High-Performance Computing for Computational Engineering Science

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RWTH AACHEN UNIVERSITY

TECHNISCHE UNIVERSITÄT DARMSTADT

NHR4CES NHR for Computational Engineering Science

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National HPC (Nationales Hochleistungsrechnen = NHR) in a Nutshell

Goals

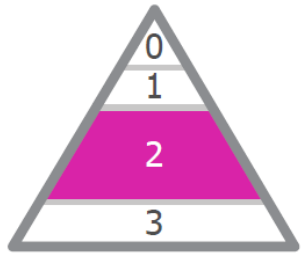
- Provide **HPC capacity** for scientific research at universities in Germany
- Coordinate interdisciplinary **cooperation across sites**
- Strengthen **HPC competence** of users and support young scientists
- Advance scientific computing

Funding

- 62,5 Mio. EUR/year for the program, 50/50 federal/state funding
- The funding can also be used for staff and operating costs!
- Previously, only investments could be funded through §91b GG

NHR centers

- ca. 75 Mio. EUR per center over 10 years (2021-2030)
- Open nation-wide: moving from definition by region to **definition by focus area**



Tier 0: European stand-alone systems

Tier1: Gauss Centres for Supercomputing

Tier 2: **NHR centers** and non-university research institutions

Tier 3: Regional HPC centers and institutes with local clusters

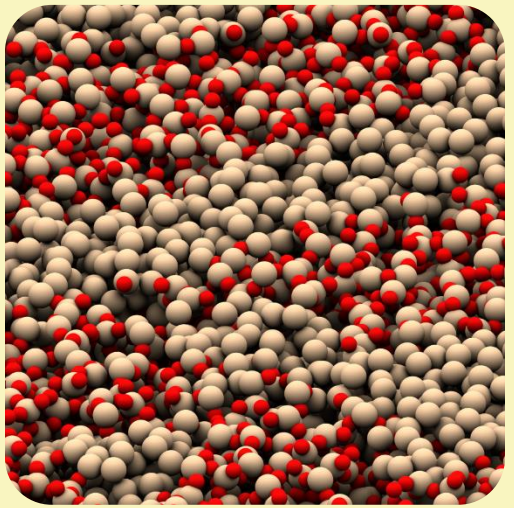
NHR Alliance - Members

- **Rhein-Westfälische Technische Hochschule Aachen**
- Zuse Institut Berlin (ZIB)
- **Technische Universität Darmstadt**
- Technische Universität Dresden
- Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg
- GWDG/Georg-August-Universität Göttingen
- Karlsruher Institut für Technologie
- Johannes Gutenberg Universität Mainz for NHR Süd-West (Goethe-Universität Frankfurt, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Johannes Gutenberg Universität Mainz, Universität des Saarlandes)
- Universität Paderborn

The NHR Center for Computational Engineering Science

Optimal support for engineering and materials science & engineering-oriented physics, chemistry, and medicine

- Hardware tailored to CE workloads
- Scientific support & method training in relevant areas
- Software stack for users



Amorphous structure of silicon monoxide with silicon atoms and oxygen atoms

Complex liquid-gas interface close to the nozzle of a coaxial atomizer

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Two technical universities joining forces

Joint scientific support & method training via
Simulation & Data Labs (**SDL**s) and Cross-Sectional Groups (**CSG**s)

Unified execution environment

Aligned procurement

CLAIX

RWTH Aachen

Lichtenberg

TU Darmstadt

Specializations

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computational fluid dynamics	**Application: Engineering**	materials science
parallel programming	**Methods: Performance engineering**	scaling
energy efficiency	**Hardware/Operation**	cluster

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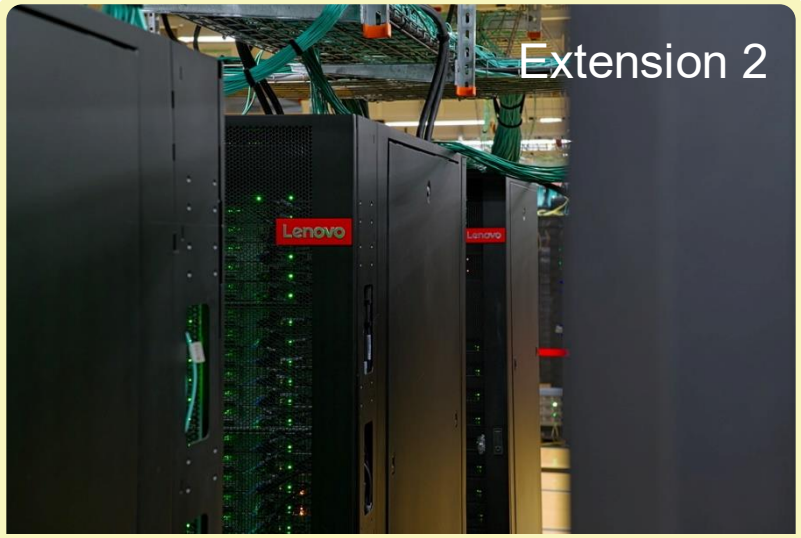
HPC Systems at TU Darmstadt

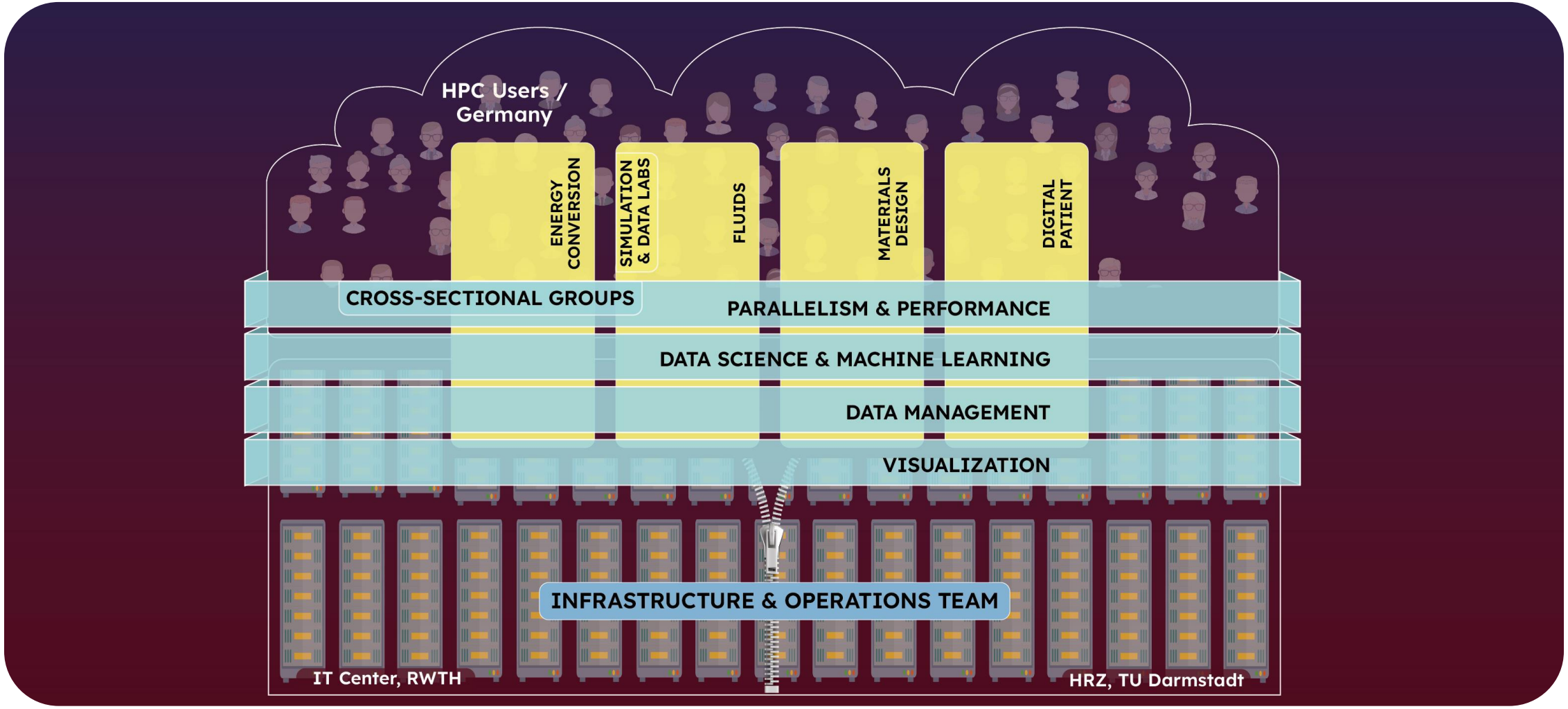
Operation since	Q4 2020
Compute nodes	630x MPI / 2x MEM
GPU nodes	4x V100 / 4x A100 / 3x DGX A100
Memory/node	384 / 1536 GB
Total # of cores	62.592
Total memory	257 TByte
CPU Peak (theo.)	ca. 4.5 PFLOPS
GPU Peak (theo.)	ca. 424 TFLOPS



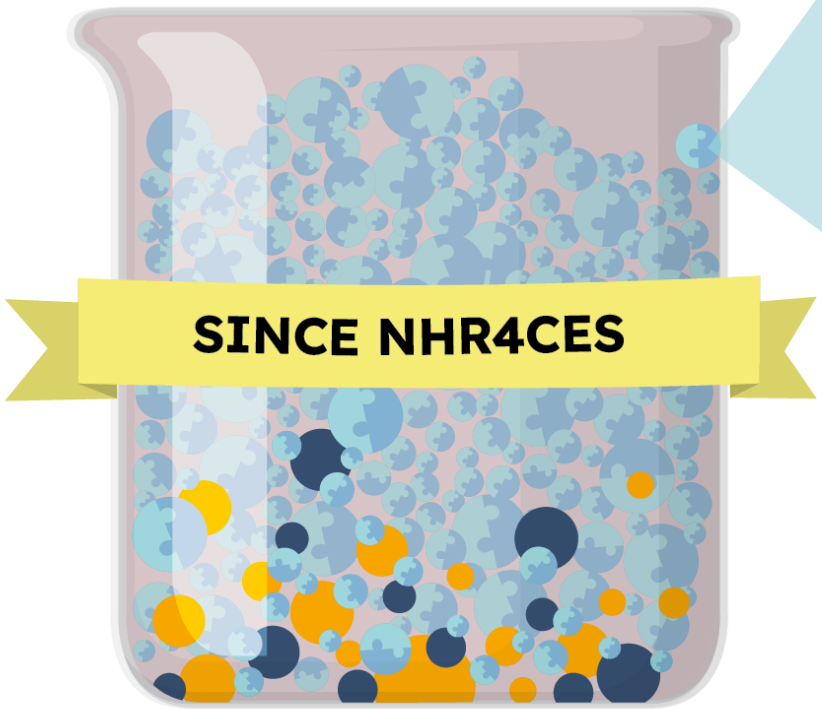
Operation since	Q4 2023
Compute nodes	576x MPI / 3x MEM
GPU nodes	5x PVC / 2x H100
Memory/node	512 / 2048 GB
Total # of cores	61.304
Total memory	306 TByte
CPU Peak (theo.)	ca. 4.0 PFLOPS
GPU Peak (theo.)	ca. 1312 TFLOPS

Disk pool	4 PByte
Flash pool	2 PByte
Flash Read Bandwidth	ca. 1216 GB/s
Flash Write Bandwidth	ca. 869 GB/s
IOPS	ca. 1.5 Mio./s

Support groups in applications and methods



Workshops & training courses



→ **More than 80 training courses with approx. 1900 participants (in total)**

approx. 40% newly created in the context of NHR

- HPC.NRW/HKHLR training courses
- IT Center/HRZ training courses
- NHR4CES training courses

Community workshops

2022

1st Community Workshop: The Role of High-Performance Computing in Computational Engineering Science

(all groups)

2023

Machine Learning in Computational Fluid Dynamics

(SDL Energy Conversion & CSG DSML)

2024

Data-Driven Healthcare: Leveraging Visualization and Data Management for Digital Patient Studies

(SDL Digital Patient & CSG Vis)

2025

Performance Engineering for Numerical Methods in Computational Fluid Dynamics

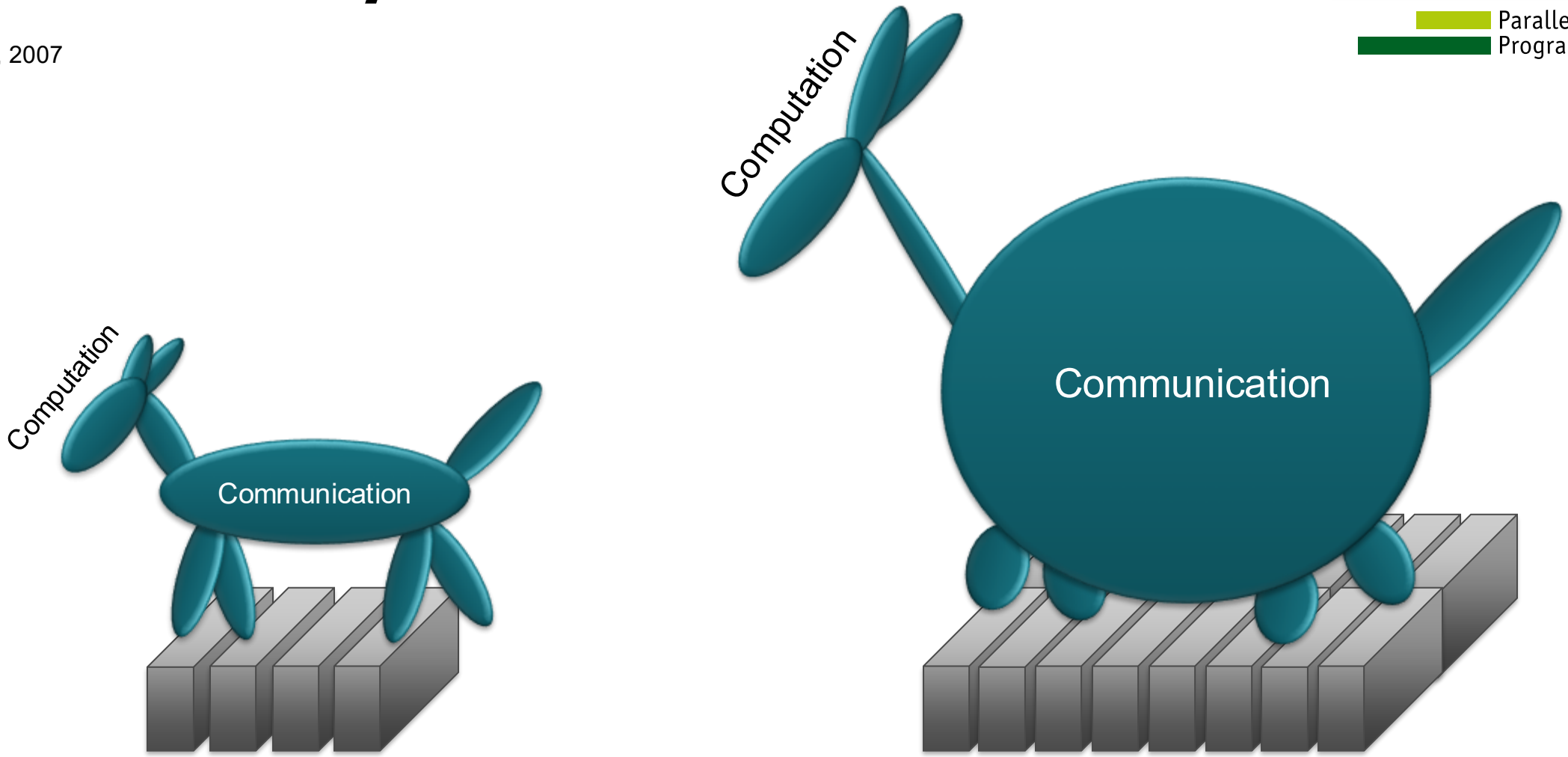
(CSG PP & SDL Fluids)

Materials Science with Advanced Data Management and Data Science Techniques

(SDL Materials Design & CSGs DM & DSML)

Scaling your code can harbor *performance surprises**...

*Goldsmith et al., 2007



Performance model

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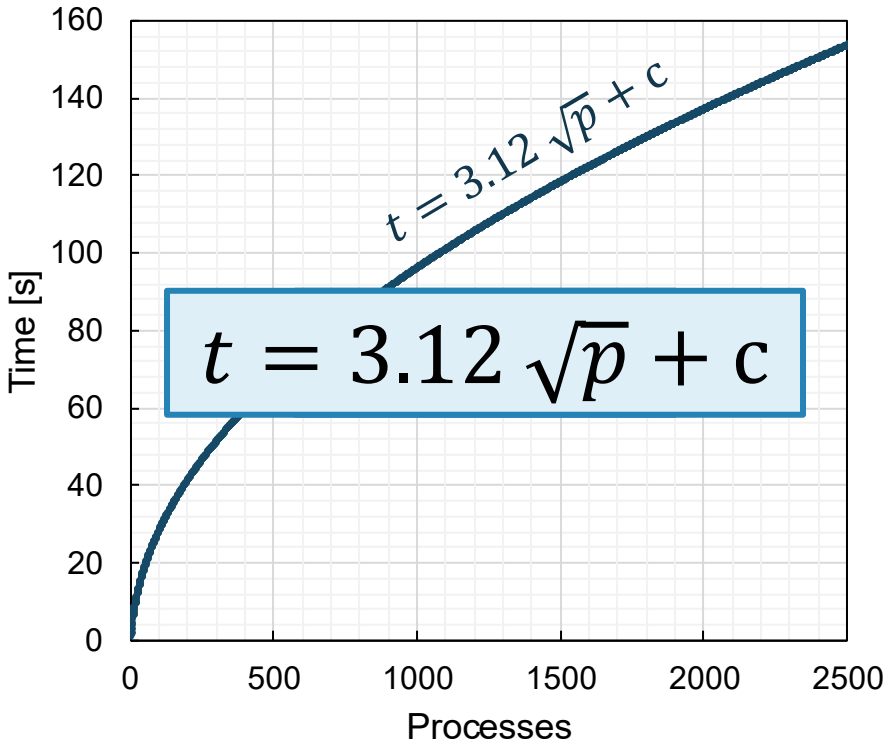
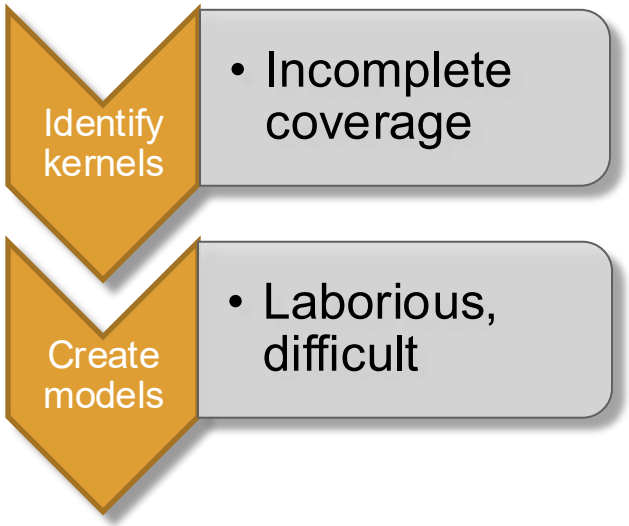
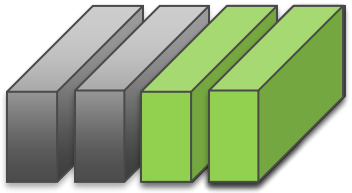
Formula that expresses a relevant performance metric as a function of one or more execution parameters



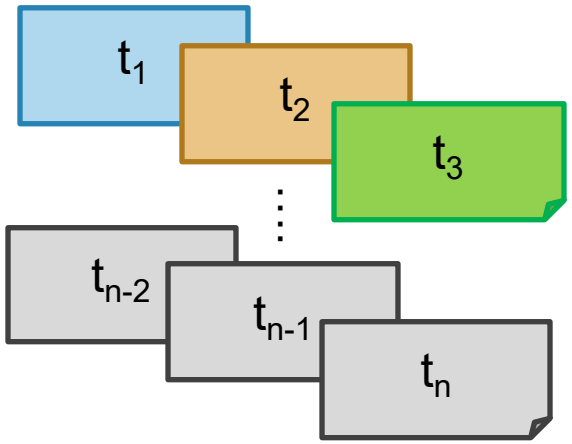
Analytical (i.e., manual) creation challenging for entire programs

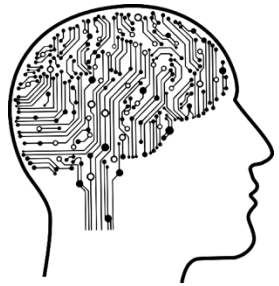


Empirical performance modeling



Performance measurements with different execution parameters $\mathbf{x_1,\ldots,x_n}$





Machine learning

$$t = f(x_1, \ldots, x_n)$$

Alternative metrics: FLOPs, data volume…

Extra-P

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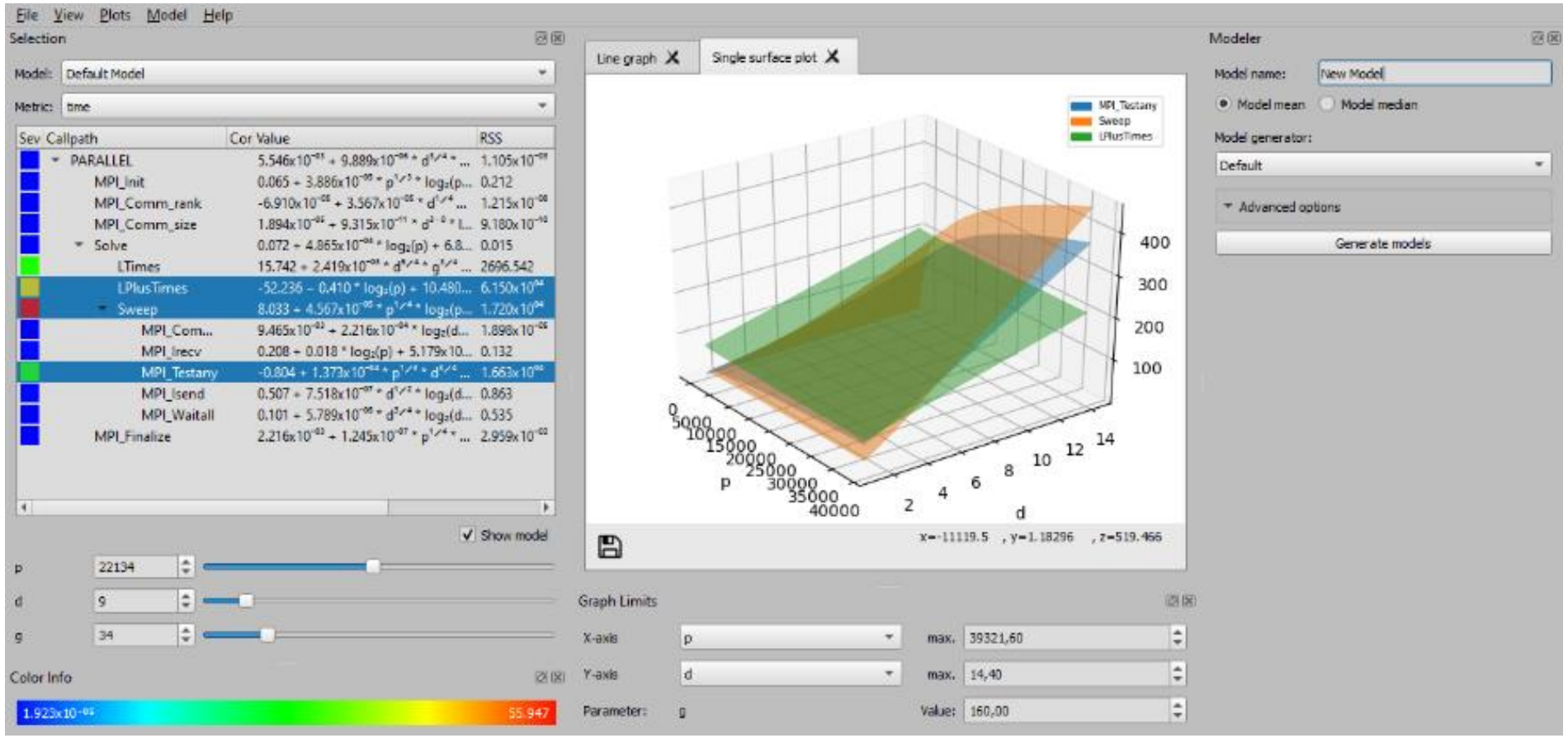
Parallel Programming



YouTube

GitHub

Community codes

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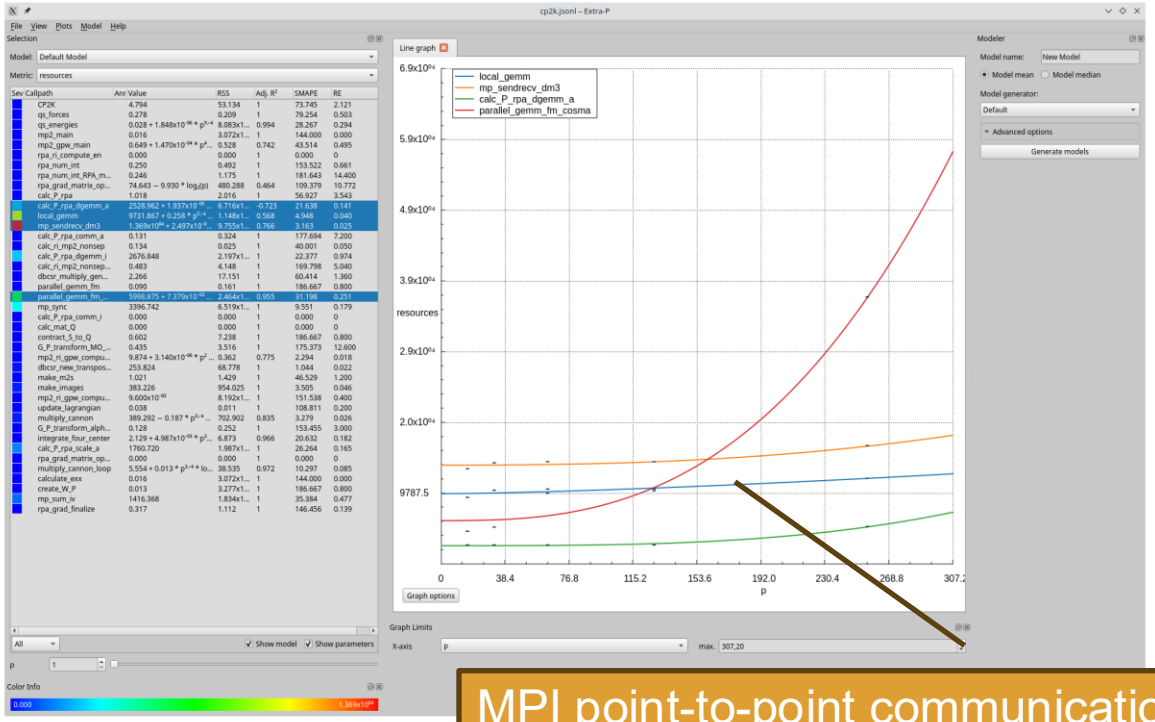
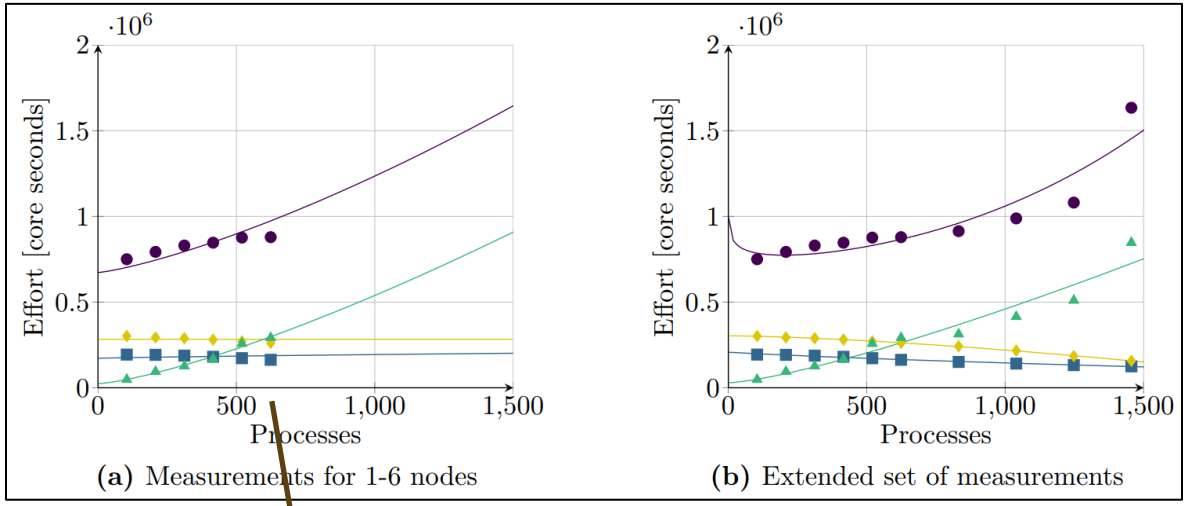
Computational chemistry (CP2K)



MPI point-to-point communication dominates resource consumption beyond 128 ranks

Fluid dynamics (OpenFOAM)



MPI_Allreduce dominates resource consumption beyond 500 processes

BoSSS

[Calotoiu et al., ProTools@SC20]

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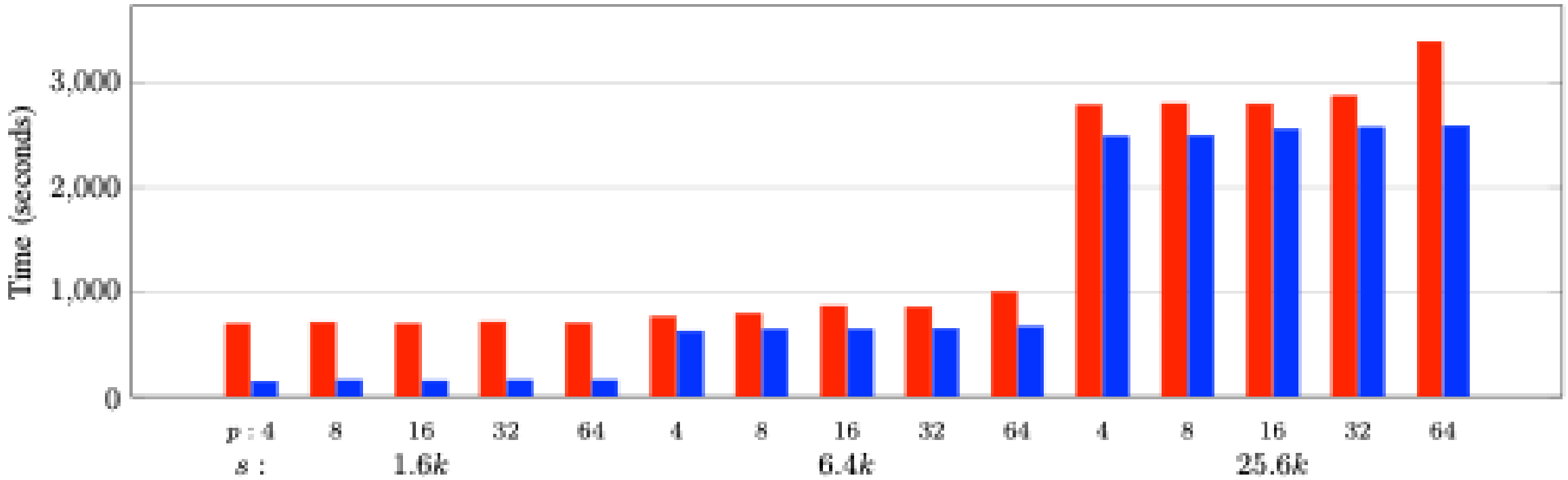
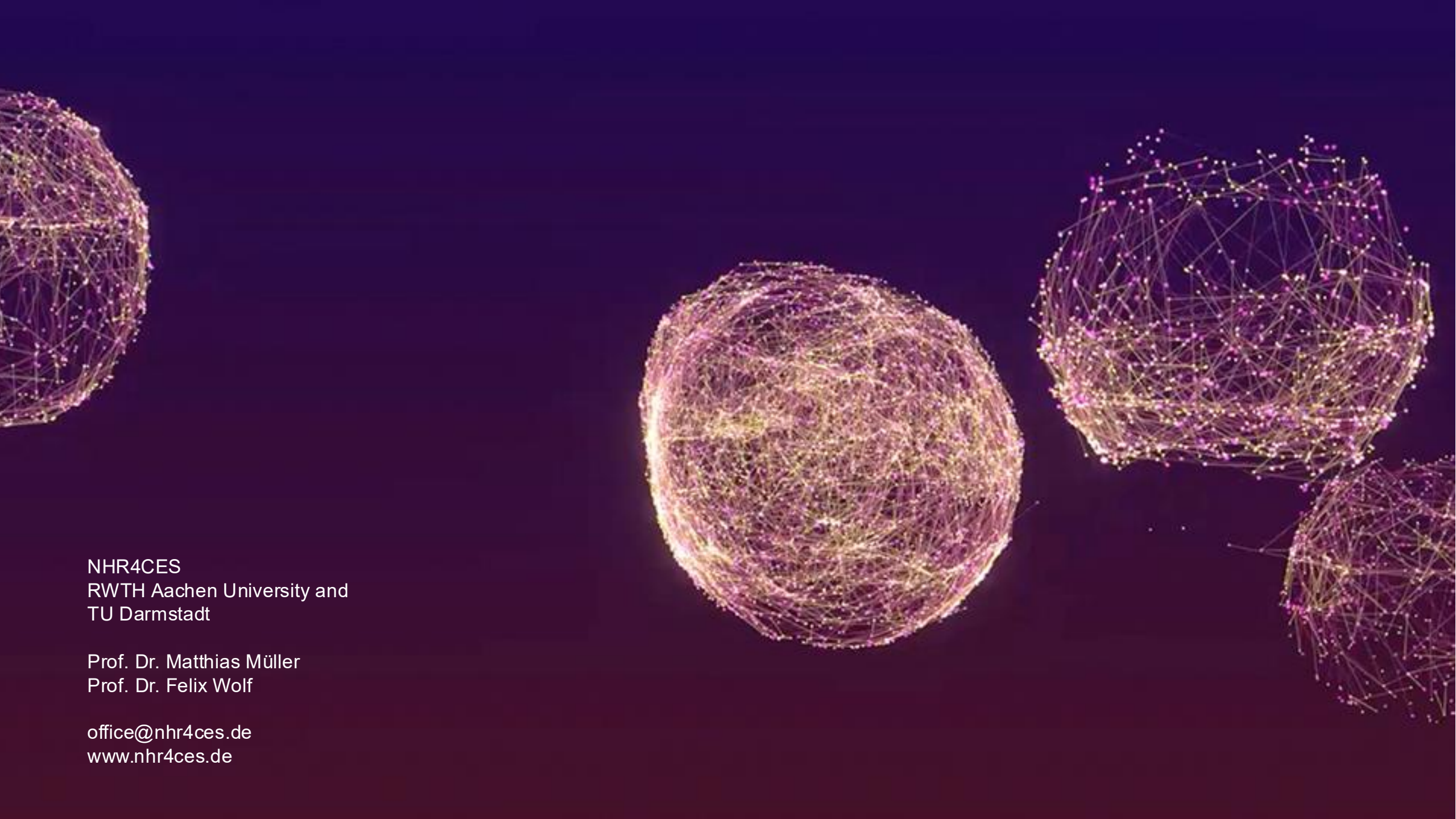
Parallel Programming



Before optimization

After optimization



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