Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

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HPC and Quantum Computing

Prof. Dr. Dieter Kranzlmüller
Ludwig-Maximilians-Universität München (LMU) &
Leibniz-Rechenzentrum (LRZ)

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Leibniz Supercomputing Centre (LRZ)
of the Bavarian Academy of Sciences and Humanities
Partner for Digital Transformation of Science & Research
BAdW
lrz
IT-Services for Science since 1962
Munich Universities, Bavaria, Germany, Europe, …
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GCS
Gauss Centre for Supercomputing
lrz
SUPERMUC-NG
ASTRO PHYSICS
LIFE SCIENCES
Quelle: F. Löchner für LRZ
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The World's Largest Turbulence Simulation
Astro physics: How stars are born
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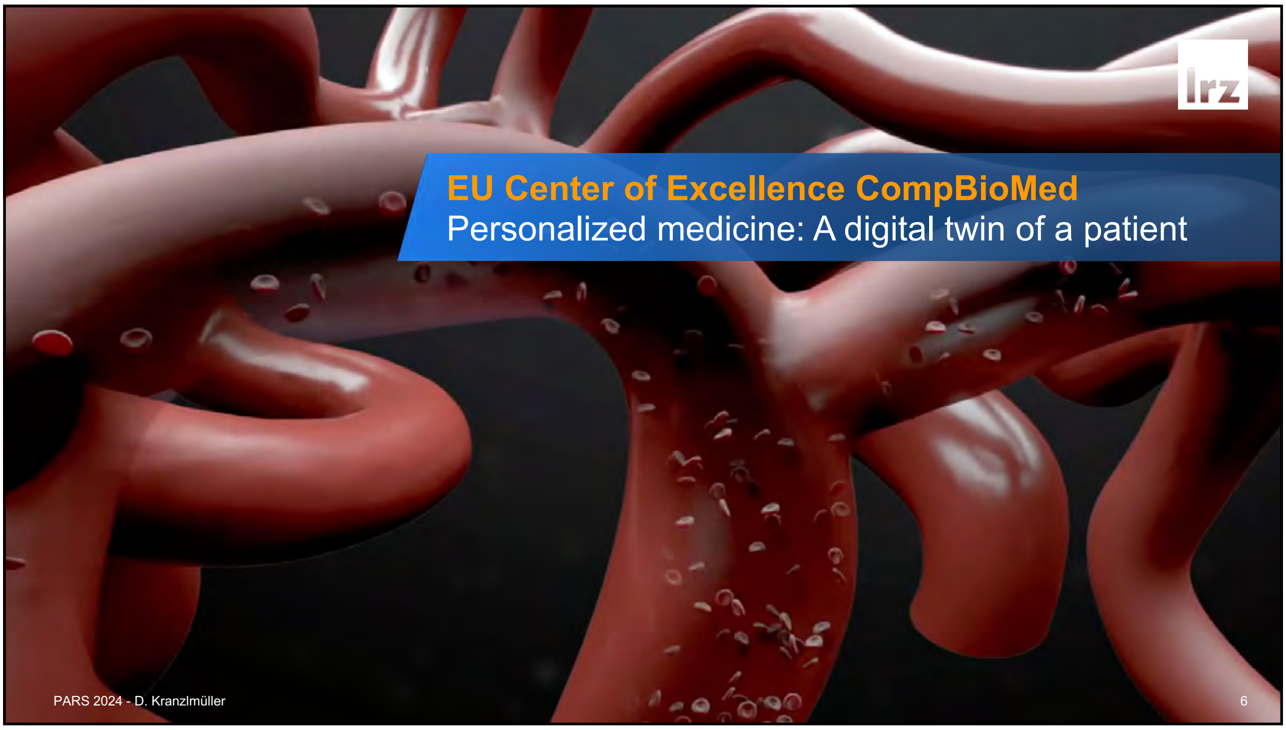
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EU Center of Excellence CompBioMed
Personalized medicine: A digital twin of a patient
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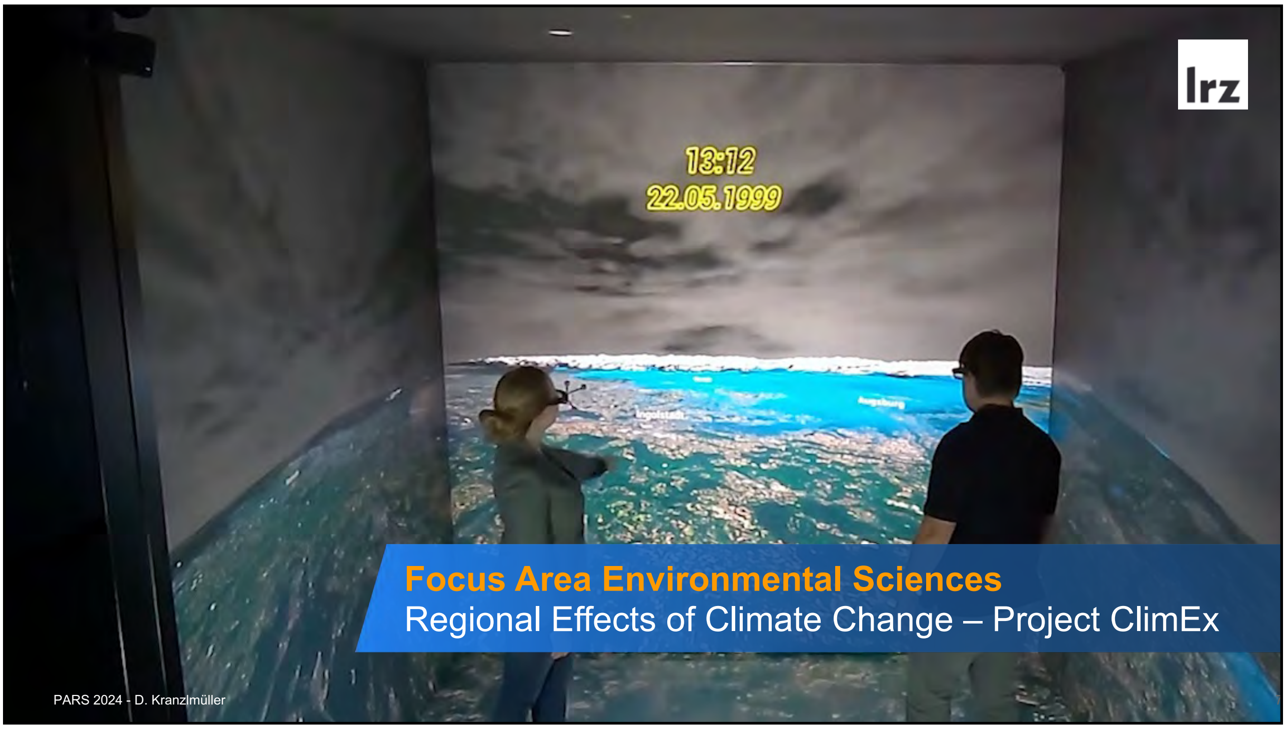
lrz
13:12
22.05.1999
Focus Area Environmental Sciences
Regional Effects of Climate Change – Project ClimEx
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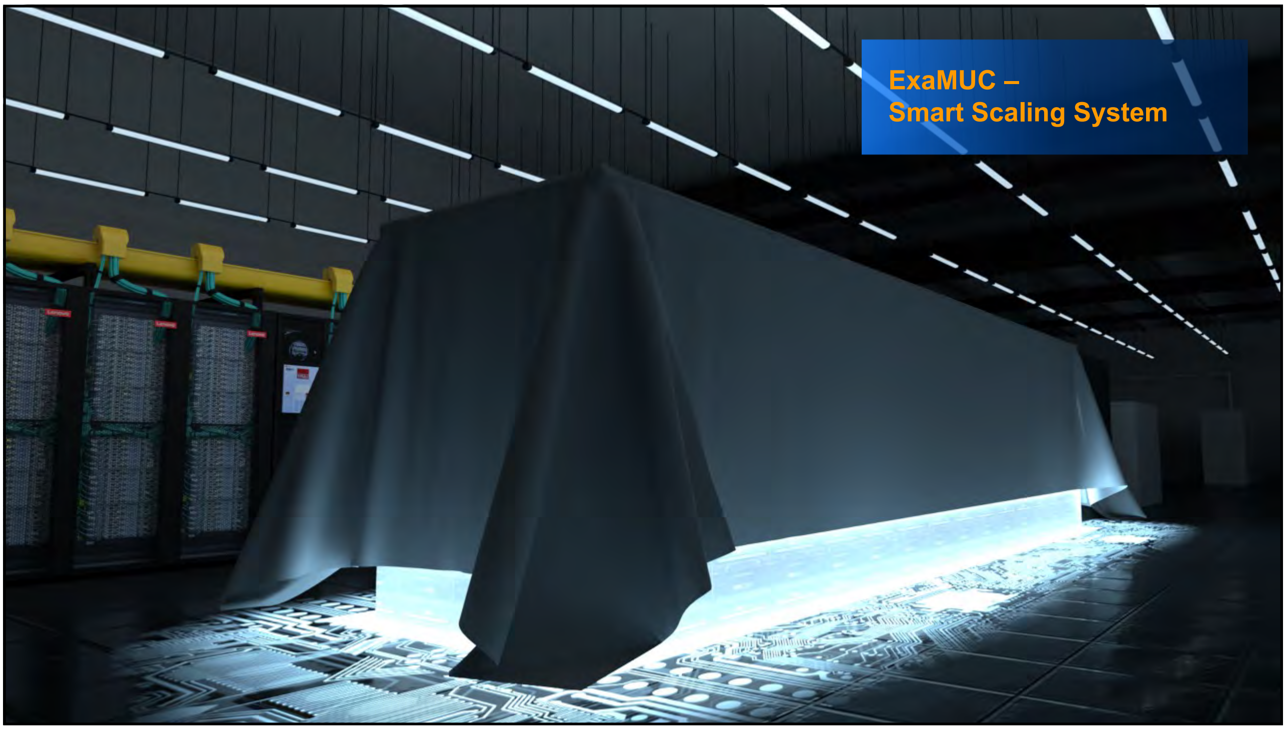
ExaMUC –
Smart Scaling System

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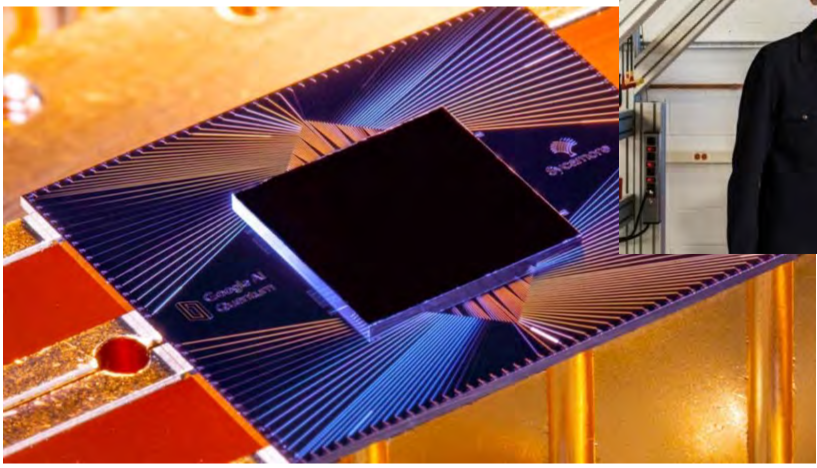
Google demonstrates „Quantum Supremacy“



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

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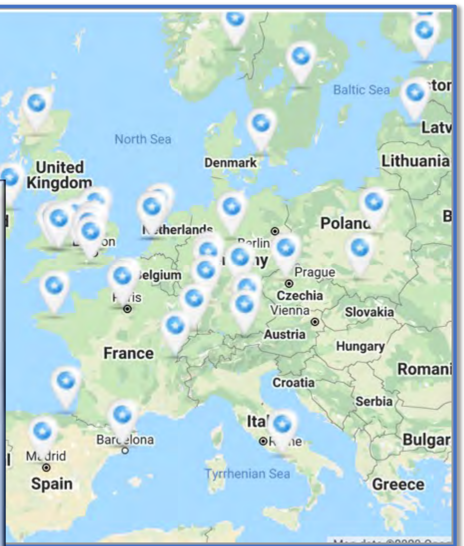
https://quantumzeitgeist.com/interactive-map-of-quantum-computing-companies-from-around-the-globe/

Quantum Computing Companies around the Globe



23.01.2024 - **World Economic Forum**:
„Quantum-secure financial sector:
4 principles to inform global regulatory approaches“

- **Quantum computing provides disruptive opportunities** to the financial sector, by advancing complex operations with projected investment expected to reach $19 billion by 2030s.
- **Mitigating the quantum security threat** is needed to fully harness these opportunities, and global regulatory approaches can trigger harmonized action.

https://www.weforum.org/agenda/2024/01/quantum-secure-financial-sector-regulations/

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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/

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/

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

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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

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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

Quantum Computer:

- 1 Qubit: 0 and 1 "simultaneously"

- Example: Schrödinger's Cat

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

https://media.giphy.com/media/LGyeWkr2m3v7a/giphy.mp4

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How does a Quantum Computer work?

Computing with Qubits

Conventional Computer:

- 1 Bit: 0 or 1

Compute ($Bit_1 + Bit_2$)

Result: 1 row of

Bit_1	Bit_2	Sum	Overflow
0	0	0	0
0	1	1	0
1	0	1	0
1	1	0	1

Quantum Computer:

- 1 Qubit: 0 and 1 „simultaneously“

Compute ($Qubit_1 + Qubit_2$)

$Qubit_1$	$Qubit_2$
$\alpha_1\|0\rangle + \beta_1\|1\rangle$	$\alpha_2\|0\rangle + \beta_2\|1\rangle$

Result:

Sum	Overflow
$\alpha_s\|0\rangle + \beta_s\|1\rangle$	$\alpha_o\|0\rangle + \beta_o\|1\rangle$

Sum	Overflow
0	0
1	0
1	0
0	1

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How to use a Quantum Computer

Applications of Quantum Computers

Conventional Computer:

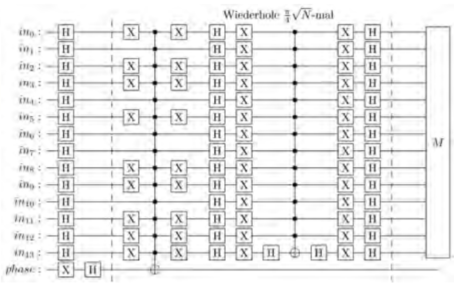
0000
0001
0002
0003
0004
0005
…

Max. 10.000 Steps

SuperMUC-NG:
26.900.000.000.000.000 Flop/s

Quantum Computer:

14 Qubits
2^{14} = 16385 States



79 Steps Grover
Speedup: 133

https://www.amazon.de/dp/B07SXGRDMM?th=1

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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

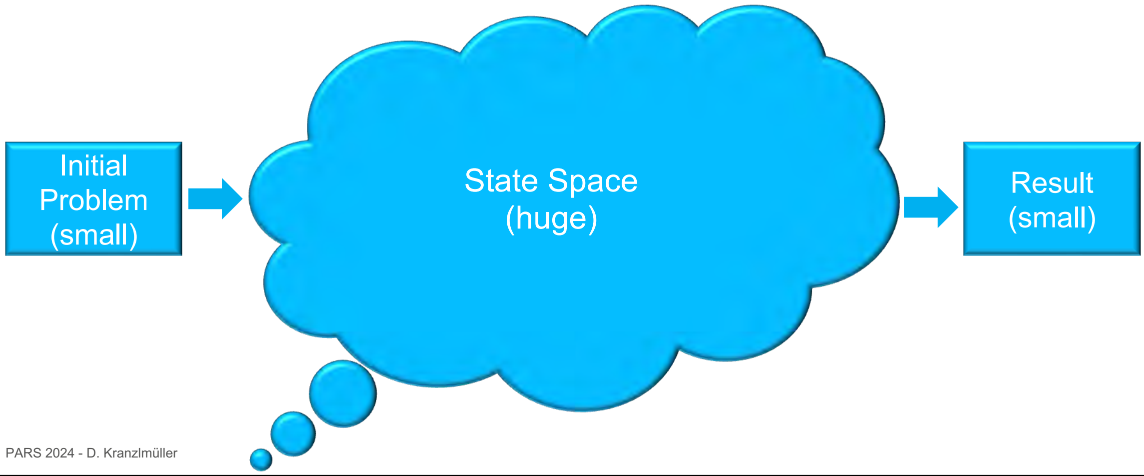
Overview Quantum Algorithms

- **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

Application of Quantum Computers

What are quantum computers particularly suitable for?

1. Computing Quantum Mechanics (Physics, Chemistry, Pharmacy, …)
2. Optimizations in large state spaces



Application of Quantum Computers

What are quantum computers particularly suitable for?

Sudoku

6	3	2	8			4	7	1
				6				
8		4						
					2		5	
								4
	2		6	8		7		
1		5	9	4			8	
								6
7	8				5			

qc@nm.ifi.lmu.de

MNM TEAM

Traveling Salesman

Von Der ursprünglich hochladende Benutzer war Kapitän Nemo in der Wikipedia auf Deutsch – https://www.cia.gov/cia/publications/factbook/maps/gm-map.gif, Gemeinfrei, https://commons.wikimedia.org/w/index.php?curid=5584283

Material Sciences, …

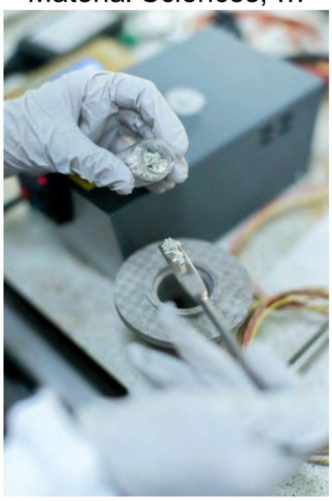


Foto von ThisisEngineering RAEng auf Unsplash

Quantum Artificial Intelligence & Quantum Machine Learning

AI and QC? (1/2)

- Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd, „Quantum Algorithm for Linear Systems of Equations“, Phys. Rev. Lett. 103, 150502 – Published 7 October 2009 https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.103.150502
  ➔ Solving systems of linear equations exponentially faster than classical computers

- Problem: Encoding “classic” data into qubits and back takes a (really) long time (today)
- But: Speed is not the only aspect in favor of quantum computers
- Hope: Quantum computers may discover correlations that remain hidden to conventional computers

- ➔ Machine quantum learning for quantum data – Quantum sensors measure the quantum mechanical properties of a system ➔ Pattern matching with QC

https://www.spektrum.de/news/revolutioniert-die-fusion-von-ki-und-quantenphysik-die-wissenschaft/2203074

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Quantum Artificial Intelligence & Quantum Machine Learning

AI and QC? (2/2)

- Hsin-Yuan Huang, et al, „Quantum Advantage in Learning From Experiments“, Science, 9 Jun 2022, Vol 376, Issue 6598, pp. 1182-1186, DOI: 10.1126/science.abn7293

- Experiment on the Google Sycamore quantum computer (40 Qubits) – Simulating the behavior of abstract material ➔ Analysis with quantum machine learning
- ➔ exponentially faster compared to the classic method

- Use of quantum sensors:
  Superconductors, particle accelerators, astronomy, …

- Vedran Dunkjo, „Quantum Learning Unravels Quantum System“, Science, 9 Jun 2022, Vol 376, Issue 6598, pp. 1154-1155, DOI: 10.1126/science.abp9885

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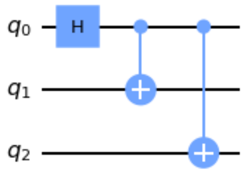
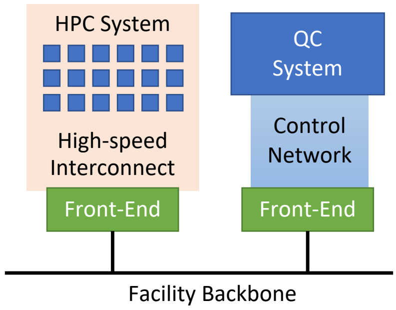
How to use a Quantum Computer in your HPC Data Center

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





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

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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

Big Data

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LRZ Integrated Supercomputing Architecture

The HPC Innovation/Integration Circle

lrz

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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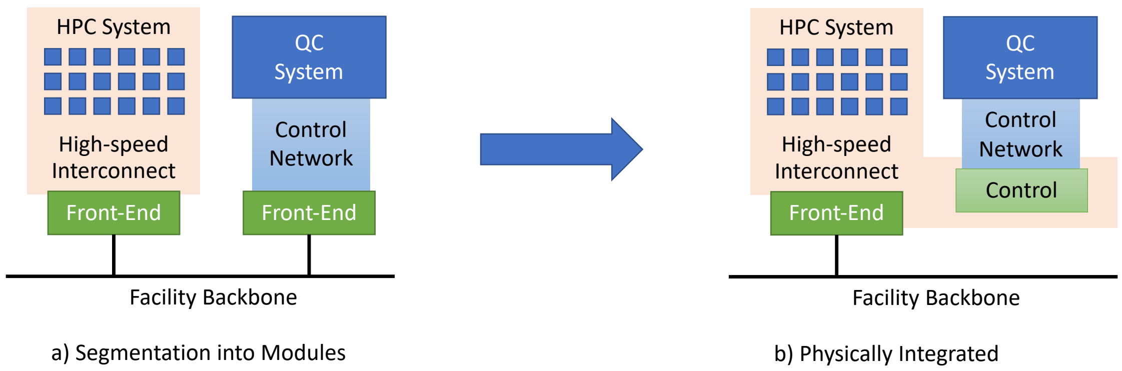
Utilizing the Ideas of the Integrated Supercomputing Architecture

From Independent Modules to an Integrated System

lrz



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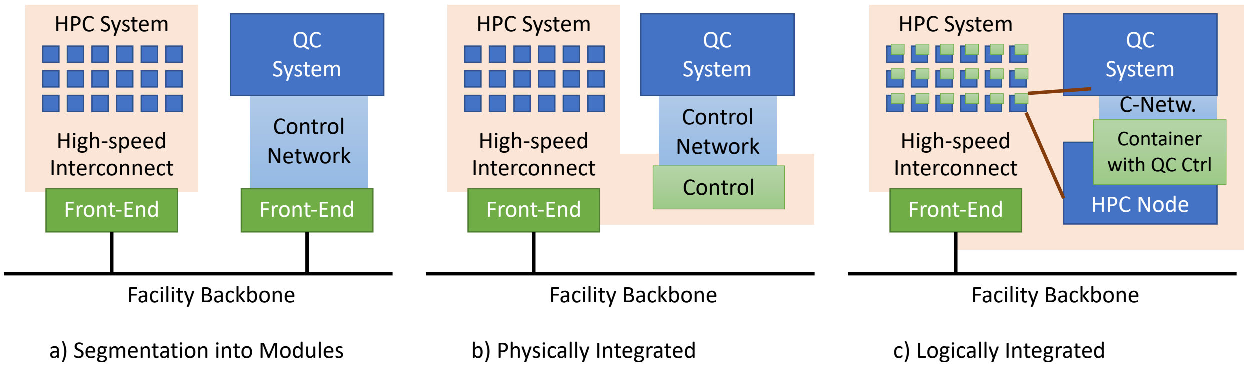
Full HPC-QC Integrated Architecture

Towards Logically Integrated Quantum Computers



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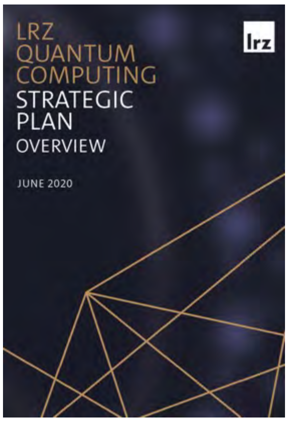
QC at LRZ

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

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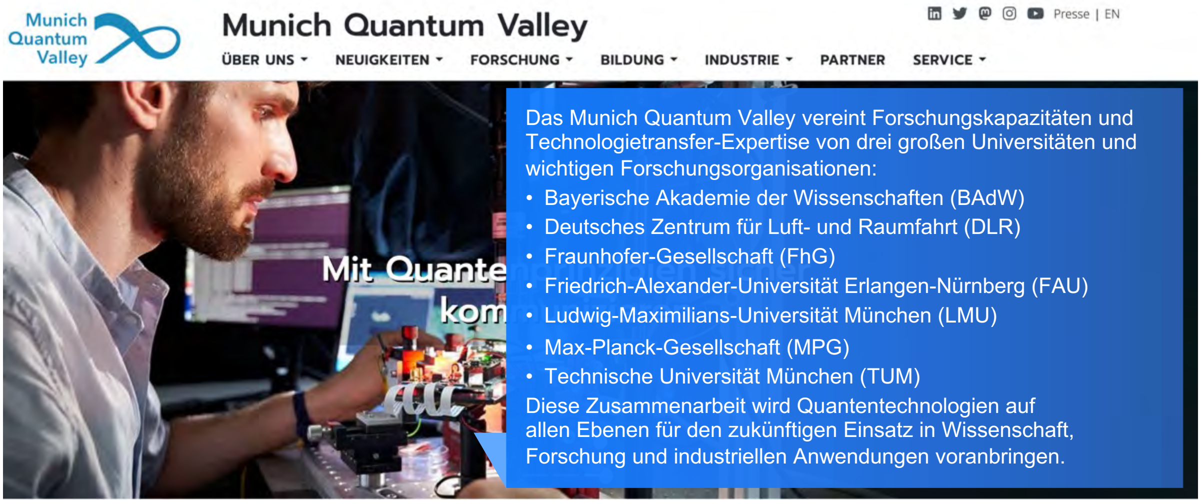
Zusammenhang QC – Integrierte Architektur

MQV – Einbindung Münchner Umfeld



Das Munich Quantum Valley vereint Forschungskapazitäten und Technologietransfer-Expertise von drei großen Universitäten und wichtigen Forschungsorganisationen:

- Bayerische Akademie der Wissenschaften (BAdW)
- Deutsches Zentrum für Luft- und Raumfahrt (DLR)
- Fraunhofer-Gesellschaft (FhG)
- Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
- Ludwig-Maximilians-Universität München (LMU)
- Max-Planck-Gesellschaft (MPG)
- Technische Universität München (TUM)

Diese Zusammenarbeit wird Quantentechnologien auf allen Ebenen für den zukünftigen Einsatz in Wissenschaft, Forschung und industriellen Anwendungen voranbringen.

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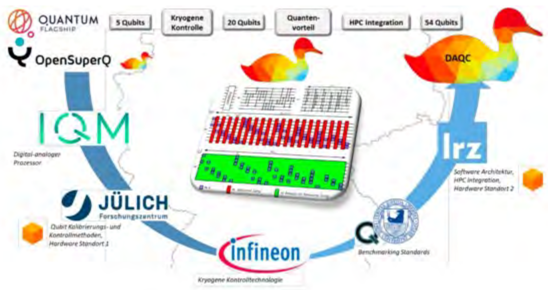
On-premise quantum systems

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

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On-Premise Quantencomputer

Digital-Analogue Quantum Computer (DAQC)

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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

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Germany's First Quantum Demonstrator

Q-Exa

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6 Quantum computers for Europe

European Integrated Quantum Computer - Euro-Q-Exa

https://www.quantum.lrz.de/bits-of-qubits/detail/quantum-computer-for-europe

- EuroHPC Joint Undertaking (JU) has signed agreements with 6 HPC centres to each host and operate a quantum computer at their sites
- LRZ will
  - connect QC to its leadership class system
  - provide access for European researchers to the Q-Exa demonstrator in 2024
  - upgrade its capabilities for Europe to 50 and later a minimum of 100 qubits
  - develop and optimize software for QC
- Euro-Q-Exa is supported by EuroHPC JU, BMBF and StMWK

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IQM Leibniz-Rechenzentrum 2022

Bringing quantum acceleration to supercomputers

MARTIN RUEFENACHT[1], BRUNO G. TAKETANI[2], PASI LÄHTEENMÄKI[3], VILLE BERGHOLM[3], DIETER KRANZLMÜLLER[1], LAURA SCHULZ[1], AND MARTIN SCHULZ[1,4]

[1] Leibniz Supercomputing Centre, Garching near München, Germany
[2] IQM, Nymphenburgerstr. 86, 80636 Munich, Germany
[3] IQM, Keilaranta 19, 02150 Espoo, Finland
[4] Technical University of Munich, Garching near München, Germany

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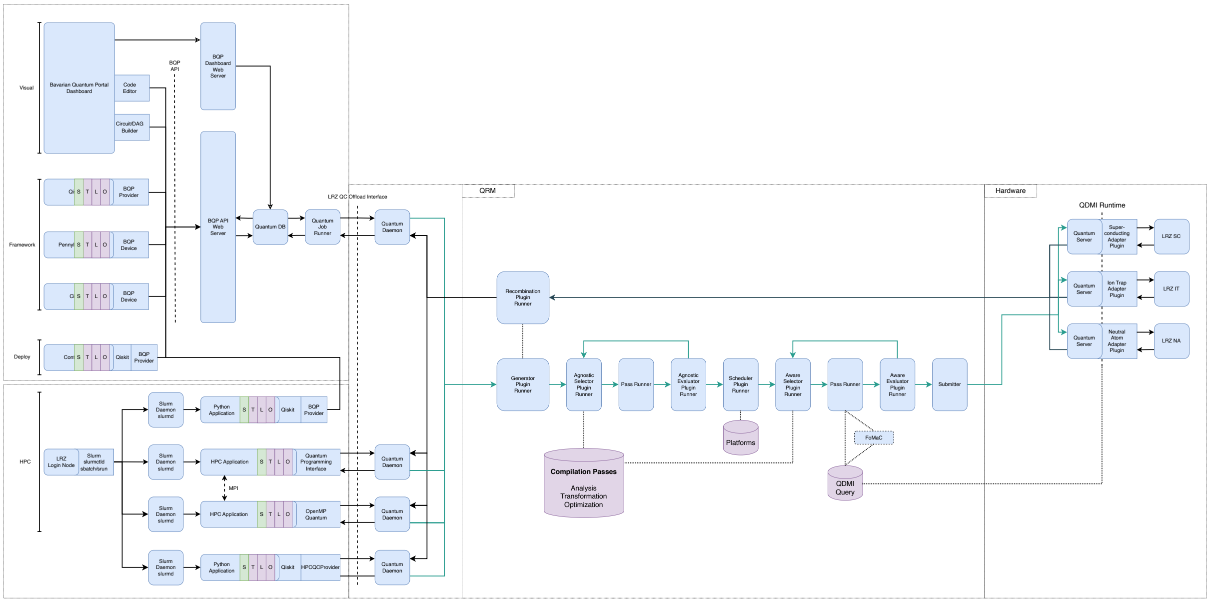
Overview of Munich Quantum Software Stack



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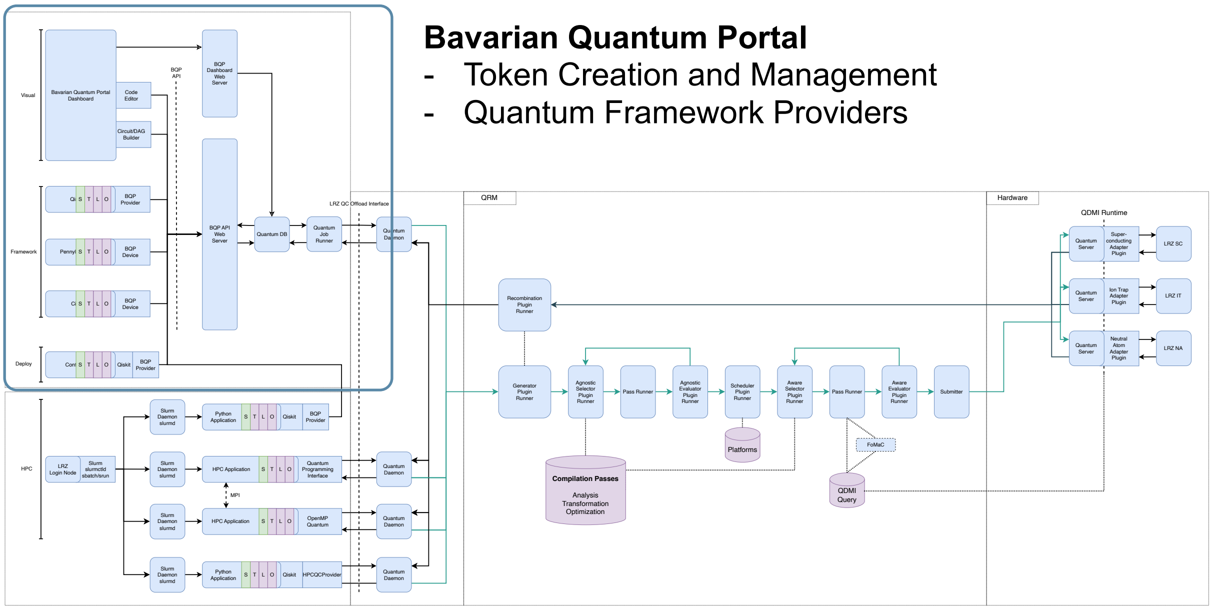
Overview of Munich Quantum Software Stack



Bavarian Quantum Portal

- Token Creation and Management
- Quantum Framework Providers

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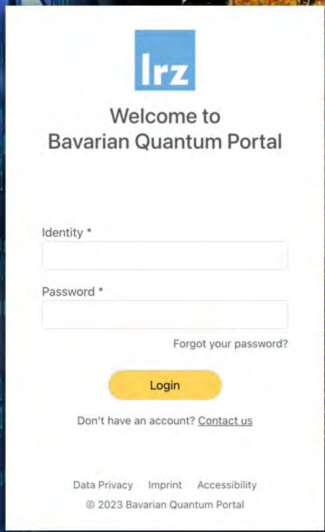
BQP Dashboard

For Users

- User login with university ID or Quantum Portal account
- Status reports for resources/budget
- Job overview and submission
- Code editor
- Circuit builder

For Administrators

- Access token management
- Allocation and Account Management
- Security Compliance



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BQP Qiskit Provider

Allows user to use Qiskit as they are accustomed.

Hooks Qiskit into the Munich Quantum Software Stack.

Token is placed in tokenfile here.

Job sent to IQM Q5 system at LRZ

```python
from bavarian_quantum_portal_provider import BQPProvider

from pprint import pprint

import termplotlib as tpl


if __name__ == "__main__":
    c = QuantumCircuit(5, 5)

    c.h(2)
    c.cx(2, 1)
    c.cx(2, 0)
    c.cx(2, 3)
    c.cx(2, 4)

    c.measure_all()

    print(c.draw())

    with open("token.txt") as tokenfile:
        provider = BQPProvider(token=tokenfile.read()[:-1])

    backend = provider.get_backend("Test Q5")

    job = backend.run(c, shots=1000)

    result = job.result()

    pprint(result.get_counts())

    proper = {
        k: v for k, v in sorted(result.get_counts().items(), key=lambda item: item[0])
    }

    fig = tpl.figure()
    fig.hist(
        list(proper.values()),
        list(proper.keys()),
        force_ascii=False,
    )
    fig.show()
```

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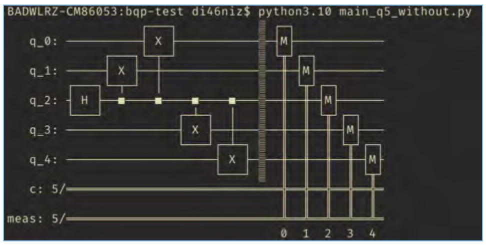
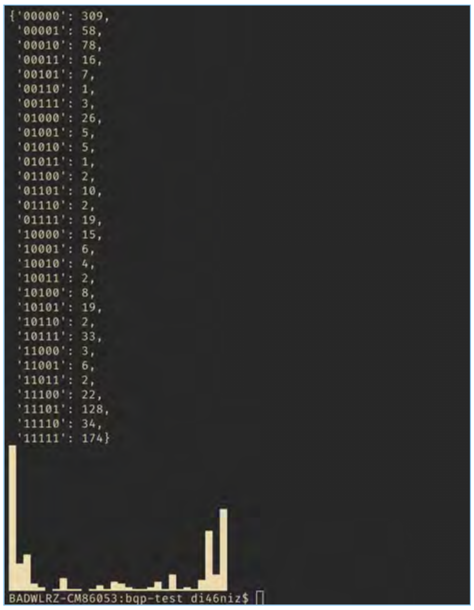
BQP Python Execution

Circuit sent to IQM Q5 at LRZ.

Returns circuit design and measurements.





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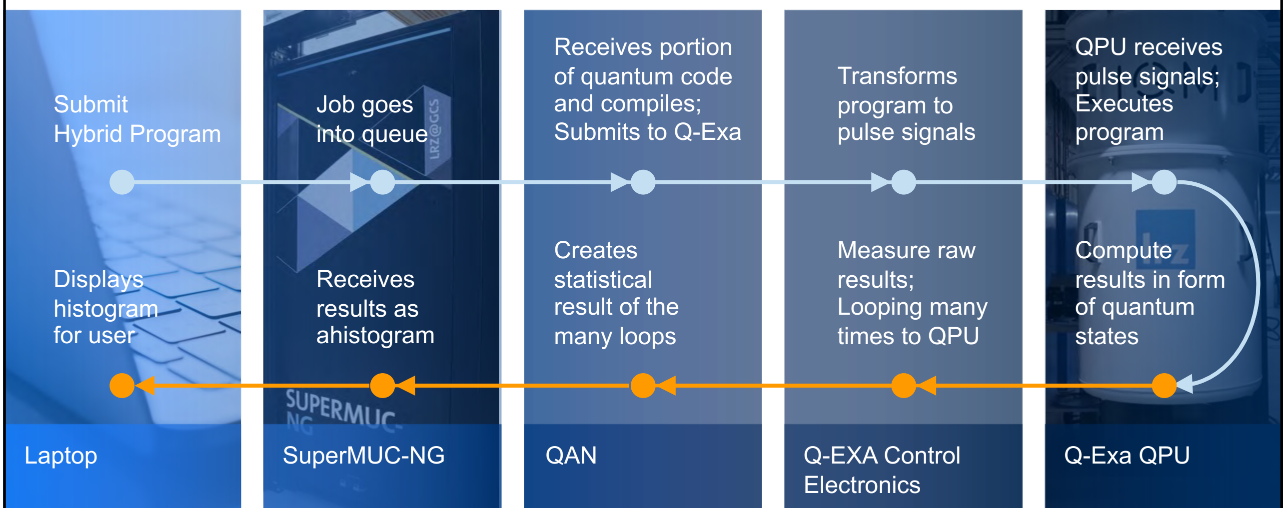
How to use a Quantum Computer?

Integration of Q-Exa with SuperMUC-NG



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Towards Quantum Computing

Challenges for Quantum Computers

Physics:
- Decoherence (environmental sensitivity)
- Error correction
- Scalability
- Clock speed (Superconducting: 1.4 MHz, Photons: 10 Hz)
- Data transfer in and out of the QC

Computer science:
- Real algorithms or algorithms for real world problems
- An abstraction for programming quantum computers
- A programming language and compiler
- A runtime system for integrated quantum and HP computers

HPC and Quantum Computing

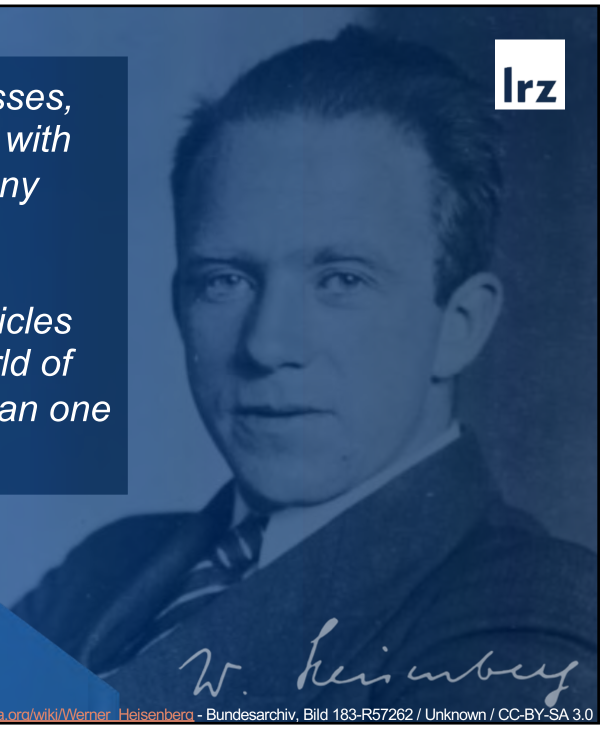
- **Integrated Supercomputing** combines HPC, AI&ML, BD and **QC**
- Quantum computers offer huge potential as accelerators for science (if they are integrated into HPC)
- QC is not only a physics challenge! It requires also lots of research in **Computer Science**

Contact:
Prof. Dr. Dieter Kranzlmüller
kranzlmueller@lrz.de / @Kranzlmueller

Foto: StMWK / Axel König

„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.“



Quelle: https://de.wikipedia.org/wiki/Werner_Heisenberg - Bundesarchiv, Bild 183-R57262 / Unknown / CC-BY-SA 3.0

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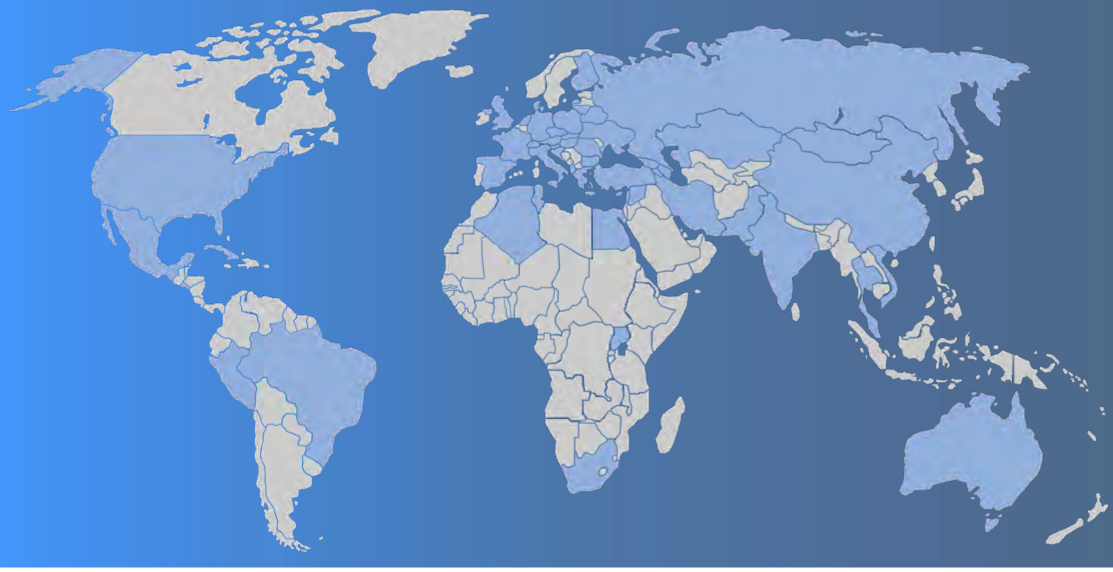
Leibniz Supercomputing Centre (LRZ) – Our Staff



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