Thoughts on the Path towards Exascale from a JSC Perspective
Supercomputing in Germany

Gauss Centre for Supercomputing

▪ Roof organisation for supercomputing centres in Germany
▪ Funded by federal state + 3 states
▪ Hosting member of PRACE

GCS members

▪ Jülich Supercomputing Centre (JSC)
▪ HLRS High Performance Computing Centre Stuttgart (HLRS)
▪ Leibniz Supercomputing Centre (LRZ)

Mission

▪ Provision of state-of-the-art supercomputing resources
▪ Open access for scientists and researchers
▪ Optimal application and user support
▪ High-level education and training of supercomputer users
Current Systems Roadmap of JSC

- **IBM Power 6**
  - JUMP, 9 TFlop/s

- **JUROPA**
  - 200 TFlop/s
  - HPC-FF
  - 100 TFlop/s

- **IBM Power 4+ JUMP (2004)**
  - 9 TFlop/s

- **IBM Blue Gene/L JUBL (2013)**
  - 45 TFlop/s

- **IBM Blue Gene/P JUGENE**
  - 1 PFlop/s

- **IBM Blue Gene/Q JUQUEEN (2012)**
  - 5.9 PFlop/s

- **JURECA Cluster (2015)**
  - 2.2 PFlop/s

- **JURECA Booster (2017)**
  - 5 PFlop/s

- **GCS Cluster Module (2018)**
  - 12 PFlop/s

- **Hierarchical Storage Server JUQUEEN Successor**

- **GCS Scalable Module (2019)**
  - 50+ PFlop/s
Exascale Computing

My preferred definition: Supercomputer that are $100 \times$ better for enabling new science

- Supercomputing as a mean for enabling science and engineering

JSC’s focal application domains

- Earth sciences
- Materials sciences
- Neurosciences and brain research
- High energy physics
Example: Lattice Quantum Chromodynamics

Key characteristics
- Regular grid, compute and memory bandwidth limited

Workload $W \propto V^{5/4}$
- $100 \times$ could mean $2.5 \times$ larger lattices
- Requires $100x$ increase in compute performance, memory bandwidth and capacity
  - Memory capacity requirements in main kernel typically $\sim 10\%$ of overall application

Scientific benefits
- Simulations closer to continuum limit
- Simulations using larger physical boxes
Example: Brain Simulations

Key characteristics

- Spiking neuronal network simulators with complex control flow
- Multi-compartment simulators with compute-intensive solvers with regular control flow
- Memory footprint limited in extreme-scale network limit

100× increase of compute architecture capabilities for

- Significantly increased network sizes
- Increase of compute capabilities to enable
  - Faster simulations
  - More complex models

Required capability improvements

- Memory capacity (at suitable memory bandwidth)
- Compute and memory performance
Technology challenges: Memory

Desirable memory performance features

- Large memory capacity $C_{\text{mem}}$
- High memory bandwidth $B_{\text{mem}}$

Different memory technologies being integrated into HPC systems

- SDRAM: DDR3, DDR4
- High-bandwidth memory technologies: HBM, HMC/MCDRAM
- Non-volatile memory technologies: NAND Flash, 3D-Xpoint

Significant differences in terms of

$$\Delta \tau = \frac{C_{\text{mem}}}{B_{\text{mem}}}$$
## Top500 #1 Trends

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Beyond HPC for Simulations

Interactive monitoring and steering of applications
- Tight integration of visualisation
- Enablement of feedback loops
- Example: steering of brain simulations

Open data infrastructures
- Facilitate data import/export within federated data infrastructures
- Examples: data-driven material sciences, analysis of earth satellite data

Interactive computing services
- Facilitate interactive access to large data resources
- Allow for elastic access to scalable compute resources
- Example: brain research
Summary

The path towards exascale should be driven by application needs
- Enable addressing larger challenges in shorter amount of time

Improvements required by applications can be diverse
- Lattice QCD: Need for increasing $B_{\text{mem}}$
- Brain simulators: Need for increasing $C_{\text{mem}}$

The path to future architectures strongly limited by key technologies
- Example: memory technologies