hpc.bw NEWSLETTER 2025/1

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HELMUT SCHMIDT UNIVERSITÄT Universität der Bundeswehr Hamburg

Welcome to the newsletter of the dtec.bw project *hpc.bw*. If you want to subscribe to the newsletter, please send a message with subject line "Subscription hpc.bw Newsletter" to: info-hpc-bw@hsu-hh.de

Editors:
Prof. Dr. Markus Bause, Prof. Dr.-Ing. Michael Breuer, Prof. Dr.-Ing. Denis Kramer, Prof. Dr. Philipp Neumann, Marie Rathmann

SEMINAR SERIES & HPC CAFÉ "COMPUTATION & DATA" & HPC CAFÉ IN FT25

Author: Marie Rathmann

We warmly invite you to the upcoming talks in our seminar series „Computation & Data and our HPC Café" at the HSU in the spring trimester (FT25) and look forward to exciting discussions on the topic! In addition to attending in presence at the HSU, it is also possible to participate digitally via BigBlueButton.

Date	Seminar Room	Speaker & Moderator	Title of Lecture & HPC Café
23.04.2025	**109**		
16:00-17:00		Julio Gutierrez (HSU/UniBw H)	Study of nozzle influence on aerosol deposition (AD) by using 3D CFD simulations
17:00-18:00		HPC Café	Peer Guidance & User Collaboration
21.05.2025	**108**		
16:00-17:00		Ruben Horn (HSU/UniBw H)	GreenHPC: An overview and practical guide
17:00-18:00		HPC Café	Peer Guidance & User Collaboration
25.06.2025	**109**		
16:00-17:00		Guillaume De Nayer (HSU/UniBw H)	High-Fidelity Fluid-Structure Interaction Simulations
17:00-18:00		HPC Café	Peer Guidance & User Collaboration

To subscribe to the seminar mailing list, send an e-mail to info-hpc-bw@hsu-hh.de, subject line „Subscription Seminar Computation & Data".
For more information, click here.

FOTO: HSU/MZ/GELHAUSEN

HPC@dtec.bw: Perspectives & New Horizon

Author: Marie Rathmann

We have successfully completed the first funding phase of the *hpc.bw* project (dtec.bw) and have achieved numerous exciting calculations and results, made possible by the CBRZ and its compute platforms HSUper and ISCC. In this context, the event „HPC@dtec.bw: Perspectives & Next Horizon" took place at HSU on March 3 and 4, 2025. Participants included project members not only from HSU/UniBw H and UniBw M, but also from DESY Hamburg and the Technical University of Munich. The auditorium was ceremoniously opened with words from the President of HSU/UniBw H, Prof. Dr. Klaus B. Beckmann, and Prof. Dr. Markus Bause.

FOTO: HSU/HPC/MARIE RATHMANN

On March 3, a wrap-up meeting was held, where the diverse results within the individual work packages were presented and discussed. These included the HPC portal for acquiring HPC competencies (Lead: Prof. Dr. Sabine Schmidt-Lauff), software sustainability within HPC (Lead: Dr. Matthias Mayr), HPC for optimization and logistics (Lead: Prof. Dr. Andreas Fink), and projects for performance engineering (Lead: Johann Duffek). The review was initiated by Prof. Dr. Philipp Neumann, who provided a comprehensive insight into the milestones achieved in the first funding phase.

In addition to the presentations, a poster session with a total of 14 posters was held, showcasing the diversity of topics and methodological approaches in the broad world of HPC across a wide range of disciplines. Users who access the dtec.bw-funded resources HSUper and ISCC presented their current research. The first day was rounded off with a joint dinner.

On the second day of the event, March 4, 2025, the kick-off meeting took place, where all project participants of the second funding phase provided an exciting outlook on their plans. In the course of the second funding phase, the dtec.bw projects *hpc.bw* and *MaST* will merge to utilize mutual synergies. The day began with presentations from the work packages of the HPC portal (Lead: Prof. Dr. Sabine Schmidt-Lauff), multi-physics/multiscale modeling (Lead: Prof. Dr. Markus Bause and Prof. Dr.-Ing. Michael Breuer), efficient methods in optimization and logistics (Lead: Prof. Dr. Andreas Fink), HPC use cases and HPC workflows for Bw (Lead: Dr. Matthias Mayr), and transcritical fluids & computational fluid dynamics (Prof. Dr. Philipp Neumann; Prof. Dr.-Ing. Michael Breuer). After a short break, the remaining work packages were presented: energy efficiency (Lead: Piet Jarmatz), HPC infrastructure and administration (Lead: Piet Jarmatz), and research software engineering and sustainability (Lead: Dr. Matthias Mayr). The day concluded with a joint tour of the HSUper or container-based research center.

We look forward to many enriching research horizons, innovative potentials in the field of HPC and methodologies, as well as diverse research collaborations and interdisciplinary networking across all status and research groups.

FOTO: HSU/HPC/MARIE RATHMANN

Performance Engineering Projects Supported in 2025

Author: Marie Rathmann

We are pleased to support the following projects from April 1, 2025, to April 1, 2026, in various ways through the research assistants of the HPC.BW team. The goal is to enable computer-aided research and the assessment of discipline-specific questions using fast algorithms, optimized implementations, and software parallelization.

To ensure optimal project support, the containerbased High Performance Computing Center (CBRZ) HSUper is available.

Keep watching this space for updates on registration, the workshop program, and more—right here:

Marco A. Öttl, M.Eng. (UniBw M)	Development of a mine burial model for the North Sea by waves and currents
Günter Reiner, Prof. Dr. (HSU/UniBw H)	Automatische Verschlagwortung und automatischer Vergleich von deutsch-sprachigen Gerichtsentscheidungen
Arne Schulz, Dr. (HSU/UniBw H)	Learning-based branching strategies for mixed-integer programming

SUCCESSFUL WORKSHOP FOR DETERMINING FUTURE HPC REQUIREMENTS AND RESOURCE NEEDS OF HSU/UNIBW H

Author: Piet Jarmatz

Recently, a workshop for HPC demand analysis was held at Helmut Schmidt University (HSU). It took place on 30.01.2025 and was organized by Piet Jarmatz who is head of HPC lab at the chair for high-performance computing. The event aimed to gather information about the future requirements for HPC systems from researchers across various disciplines. Researchers from over 30 different research fields and depart-ments attended the event. The primary goal was to systematically capture and record all relevant re-quirements and needs, so that it becomes clear and well-documented which HPC demands exist at HSU and what the specific reasons for the various requirements are. The event that lasted for four hours, began with introductory presentations that highlighted the growing importance of HPC in research and education, gave an overview of existing HPC systems deployed at HSU, and discussed relevant aspects for future systems. To secure the outcomes, workshop results have been collected by the HPC team. This includes gathering of conversation protocols, questionnaires for HPC demand analysis, and reports from individual brainstorming working groups. An evaluation of the results was conducted later by the HPC Steering Committee and the university management.

Currently, HSU operates two HPC systems, the Linux based cluster HSUper and the VMware based cloud ISCC. HSUper has more than 200 users. In general, there is a large number of small jobs with less than 10 compute nodes running on HSUper, while only a small number of jobs actually uses a large number of more than 100 nodes. In 2025, HSUper showed a very high utilization, especially of the CPU partition, leading to long waiting times for larger jobs in the queue. The GPU partition was utilized by 38 different users, most of their jobs only use a single GPU device. The workshop also highlighted and examined the development of several other HPC computing centers worldwide in order to gain a broader perspective and enable comparison with HSU systems. It was discussed which types of resources should be shared central HPC infrastructure at all. Especially highly individualized island solutions and systems that strive to maximize single-thread performance instead of enablingparallelism should not be integrated into central HPC resources. No precise hardware models and no precise technical data were decided upon at the workshop. Instead, discussions took place about criteria, requirements or minimum requirements, reasonable ratios of components or sub-systems, and the corresponding reasons behind them.

FOTO: ADOBE STOCK 294794307_(C)_pdusit

There were impulse lectures, as well as demand descriptions and brief presentations of application examples from individual research groups. It was reported on current research, for example for solving optimization problems and decision analysis, where often a higher CPU clock frequency is required and GPUs are not yet usable. The presentations also covered AI infrastructure for research and teaching at HSU, summarizing the computational demand from the HSU AI institute. Especially generative models and large language models generally require a large number of GPUs and more VRAM per GPU. Applications such as LLMs or the analysis of satellite images tend to require GPU-supernodes. There was a presentation of Kubernetes, which enables flexible universal container orchestration and has become the de facto standard for cloud computing, but is more complex in setup and administration. Kubernetes was also compared to systems based on the Slurm scheduler, but a comparison is difficult as the requirements are very heterogeneous and some groups need both types of software stacks. It was found that depending on the specific project, different software is required, so that the benefits of Kubernetes and Slurm are application specific. There were several talks about the need for CPU computing power, which is primarily needed for numerical simulations, fluid dynamics, materials science and new professorships. The demand for CPU power will increase strongly in the coming years and a system with several hundred compute nodes will be required. For applications such as ‚on-the-fly learning', GPU nodes with strong CPUs or a tight interconnection of CPU and GPU nodes are required. ‚On-the-fly computing', where numerical simulations and machine learning are used simultaneously and depend on each other, could be a future unique selling point of research at HSU. A close coupling to the existing HSUper is desired, as well as an integration of the new HPC systems into teaching.

After the presentations, the workshop continued with two brainstorming sessions. In each of these brainstorming sessions, four working groups were formed to discuss specific aspects: Cluster Architecture, CPU Requirements, GPU Requirements, and Storage Needs. Each group consisted of experts from various research fields. The discussions in the working groups revealed a wide range of requirements for HPC systems, reflecting the diversity of research applications at HSU. This includes the need for a balance between CPU and GPU performance, with some applications requiring strong CPU capabilities and others demanding high-performance GPUs. It also includes the importance of compatibility with existing systems, such as HSUper. A detailed statistical analysis of the survey results and a review of the conversation transcripts has been conducted, but the detailed findings will not be made public at this time, so as not to compromise ongoing procurement processes. Overall, the workshop was a significant success in bringing together experts from various fields to discuss the future of HPC at HSU. The event provided valuable insights into the requirements for next-generation HPC systems. The highly valuable outcomes are actively used by the HPC Laboratory, Steering Committee, and University Management to inform future in-vestments in HPC systems. Researchers can look forward to new, exciting projects that will be enabled by these developments.

SAVE THE DATE

INVITATION: preCICE WORKSHOP @HSU/UNIBW H SEPTEMBER, 8-12, 2025

Author: Marie Rathmann, on behalf of the preCICE Organization Team

The 6th preCICE Workshop will be held at the Helmut Schmidt University/University of the Federal Armed Forces Hamburg (HSU/UniBw H) on September 8-12, 2025. The workshop is a coming together of the preCICE community to share ideas, experiences and knowledge about using preCICE, and to learn from others in the process.

Workshop #6 2025 preCICE
HSU Hamburg Germany September 8 - 12

Like always, we plan to have user and developer talks, hands-on training sessions, discussions with the developers about your applications and use cases, and plenty of opportunities for networking.

The workshop will include a hands-on training course. The course is suited for both beginners and current preCICE users, since advanced topics will also be covered. We will extend the course by a new module on HPC.

In the developer talks, the maintainer team will present recent updates on dynamic meshes, mesh-particle coupling, and macro-micro coupling – to only mention a few highlights. And we will continue the standardization process of adapters and application cases, where you can help shaping the future.

Keep watching this space for updates on registration, the workshop program and more here:

HPC Portal

REIMAGINING THE SEMINAR SERIES „COMPUTATION & DATA": THE HPC CAFÉ

Author: Alexander Kolling

For the last two year, the seminar series *Computation & Data* has served as a space for knowledge ex-change on topics related to High Performance Computing (HPC). However, participation patterns and logistical challenges have highlighted the need for a fresh approach.

Starting in the second quarter of 2025, the format will undergo a transformation to create a more interactive and engaging learning environment.
The seminar series, organized as part of the HPC initiative, has traditionally followed a structured format: two invited speakers present their research on HPC-related topics, followed by a brief Q&A session. Meetings take place once a month and typically attract a small but engaged audience.

Recognizing the potential for improvement, the seminar series is being redesigned with three main objectives:

Shifting from Passive to Active Learning

The new format will move beyond passive knowledge transfer by fostering interactive learning experiences. While expert talks will still be a core element, the goal is to encourage deeper engagement through guided discussions, structured moderation, and interactive elements.

Introducing the HPC Café – A Space for Collaboration

A major innovation is the introduction of the HPC Café, a dedicated space for informal peer-to-peer learning. This additional hour will provide a structured yet relaxed setting where participants can discuss HPC-related challenges, exchange ideas, and receive support from experienced researchers. The café format aims to lower barriers for early-career scientists, who may hesitate to present their work in a formal seminar setting.

Speaker Engagement and Discussions

Each session will now feature only one invited talk instead of two. This change will allow for more in-depth discussions. A rotating moderation team from our HPC group will be introduced to ensure that discussions remain structured and engaging while also being available for HPC-related questions.

To ensure the success of these changes, a structured evaluation process will be implemented, including participant surveys and feedback loops. The hope is that this transformation will not only revitalize the seminar series but also foster a more connected and collaborative HPC research community.

KICK-OFF MEETING: CFD DESIGN OPTIMIZATION OF SUBMARINE VELOCITY LOG

Author: Markus Bause

On February 20, the kick-off meeting of the project ***CFD Design Optimization of Submarine Velocity Log*** *by Markus Bause and Marius P. Bruchhäuser, Chair of Numerical Mathematics, Helmut Schmidt University/University of the Federal Armed Forces Hamburg (HSU/UniBw H), was held. It was hosted by the Marinearsenal (Naval Arsenal) in Kiel. The project is part of the hpc.bw work package Multi-physics and Multiscale Simulation that comprises research in the field of accurate discretization methods, technology of efficient algebraic solver and their implementation for the numerical simulation of complex flow and multi-physics phenomena. The team from HSU/UniBw H was made complete by the mechanical engineering student and member of the German Navy Friedrich Jung.*
Cooperation partner in the project is the 1st Submarine Squadron, based in Eckernförde. Next to members from this group, the BAAINBw Bundesamt für Ausrüstung, Informationstechnik und Nutzung der Bundeswehr and the Marinearsenal (Naval Arsenal) further joined the meeting and contributed by ex-pertise on submarines. The missions of the partners are summarized in following.

1st Submarine Squadron, based in Eckernförde, operates six Type 212A submarines, one Elbe class ten-der, and the Oste class intelligence collectors. The Submarine Training Centre and the Navy Hydroacoustic Analysis Centre are also part of the Squadron. The submarines' two key capabilities are the collection of information using long-range sonar and the engagement of submarine and surface targets. Although developed for worldwide deployment, their size, design and manoeuvrability make the submarines particularly suited to operations in shallow and littoral waters. Their air-independent propulsion enables them to stay submerged for extended periods of time, for example to covertly gather information on the situation in a specific sea area. The submarines can also be used to covertly deploy special forces, for example for rescue and evacuation missions.

The main mission of **BAAINBw Bundesamt für Ausrüstung, Informationstechnik und Nutzung der Bundeswehr** is to provide the Bundeswehr with the efficient and safe defence equipment it requires. This also includes information technology. We focus on the development, testing, procurement and in-service support management of materiel. BAAINBw Bundesamt für Ausrüstung, Informationstechnik und Nutzung der Bundeswehr handles a broad range of products including highly complex weapon and IT Informationstechnik systems, tanks, aircraft, vessels as well as clothing for service personnel.
The mission of **Marinearsenal (Naval Arsenal)** is to ensure the operational readiness of the German Navy. Its scope of responsibility includes, besides ships and boats, the Navy agencies and installations ashore such as the Navy schools, radio transmission sites, ammunition depots and others. The core tasks are to plan and carry out maintenance measures above organizational-level maintenance and to repair command and weapons control systems in the arsenal installations. The Naval Arsenal performs repairs that cannot be carried out by the Navy units themselves with their on-board maintenance resources.
In a fruitful discussion of all participants the expected project's outcome, its challenges and problem set-tings for the CFD simulations were addressed and evaluated. Afterwards, the opportunity to see one of the submarines of the German Navy from inside was offered to the group from HSU/UniBw H. The HSU/UniBw H group thankfully accepted the offer and had a fantastic view and impression from work and life in a submarine. Technical constructions in the submarine, safety/emergency devices and weapon systems are highly impressive.

The goal of the *hpc.bw* project CFD Design Optimization of Submarine Velocity Log is the numerical simu-lation of the flow around the bow of a submarine of class U212 and the elucidation of the boundary layer thickness to evaluate the feasibility of a redesign of a velocity log. The velocity log is used to provide inertial system aiding, precision positioning, and speed log capability. It is mounted on the submarine's bow for test drives and used for checking and calibrating the submarine's systems. To reduce fluid-structure interaction in diving drives, perturbing the measurements, an optimal design of the velocity log is desirable. On the one hand, it's aimed at reducing the height of the velocity log to a minimum with less impact of fluid-structure. On the other hand, the height has to meet the boundary layer's height of the flow around the submarine since the boundary layer is dominated by turbulent flow phenomena, strongly perturbing measurements in this region.
The elucidation of the flow around the bow of the submarine of class U212 by methods of Computational Fluid Dynamics (CFD) continues to be a challenging task. The underlying mathematical model of incom-pressible viscous flow around the submarine is given by the nonstationary Navier-Stokes equations. Strong gradients of the velocity field and pressure function close to the submarine's body and surface demand for highly adapted and locally refined computational meshes. A-posteriori error estimation for goal quantities of physical interest by duality techniques and combined adaptive refinement of the space-time mesh offer an efficient approach to overcome this challenge, construct economical meshes and ensure high quality approximation of the goal quantities[4]. Nevertheless, such discretizations and computations in three space dimensions for the sake of physical realism lead to high-dimensional algebraic non-linear systems. The number of unknowns, being necessary for the simulation of flow round the submarine's bow, is expected to be in the order of magnitude of at least 10^8 per time step. Conducting 10^4 time steps then leads to 10^{12} unknowns on the entire space-time mesh. In the group of Numerical Mathematics, robust and fast Geometric Multigrid (GMG) Preconditioners with local Vanky-type smoothers for arbitrary order space-time finite discretizations of partial differential equations have recently been developed[3,5]. Their efficiency and parallel scalability were demonstrated for complex flow phenomena and related problems. Recently, **matrix-free** implementations of GMG preconditioners for space-time finite element approaches were proposed and investigated[1]. Their improved performance and parallel scaling properties were carefully studied[1]. All algorithms mentioned before have been implemented in the deal.II library with MPI parallelisms for running on supercomputers like HSUper. The feasibility of con-ducting complex flow simulations with high accuracy on HPC systems offers the potential to overcome the challenges of the project CFD Design Optimization of Submarine Velocity Log. It will leverage the elucidation of the thickness of the boundary layer of flow around the submarine bow. Finally, training a neural network by using the high-fidelity simulation data allows to solve optimal control problems with partial differential equations as constraints in an efficient manner[2]. Such a hybrid approach of combined FEM HPC simulations and Scientific Machine Learning techniques is expected to solve the partner's challenging project of elucidating and optimizing the design of the velocity log.

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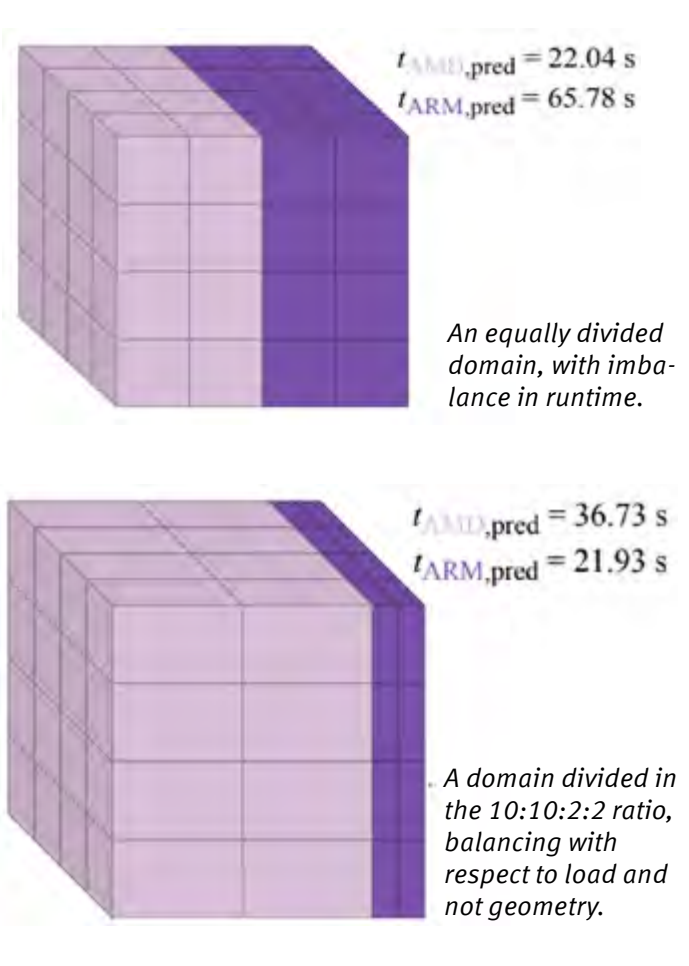
PROJECT UPDATE: STATIC LOAD BALANCING IN COUPLED SIMULATIONS

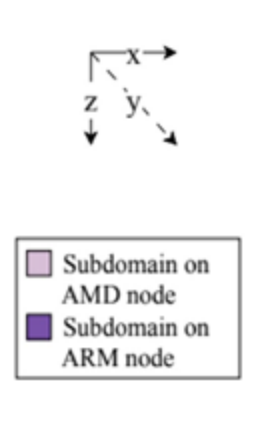
Author: Amartya Das Sharma

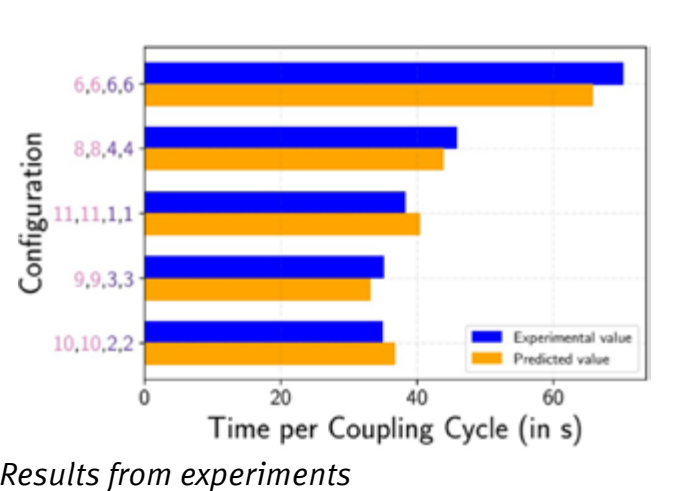
As part of the *MaST* project, we continue to refine and enhance our molecular dynamics simulation code ls1 mardyn and our continuum-molecular simulation coupling tool MaMiCo.
After the latest MaMiCo coding week, we successfully added the capability of static load balancing to both ls1 mardyn and MaMiCo. Using this new feature, we are now able to allocate computing resources to our simulations in a more efficient manner, by dividing the simulation domain into smaller and larger volumes geometrically, in a way that attempts to balance the computing load among the processors used. This was shown to be very useful in a variety of applications. For example, in a study with a simulation running on 64 processes, where the processes were divided among a faster AMD node slower ARM node, it was shown that dividing the regions in a ratio of 10:10:2:2 with larger regions given to the faster node, we obtained an approximate 50.2% improvement in runtime.
More experiments were run, with heterogeneous hardware and heterogeneous densities, and we observed 40-50% improvement of performance in the best case. The results were compiled and have now been submitted to a conference for review.



An equally divided domain, with imbalance in runtime.

A domain divided in the 10:10:2:2 ratio, balancing with respect to load and not geometry.





Results from experiments

hpc.bw@DAY OF RESEARCH, HSU/UNIBW H, MARCH 18, 2025

Author: Alexander Kolling

On March 18, the HSU/UniBw H hosted its annual Day of Research, bringing together scientists from various disciplines to showcase their work for other scientists and everyone interested.
This year's focus on interdisciplinarity was reflected in a diverse program, including poster exhibitions, lab tours, and presentations. The event was opened by HSU President Prof. Dr. Klaus B. Beckmann and Vice President Prof. Dr. Margarete Schuler-Harms, who emphasized the importance of cross-disciplinary research in tackling complex challenges.

The *hpc.bw* project was strongly represented, featuring a core poster on the project itself as well as five additional posters highlighting ongoing research within the project:

- *hpc.bw* (dtec.bw) – Competence Platform for Software Efficiency and Supercomputing
- *xbat*–An Easy-to-Use and Universally Applicable Benchmarking Automation Tool for HPC Software within the Project hpc.bw (dtec.bw)
- Fluid–structure interaction simulations of wind gusts impacting a hyperbolic paraboloid tensile structure
- Numerical simulation of artificial wind gust generation within a wind tunnel
- High Performance Computing meets Adult Education. Self-learning opportunities for HPC competence acquisition
- Optimal Design in Nonlinear Optics by Neural Networks

The team and associated members engaged in fruitful discussions with fellow researchers and interested visitors, identifying potential synergies with other projects.
We consider Research Day 2025 a success and were particularly impressed by the wide range of interdisciplinary and transdisciplinary projects presented. The event highlighted the strength of collaboration across disciplines and the innovative research happening at HSU/UniBw H. We look forward to continuing these conversations and building new connections in the future!

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