschi et al., ArXiv: 2001.10554

High-performance Quantum Computing

The Atos Quantum Learning Machine (QLM) at LRZ

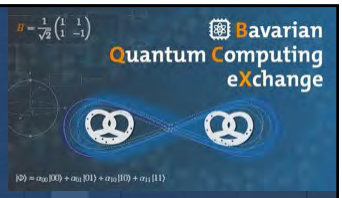
- Hardware simulator with a complete end-to-end software environment
- The software environment fully compatible with the most used development platforms (Qiskit, Cirq, Rigetti, ProjectQ) and can simulate noise on current quantum systems
- Preliminary work to make the system available to our users
- Press release and public announcement in March
- 2-day workshop with Atos for first wave of users on May, 4-5
- Development of synergies with other building blocks of our QC strategy

System arrived at LRZ
November 26, 2020

Quantum user community and education

The Bavarian Quantum Computing eXchange (BQCX)

Founded in July 2019



Bringing together and understanding the different community components

Provide a monthly forum for presentations of field experts and companies

Opportunity of visibility and networking for community members

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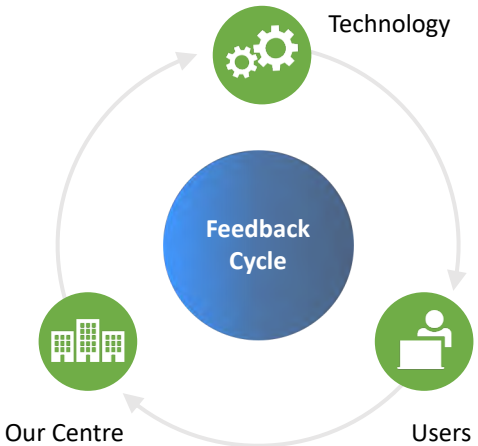
Quantum user community and education

Community alignment

- Survey of user needs (special focus: educators)
- Market surveys and tech scouting
- Focus groups
- Following / anticipating the user requests, within the LRZ role of science enabler
- Connecting with the ecosystem and its funding opportunities



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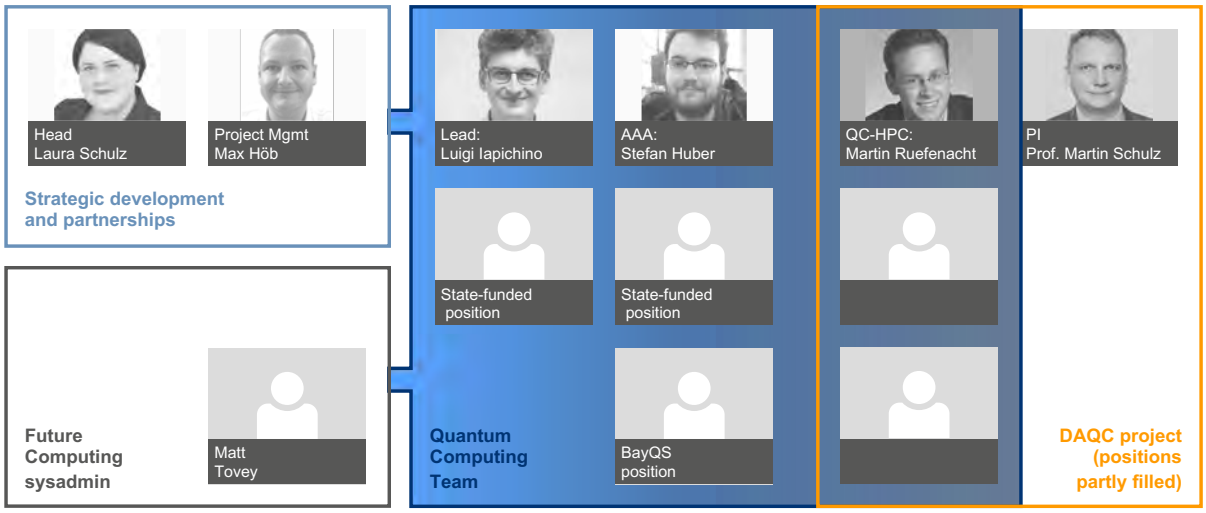
Quantum Computing at LRZ

Who we are



Integrating Quantum and High Performance Computing Expectations and Challenges

- Exascale HPC requires performance improvements beyond pure FLOP/s
- **Integrated** supercomputing architectures combine HPC, AI&ML, BD and **QC**
- Quantum computers offer huge potential as accelerators for science if they are integrated into HPC

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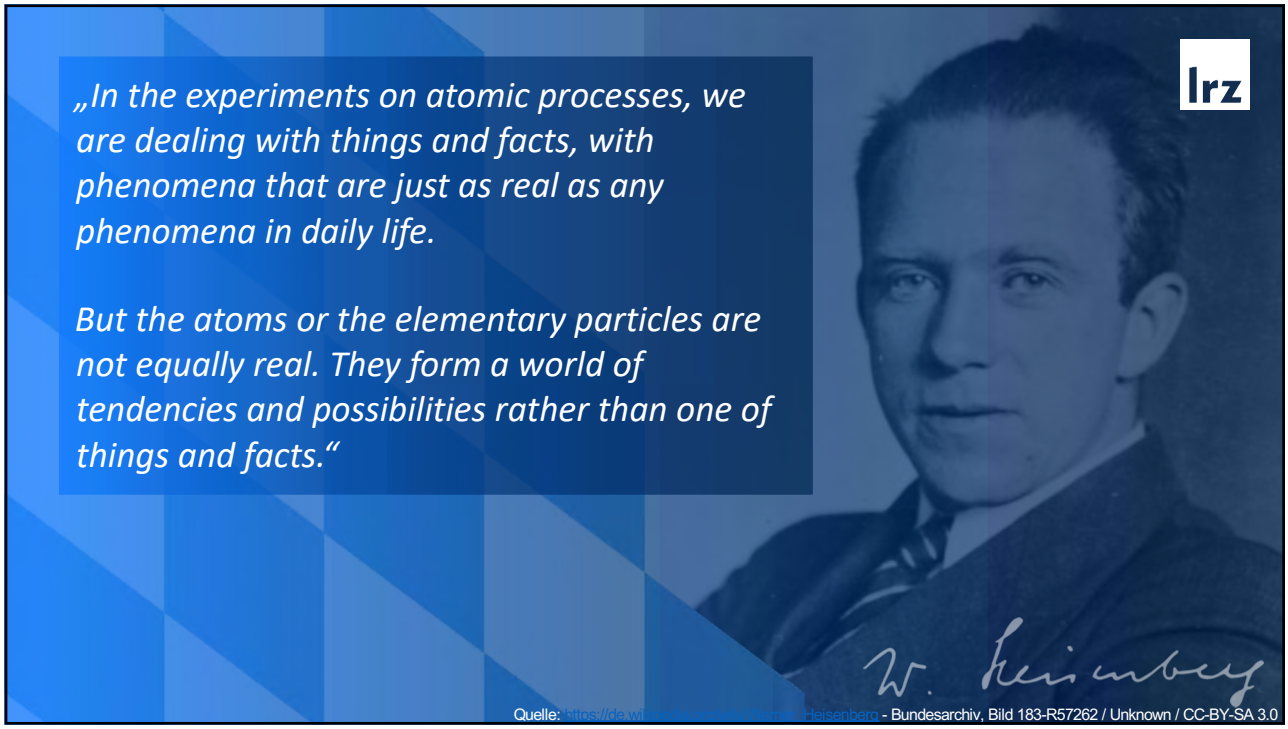
„In the experiments on atomic processes, we are dealing with things and facts, with phenomena that are just as real as any phenomena in daily life.
But the atoms or the elementary particles are not equally real. They form a world of tendencies and possibilities rather than one of things and facts.“
lrz
W. Heisenberg
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