

## hpc.bw (dtec.bw) -

# Competence Platform for Software Efficiency and Supercomputing

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## 1 Phase 1 (2021-2024)

Strengthening Research and Development by HPC in an Interdisciplinary Endeavor

The project „hpc.bw – Competence Platform for Software Efficiency and Supercomputing“ has started in January 2021 and will run for a total of six years until December 2026. It is funded within the framework of dtec.bw and is part of the KoDiA research cluster. The aim of hpc.bw is to strengthen innovative cross-location research in the field of High-Performance Computing (HPC) and to promote the transfer of relevant expertise to a wide range of disciplines. In the following, the key achievements of the first phase of hpc.bw are listed.

- 1 Container-based HPC center “CBRZ” with PetaFLOP cluster “HSuper”
- 2 Interactive Scientific Computing Cloud “ISCC”
- 3 Web-Based HPC Competencies Platform “HPC Portal”
- 4 18 Supported performance engineering projects
- 5 > 100 Journal papers empowered by hpc.bw
- 6 Sustainable strengthening of innovative and interdisciplinary Cross-Sectional Research within HPC
- 7 Transfer of relevant HPC knowledge across Disciplines
- 8 Promotion of interdisciplinary exchange between HPC related problems



Seminar Series  
Computation & Data



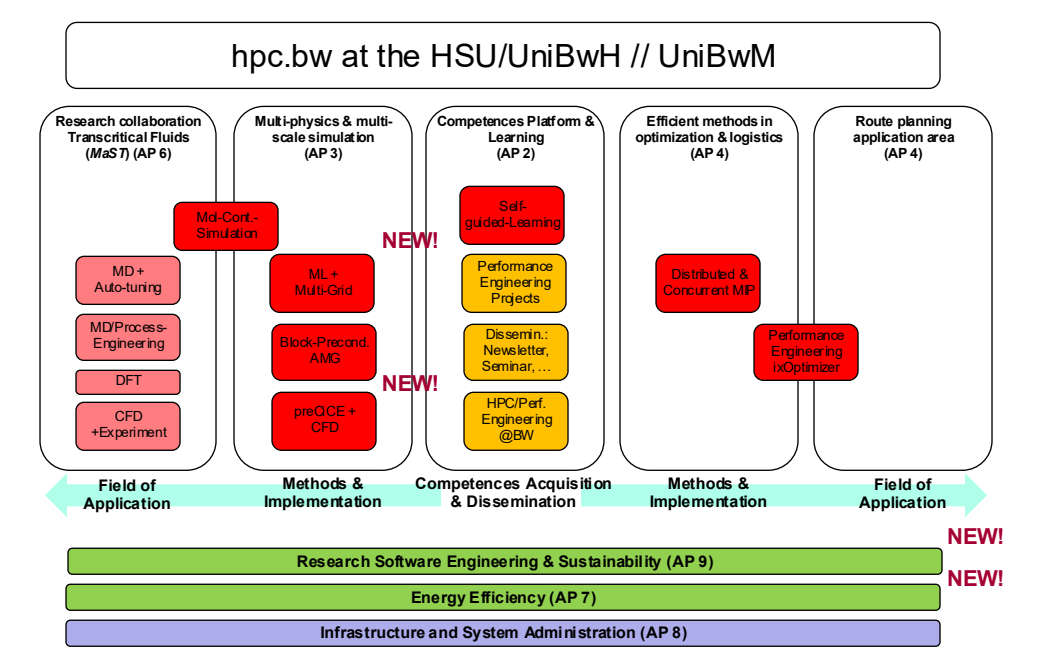
HSuper  
Workshops

## 2 Phase 2 (2024-2026)

Strengthening the HPC Applications

Building on the achievements of the CBRZ infrastructure and the successful initiation of interdisciplinary HPC application projects during the first founding phase, the second founding phase will emphasize the advancement and strengthening of discipline-specific HPC applications and their implementation. There is also a new focus on sustainability and energy efficiency implemented. Below are key components of discipline-specific applications.

- ▶ **Multi-Physics and Multi-Scale Simulation (AP 3):**  
Implementation of efficient solvers and coupled problems
- ▶ **Molecular-Continuum Simulation (AP 6):**  
Simulation of transcritical fluids and block methods/implementation
- ▶ **Logistics/Optimization (AP 4):**  
Performance analysis and engineering of optimization software



## Selection of Applications

### AP 3 Numerical Simulation

Submarine Design Optimization by Hybrid SciML and FEM HPC

#### Objective:

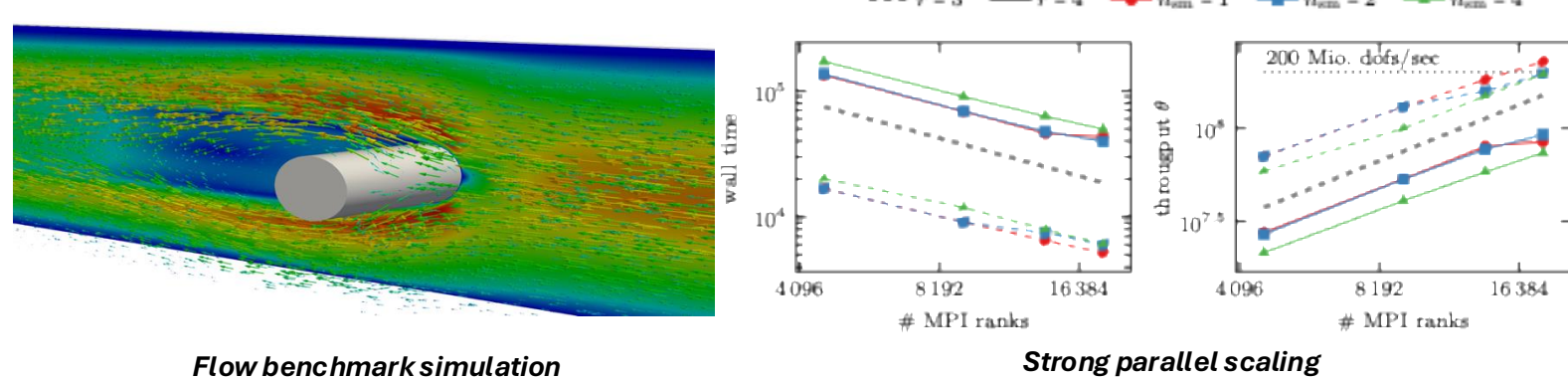
Improved design of submarine velocity log for accurate velocity information (speed through water) by HPC ambient flow elucidation and ML structure optimization

#### Application Background:

- Calibration of submarine systems and operation of autonomous underwater vehicles by monitored data
- Velocity log with high accuracy and low impact for vehicle motion and speed measurement
- Submarine: Complex ambient flow profile
- Boundary layers: Elucidation for velocity log design

#### Methodologies:

- High-resolution 3D HPC simulation of turbulent flow
- Self-adaptive space-time finite element methods with goal-oriented error control: High accuracy of goal quantities
- Robust grid-independent algebraic solver: Geometric Multigrid Preconditioner for GMRES iterations
- Implementation in open source inhouse code based on deal.II FE library: Data structure efficiency (matrix-free) and excellent HPC scalability
- Optimal shape design by neural network techniques: Cost efficiency



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Chair of Numerical  
Mathematics

### AP 6 Computational Fluid Dynamics

Macro/Micro-Simulation of Phase Decomposition in the Transcritical Regime

#### Objective:

Understanding behavior of multi-component multi-phase flows, particularly in transcritical mixtures with high pressure and low temperatures

#### Multiscale Considerations:

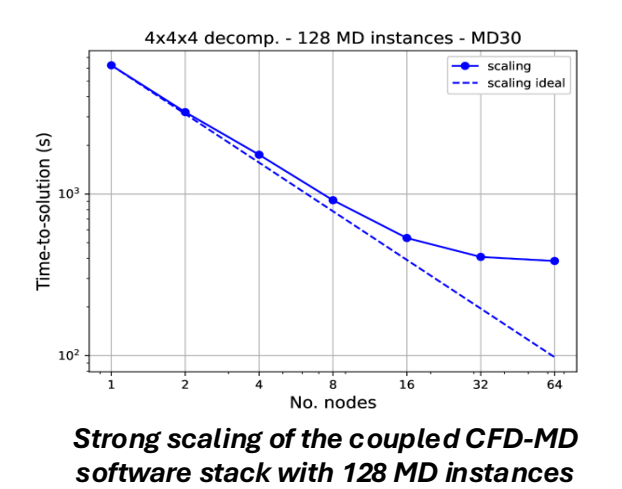
Analyzing evolving flow processes requires multiscale analysis, from molecular properties to large-scale continuum flow field simulation, requiring high-performance and robust simulation and coupling code

#### Specific Applications:

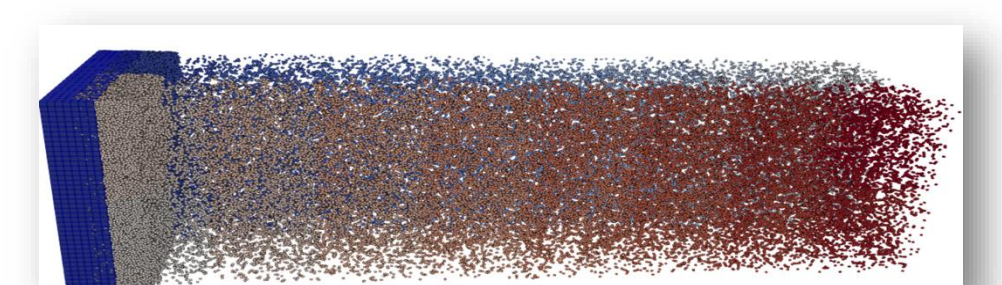
Studying droplet and bubble formation in transcritical systems, using a coupled multiscale approach, utilizing ls1-marydn + AutoPas for molecular dynamics, OpenFOAM for CFD and MaMiCo + preCICE for coupling

#### Methodologies:

- CFD
- Molecular dynamics simulation,
- Classical density functional theory
- Computational fluid dynamics
- Hybrid molecular-continuum approaches
- Experiments with high pressure chamber for validation



Strong scaling of the coupled CFD-MD software stack with 128 MD instances



A coupled macro-micro-simulation

### AP 4 Logistics/Optimization

Utilizing HPC in Business Applications to Solve NP-Hard Combinatorial Optimization Problems

#### Objective:

Utilizing HPC in economics and business applications such as in logistics to solve NP-hard combinatorial optimization problems

#### Field of Study:

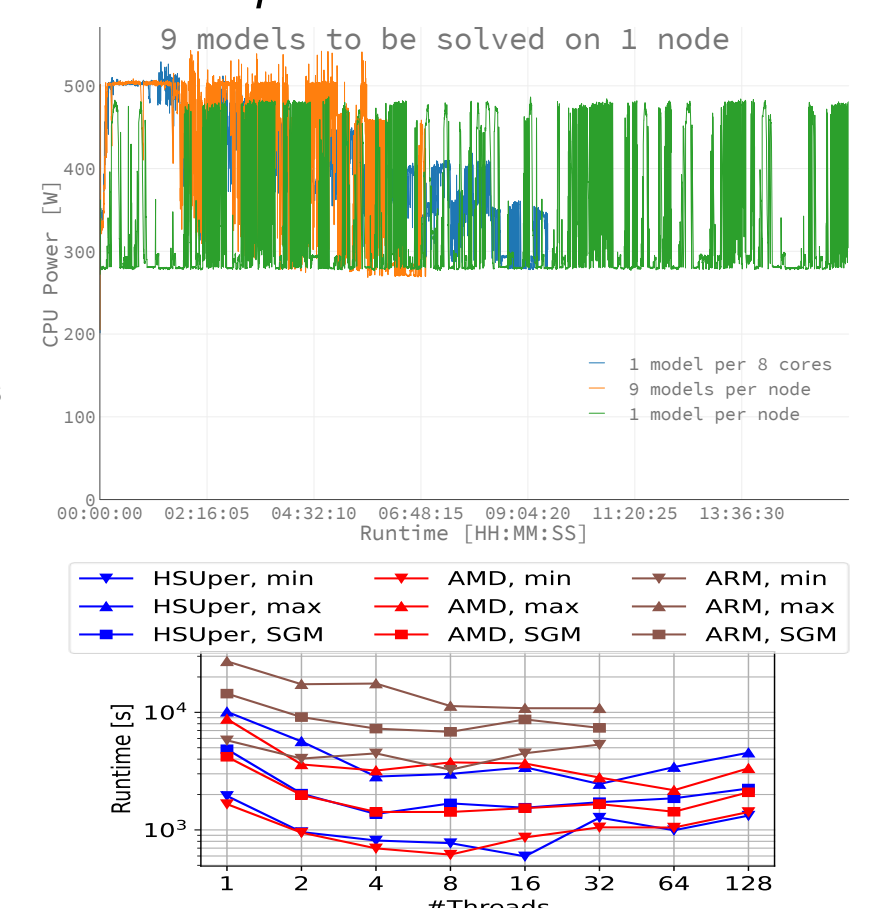
Performance, scalability and energy consumption of optimization software for time-dependent traveling salesperson problems on various hardware architectures

#### Challenges:

- Performance variability and its influence on the computing time of the solver
- Commercial solvers such as Gurobi and CPLEX (IBM) are closed-source

#### Approach:

- Testing optimization software such as Gurobi, CPLEX (IBM) and HiGHS on various HPC hardware architectures and configurations
- Investigation of hardware and solver parameters on computation time



#### Project-related publications:

Duffek, J./Dethof, F./Neumann, N./Kebler, S./Bechelaoui, I./Fink, A./Kleinschmidt, J./Kolling, A./Leinen, W./Mayr, M./Preuß, H./Rathmann, M./Schlumbohn, S./Schmidt-Lauff, S./Schumann, Y./Stierner, M. (2024): hpc.bw: An Evaluation of Short-Term Performance Engineering Projects. In: Schulz, M./Fay, A./Niggemann, O./Matiaska, W./Schulz, D. (2024): dtec.bw-Berträge der Helmut-Schmidt-Universität Universität der Bundeswehr Hamburg. Forschungsaktivitäten im Zentrum für Digitalisierungs- und Technologieforschung der Bundeswehr dtec.bw. Band 2, openHSU, pp. 223-228; <https://doi.org/10.24405/16802>.

Margenberg, N./Munch, P./Bause, M. (2025): An hp multigrid approach for tensor-product space-time finite element discretizations of the Stokes equations, SIAM J. Sci. Comput., under review (2025), 23 pages; <https://doi.org/10.48550/arXiv.2502.09158>.

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 Super-computer with Competence Platform for the Universities of the Federal Armed Forces. In: Schulz, D./Fay, A./Matiaska, W. and Schulz, M. (eds.): dtec.bw-Berträge der Helmut-Schmidt-Universität. Forschungsaktivitäten im Zentrum für Digitalisierungs- und Technologieforschung der Bundeswehr dtec.bw. Band 1, openHSU, pp. 305-310; <https://doi.org/10.24405/14569>.

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Tippmann, N./Auweter, A./Das Sharma, A./Leinen, W./Neumann, P. and Fink, A. (2024): xbat: A Continuous Benchmarking Tool for HPC Software. In: Schulz, M./Fay, A./Niggemann, O./Matiaska, W./Schulz, D. (2024): dtec.bw-Berträge der Helmut-Schmidt-Universität Universität der Bundeswehr Hamburg. Forschungsaktivitäten im Zentrum für Digitalisierungs- und Technologieforschung der Bundeswehr dtec.bw. Band 2, openHSU, pp. 91-97; <https://doi.org/10.24405/16783>.

Viot, L./Piel, Y. and Neumann, P. (2023): From Desktop to Supercomputer: Computational Fluid Dynamics Augmented by Molecular Dynamics Using MaMiCo and preCICE. In: Bienz, A./Weiland, M., Baboulin, M., Kruse, C. (eds) High Performance Computing. ISC High Performance 2023. Lecture Notes in Computer Science, vol 13999. Springer, Cham. DOI: [https://doi.org/10.1007/978-3-031-40843-4\\_42](https://doi.org/10.1007/978-3-031-40843-4_42).



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