Competence Platform for Software Efficiency and Supercomputing

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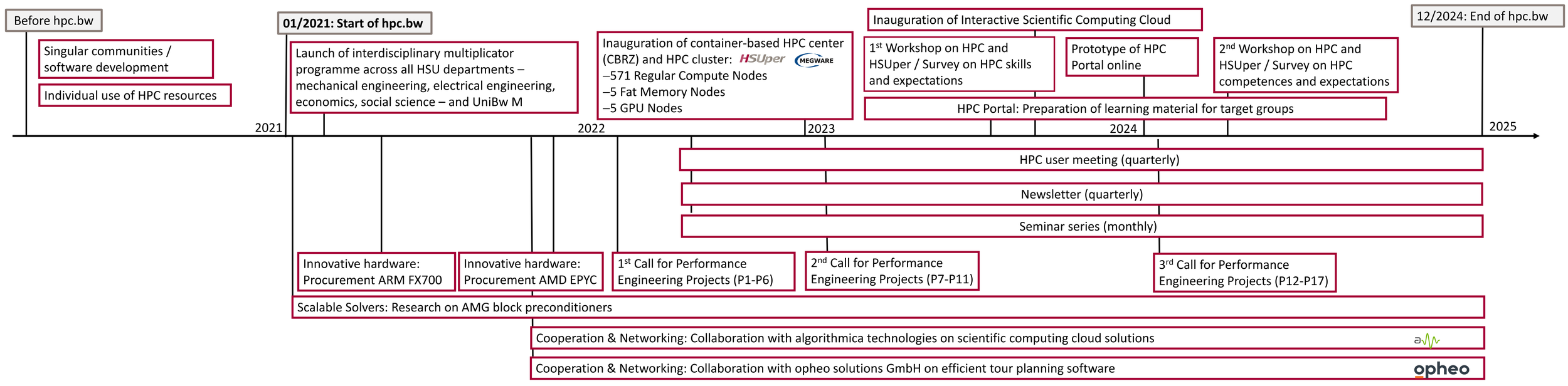
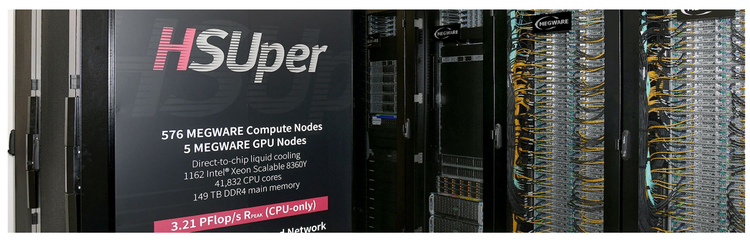
Timeline of hpc.bw: Strengthening research and development by HPC in an interdisciplinary endeavor



Supercomputer HSUper

- 581x dual Intel 8360Y (41.832 compute nodes)
- 2x 1-PB-storage system (Ceph, BeeGFS), InfiniBand HDR100
- 571 nodes, dual-socket Intel Icelake (2x36 cores), 256 GB RAM
- 5 nodes, dual-socket Intel Icelake, 1 TB RAM
- 5 nodes, dual-socket Intel Icelake (2x36 cores), equipped with 2 A100 GPUs, 256 GB RAM



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Calls for Projects for Performance Engineering

- ✓ P1 Monte Carlo simulations of real fluids (HSU)
- ✓ P2 DigiTaKS* Learning behaviour of students in dealing with digital media and tools (HSU)
- ✓ P3 benEFIT- Numerical simulation of non-destructive testing of concrete (HSU)
- ✓ P4 Enabling High-Throughput Studies of Reactive Materials (HSU)
- ✓ P5 C-STAR Electric Propulsion Demonstrator Multiphysics Modelling/ Modelling Hypersonic re-entry from the Martian Thermosphere down to the Troposphere (UniBw M)
- ✓ P6 Optimization of an IGA Code in MATLAB for parallel computing (UniBw M)
- ✓ P7 Case Study "Personnel Scheduling in RoRo Terminals" (HSU)
- ↻ P8 The 2-stage no-wait hybrid flow job scheduling problem (HSU)
- ↻ P9 Single machine scheduling with position dependent maintenance (HSU)
- ↻ P10 HPC for semi-parametric statistical modelling on massive data sets (HSU)
- ↻ P11 Performance portability for the MIRCO BEM solver for rough surface contact (UniBw M)
- ↻ P12 Density Functional Theory Calculations of Positron Lifetimes (UniBw M)
- ↻ P13 Nozzle Design in Cold Spray Applications (HSU)
- ↻ P14 MD-Simulations for damping assessment in MEMS resonators: (HSU)
- ↻ P15 Enabling global sensitivity analysis of large-scale FEM models using QUEENS (UniBw M)
- ↻ P16 DSMC-based simulation for the development ABEP systems (UniBw M)
- ↻ P17 Molecular Monte Carlo simulations on GPUs (HSU)

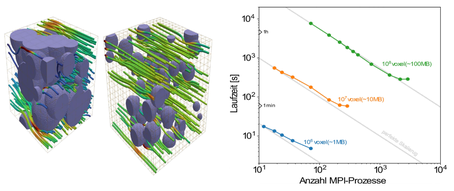
Types of hpc.bw team support:

- Problem identification
- Setup, familiarization on usage/code
- Introduction of best practices
- Profiling/benchmarking on test cases
- Selection on promising bottlenecks
- Introduction of changes/optimizations
- 1 on 1 mentoring/help
- Investigation of possible solutions
- Communication of solution clues
- Preparation of 'proof-of-concept'

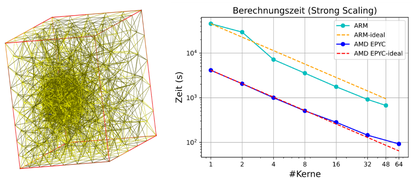
Research areas with HPC needs

- Numerical simulation and development of parallel simulation methods
- Artificial intelligence / machine learning / data analyses
- Bioinformatics problems, e.g. in medicine
- Optimization problems, e.g. in logistics

Simulation in material science
(Prof. Kramer, HSU)

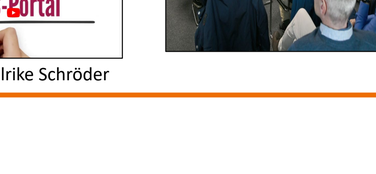


Molecular-continuum simulation
(Prof. Neumann, HSU)



Simulation of turbulent flows
(Prof. Breuer, HSU)

Monte Carlo simulation of real fluids
(Prof. Meier, HSU)



HPC Competences Platform: Interdisciplinary Cooperation – Continuing Education and Lifelong Learning & HPC

"Culture of Digitalization" (Stalder, 2021) & Computer Science

- "Data as the raw material of the future" (DARP 2022, 324)
- *Algorithmicity*: Automated decision-making processes that generate Information and become the basis for collective behaviour
- *Referentiality*: Referential processes that enable references on the basis of data and thus have a meaningful and formative effect on knowledge and practices
- *Collectivity*: Collective frames of reference that stabilise meanings, generate options for action and agency

Strengthening of HPC discipline & bringing together different potentials

- Construct knowledge on the basis of data
- Open Educational Resources and Open Access regarding HPC competences
- Overcoming boundaries
- Strengthening interdisciplinary research and cooperation
- Profiling HPC discipline
- Discovering new research horizons

Acquisition of Future Skills (Ehlers, 2020)

Selection of Future Skills in relation to HPC Portal:

- *Digital and design competence*: Knowing and using rigorous metrics and promoting value
- *Ethical and initiative competence*: sustainability of HPC resources
- *Reflection-, decision-making and system competence*: Understanding, weighing up and managing risks in relation to hard- and software
- *Ambiguity and innovation competence*: dealing with complexity and uncertainty of HPC knowledge

HPC Portal: Interim conclusion and next steps

- Methodical and didactic preparation of teaching and learning materials
- Open Educational Resources for self-directed learning processes and for exploring new research potential
- HPC competences transfer along digital, on-site and hybrid learning settings
- Informal learning with the aim of creating networking and exchange opportunities in various target groups and disciplines
- Example offers: Seminar series, HPC workshops for beginners and advanced users, newsletter, forum, blog post, videos, cluster tours

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Target Groups of HPC Competence Platform

Interdisciplinary users without affinity for Computer Science

- Currently no affinity for computational processes
- Writing only individual lines of code or having no experience with HPC, programming or optimizing software

Beginners

- Basic knowledge of computer science
- Driven by scientific questions to be addressed using HPC
- Ability to write short parts of programmes, e.g. larger macros, scripts or interfaces for commercial software

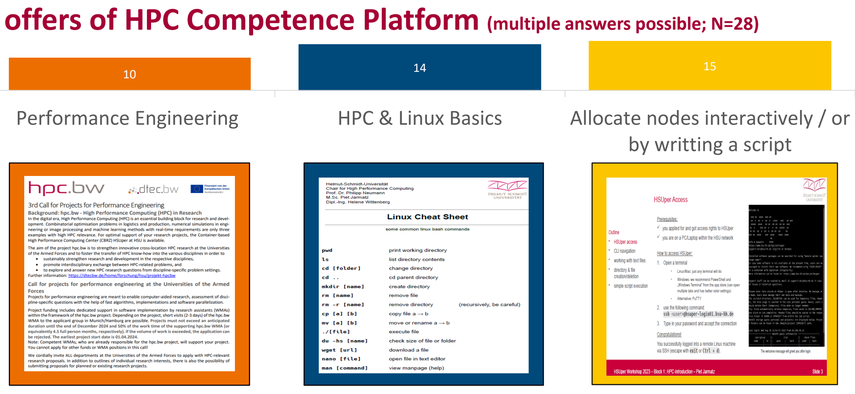
Advanced users

- Intermediate knowledge of computer science
- Advanced knowledge about software development, e.g. writing own programmes and having parts of these programmes parallelized (for execution on HPC systems)

Advanced software developers

- Comprehensive knowledge of computer science
- Ability to parallelize/optimize software mostly independently
- Detailed knowledge of job scheduling systems etc.

Selection of survey results on needs & requirements and related offers of HPC Competence Platform (multiple answers possible; N=28)



Project related publication:
Neumann, P./Duffek, J./Kleinschmidt, J./Leinen, W./Breuer, M./Schmidt-Lauff, S./Fink, A./Mayr, M./Firmbach, M./Popp, A. & Auweter, A. (2022): hpc.bw: A Supercomputer with Competence Platform for the Universities of the Federal Armed Forces. In: Schulz, D./Fay, A./Matiaske, W. and Schulz, M. (eds.): dtec.bw-Beiträge der Helmut-Schmidt-Universität. Forschungsaktivitäten im Zentrum für Digitalisierungs- und Technologieforschung der Bundeswehr dtec.bw. Band 1. Hamburg: OpenHSU, pp. 305–310. https://openhsu.ub.hsu-hh.de › openHSU_14569

Mentioned publications in the poster:
DARP (2020): Deutscher Aufbau- und Resilienzplan.
Ehlers, U.-D. (2020): Future Skills. Lernen der Zukunft – Hochschule der Zukunft. Wiesbaden: Springer VS.
Stalder, F. (2021): Kultur der Digitalität. Frankfurt am Main: Suhrkamp.

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