hpc.bw NEWSLETTER 2025/2

Finanziert von der Europäischen Union
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Editors:
Prof. Dr. Markus Bause, Prof. Dr.-Ing. Michael Breuer, Prof. Dr.-Ing. Denis Kramer, Prof. Dr. Philipp Neumann, Marie Rathmann

PROJECT UPDATES

Injection Process Investigated Using Molecula Dynamics Simulation

Author: Simon F. Homes & Bertalan Polgar

In the scope of the MaST project, which is a part of hpc.bw, a study using the molecular dynamics software ls1 mardyn was conducted to explore the behavior of liquid cyclopentane when injected into a gaseous nitrogen environment at the nanoscale. By employing over ten million molecules, which is significantly more than in prior studies, our investigation provided detailed insights into jet breakup characteristics and thermodynamic property distributions, as well as the dynamic behavior of the gas phase during injection.

The Lennard-Jones potential was selected to describe the intermolecular interactions that was parameterized to match the critical temperature of nitrogen and cyclopentane, as well as the saturated liquid density of cyclopentane. The unlike interaction parameter of the two components was fine-tuned to experimental vapor-liquid equilibrium data. Sophisticated domain boundary conditions and subregions were set up to meet the simulation requirements.

Five scenarios with varying injection velocity and ambient thermodynamic conditions were analyzed. Results show that the Rayleigh instability theory remains valid at the nanoscale. Increasing injection velocity and ambient pressure extends the liquid jet before breakup occurs. Under highly supercritical conditions, droplet formation is entirely suppressed and a continuous phase transition without a distinct phase interface prevails. In the gas phase, vortex rings form around the jet, while also shockwaves are induced at a higher injection velocity.

We would like to take this opportunity to thank the team of HSUper for the fruitful collaboration and their excellent support.

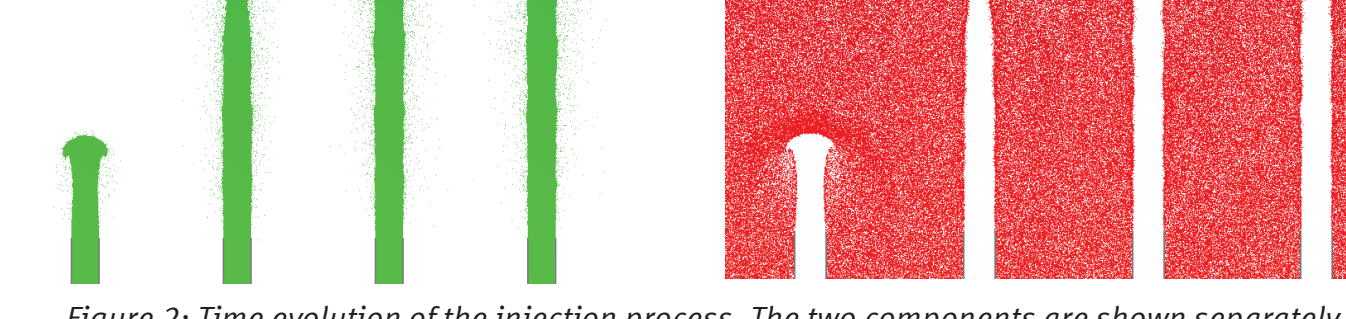


Figure 1: Liquid jet breakup following the Rayleigh instability theory

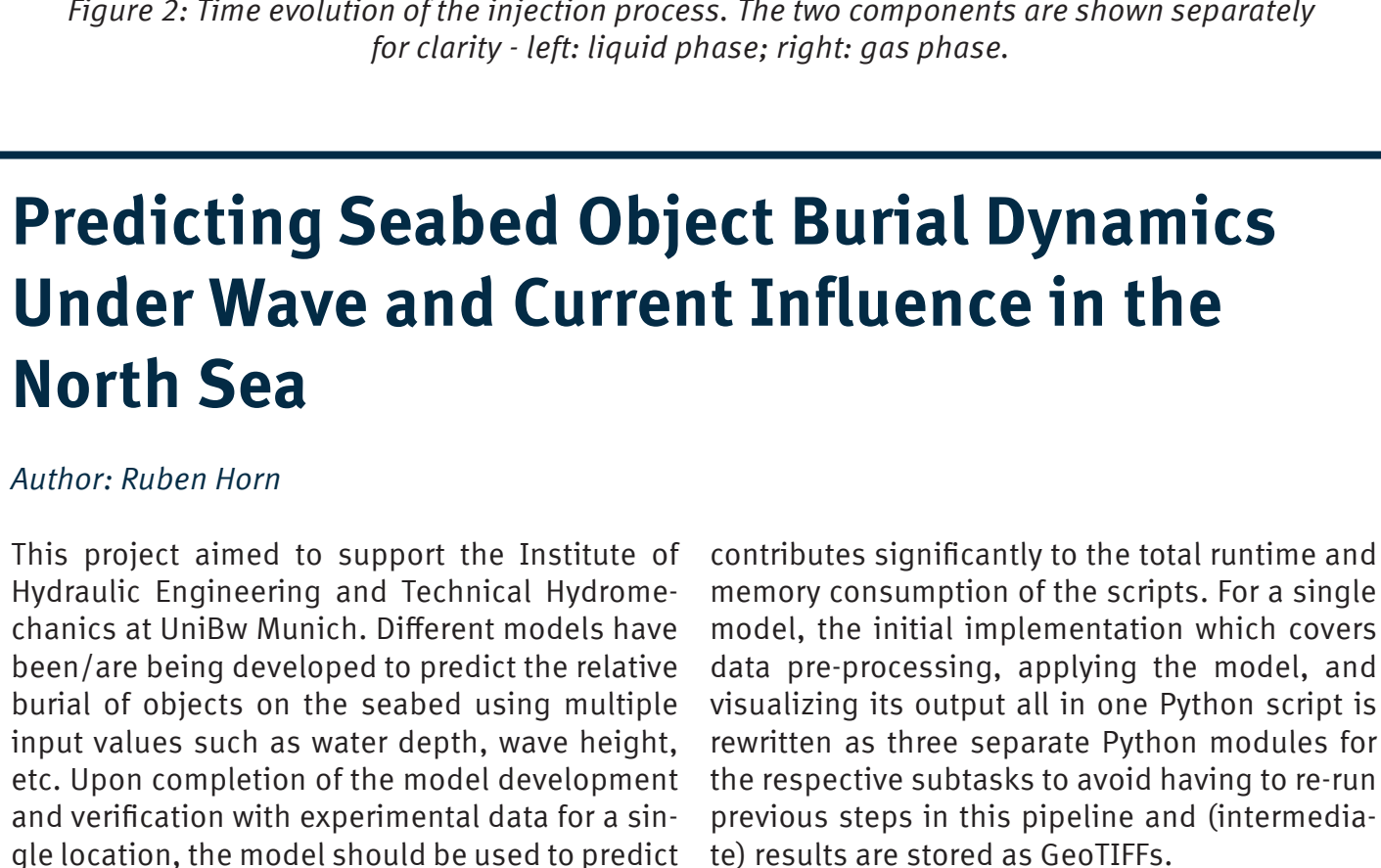


Figure 2: Time evolution of the injection process. The two components are shown separately for clarity - left: liquid phase; right: gas phase.

Predicting Seabed Object Burial Dynamics Under Wave and Current Influence in the North Sea

Author: Ruben Horn

This project aimed to support the Institute of Hydraulic Engineering and Technical Hydromechanics at UniBw Munich. Different models have been/are being developed to predict the relative burial of objects on the seabed using multiple input values such as water depth, wave height, etc. Upon completion of the model development and verification with experimental data for a single location, the model should be used to predict the burial for a wider area. To this end, the input values are provided as geographically annotated raster data (GeoTIFF image files) of the German North Sea spanning 215km2. The highest resolution of 10×10m is used. The initial implementation of the models as standalone Python scripts using the NumExpr package for parallel execution on the CPU required between eight and ten hours and 100 to 150GB of memory, running on a 64-core server with AMD Operon 6378 CPUs. This system also contains an Nvidia RTX A6000 GPU, which was not used by the initial implementation.

The primary performance bottleneck is the use of global variables which store intermediate values of the model for the entire raster, resulting in frequent allocations of large amounts (GB) of heap memory. Since the variables were created in the global scope, they were never dereferenced and therefore never released, so the memory consumption keeps increasing over time. The output of the model was visualized using the Matplotlib package. Since Matplotlib is illequipped to handle very high resolution raster data, it contributes significantly to the total runtime and memory consumption of the scripts. For a single model, the initial implementation which covers data pre-processing, applying the model, and visualizing its output all in one Python script is rewritten as three separate Python modules for the respective subtasks to avoid having to re-run previous steps in this pipeline and (intermediate) results are stored as GeoTIFFs.

Since the models are embarrassingly parallel, that is the output of a single cell depends only on the inputs associated with this cell, it can be expressed using a function of scalar input values. This avoids the allocation of large raster variables for intermediate values. As a NumPy universal functions (ufunc), it can be applied across all cells in the raster data. To accelerate this computation, the Numba package is used, which utilizes just-in-time compilation to convert the Python function into LLVM intermediate representation and can even target CUDA-capable GPUs. Using a custom wrapper class, a pure-Python function, which largely re-uses the code from the initial implementation, can thus be transparently accelerated for multicore or many-core targets.

Persisting the output of each iteration of the model takes a significant amount of time due to the bandwidth limit of the storage, which delays the next iteration (cf. fig. 3a). Therefore, the file output is carried out in parallel to the computation of the next iteration (cf. fig. 3b) to reduce the impact of this bottleneck.

(a) Sequential computation/output. *(b) Parallel computation/output.*

Figure 3: Illustration of sequential and parallel computation/output.

Interactive visualization in the browser using the HoloViews and Datashader packages progressively loads only the required data depending on the zoom and pan by the user, which results in acceptable responsiveness when visualizing very large raster data. Alternatively, the GeoTIFFs are converted into 8-bit tiles with a resolution of 250×250 served over HTTP depending on the map location and zoom. For static visualization, the data can be cropped to specific coordinates during pre-processing, resulting in smaller files which can be trivially plotted. Compared to the initial implementation of the model, which requires 37 minutes and 85.35GB of memory over 6 time steps on the 64-core server without visualization, the new implementation requires under 4 minutes (9.45×speedup) and 14.98GB of memory (−82.45 %). The model can now even be run on a highend laptop or workstation, and the introduced modularity of the project avoids duplicate code.

Open-Source Release of the (Extended Benchmarking Automation Tool) *xbat*

Author: Willi Leinen

Benchmarking plays a key role in optimising runtime, reducing energy consumption, and improving hardware efficiency of applications in high-performance computing (HPC) systems. Yet for many users—especially those without in-depth hardware knowledge—accessing and interpreting performance metrics can be a complex and error-prone task.

To make this process more accessible, MEGWARE Computer Vertrieb und Service GmbH has developed xbat **(extended benchmarking automation tool)**. Designed to be both powerful and user-friendly, xbat automates benchmarking workflows and simplifies performance analysis. xbat was released fully open-source in April 2025, further supporting transparency, collaboration, and community-driven development in the HPC community.

The **dtec.bw** projects **MaST** and **hpc.bw** contributed during the beta testing phase and studied via xbat the performance of the open-source molecular dynamics research software ls1 mardyn and of the closed-source mathematical optimisation package Gurobi on the HSUper cluster. Results of this collaboration are published in xbat: a continuous benchmarking tool for HPC software and are shown on the project poster **xbat – An Easy-to-Use and Universally Applicable Benchmarking Automation Tool for HPC Software within the Project hpc.bw (dtec.bw)** at the ISC High Performance 2025 conference.

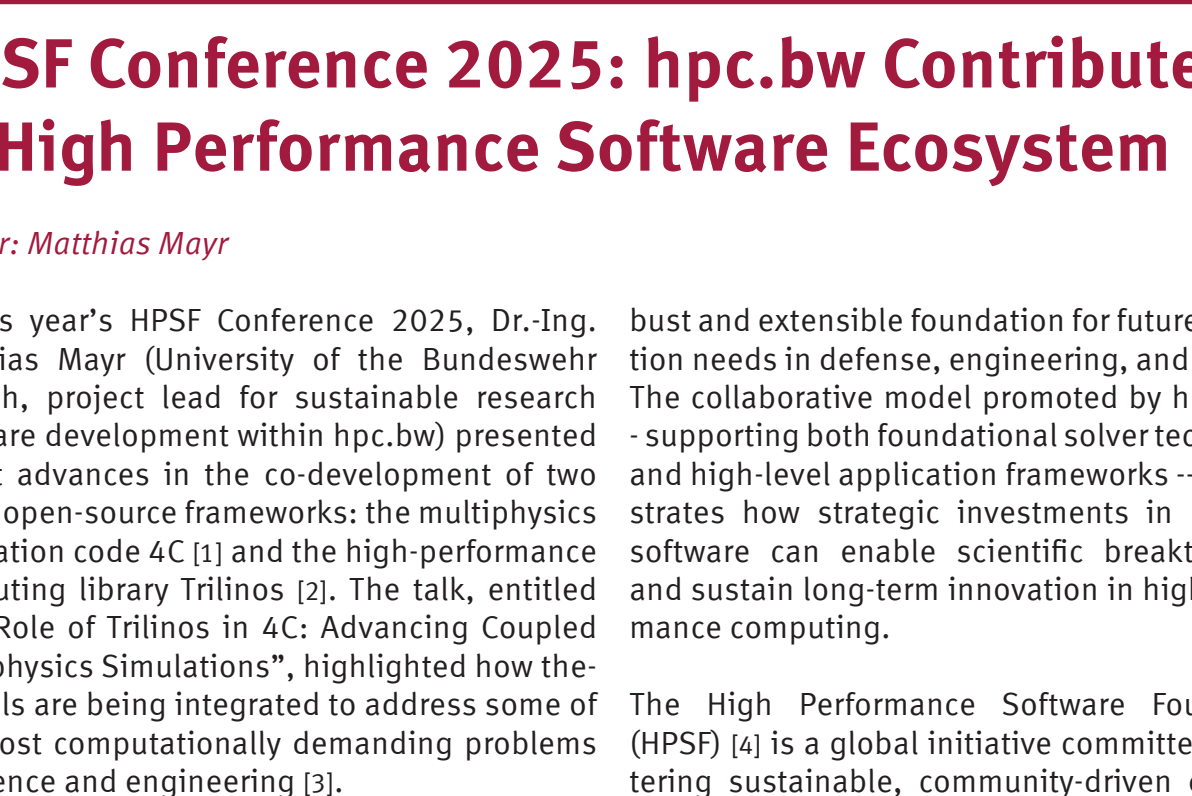
ACTIVITIES

hpc.bw @ISC High Performance 2025

Author: Willi Leinen

hpc.bw presented two posters in the project poster gallery of the ISC High Performance 2025 conference from Tuesday to Thursday (10.06.–12.06.2025). The poster *hpc.bw (dtec.bw) – Competence Platform for Software Efficiency and Supercomputing* provided an overview of the hpc.bw project and showed results about selected applications, whereas the poster *xbat – An Easy-to-Use and Universally Applicable Benchmarking Automation Tool for HPC Software within the Project hpc.bw (dtec.bw)* focused on the xbat software and its usage within the hpc.bw project. Many people were interested in the project results and we had several fruitful discussions with people creating HPC learning materials or HPC benchmarking and performance analysis software.

You can find the xbat poster here DOI 10.24405/20152
and there hpc.bw poster here DOI 10.24405/20153.



Photos: Rachel Williamson

HPSF Conference 2025: hpc.bw Contributes to High Performance Software Ecosystem

Author: Matthias Mayr

At this year's HPSF Conference 2025, Dr.-Ing. Matthias Mayr (University of the Bundeswehr Munich, project lead for sustainable research software development within hpc.bw) presented recent advances in the co-development of two major open-source frameworks: the multiphysics simulation code 4C [1] and the high-performance computing library Trilinos [2]. The talk, entitled "The Role of Trilinos in 4C: Advancing Coupled Multiphysics Simulations", highlighted how these tools are being integrated to address some of the most computationally demanding problems in science and engineering [3].

Central to this work is the support provided by the hpc.bw project, which funds the development of scalable multi-level solvers for coupled multiphysics systems within the Trilinos ecosystem. In particular, the algebraic multigrid package MueLu within Trilinos has been extended to serve as a flexible and efficient preconditioning framework for systems arising in the 4C environment. These efforts are not only pushing the boundaries of numerical performance but also shaping new directions in open-source scientific software co-design.

4C (Comprehensive Computational Community Code) is developed to simulate a broad range of coupled phenomena, including fluid-solid interaction, contact mechanics, and beam-solid coupling. By leveraging Trilinos' parallel linear algebra and solver infrastructure, and co-developing components such as MueLu under the umbrella of hpc.bw, the project is building a robust and extensible foundation for future simulation needs in defense, engineering, and beyond. The collaborative model promoted by hpc.bw —- supporting both foundational solver technology and high-level application frameworks -- demonstrates how strategic investments in research software can enable scientific breakthroughs and sustain long-term innovation in high-performance computing.

The High Performance Software Foundation (HPSF) [4] is a global initiative committed to fostering sustainable, community-driven development of high-performance computing (HPC) software. By bringing together academic researchers, industry practitioners, and open-source developers, HPSF promotes best practices in software engineering, reproducibility, and performance portability. The annual HPSF Conference serves as a central forum for presenting cutting-edge advances in HPC software, facilitating collaboration across disciplinary and institutional boundaries.

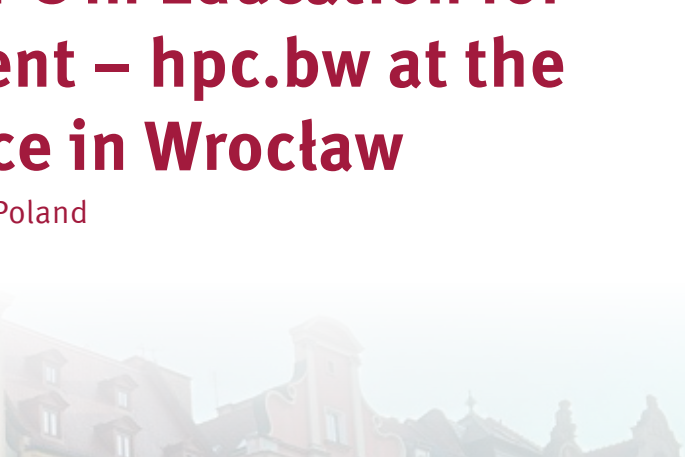


Photo: Christian Glusa

[1] https://4c-multiphysics.org
[2] https://trilinos.github.io
[3] https://www.youtube.com/watch?v=L0y-XtxEhyw
[4] https://hpsf.io

Exploring the Role of HPC in Education for Sustainable Development – hpc.bw at the International Conference in Wrocław

hpc.bw at the 14th ESREA Conference in Wrocław, Poland

Photo: Marie Rathmann

Author: Alexander Kolling

From June 12 to 16, 2025, the international conference **„Critical Learning for Sustainable Development: Communities' and Universities' Discourses"** took place in Wrocław, Poland. The event brought together researchers from various disciplines and countries to explore the role of adult education in achieving the Sustainable Development Goals (SDGs). The hpc.bw project participated in the conference with a scientific poster and a short presentation. You can find the poster here: DOI10.24405/20175

The focus was on the **intersection between HPC resources, the potential of adult education, and their relevance to the SDGs**. Today, HPC already plays a crucial role in foundational research for fields such as climate modeling, materials science, and sustainable resource management. However, in the **humanities and social sciences, HPC remains largely unknown and underutilized** - leaving a significant research potential untapped. Especially in adult education, such technological resources are rarely used. Contributing factors include a lack of competencies, limited access to infrastructure, and low awareness of the potential of HPC resources.

The goal of hpc.bw and the High Performance Computing Competences Platform is to address these gaps. On the one hand, it is essential to raise awareness of how HPC can be used in the humanities and related fields. On the other hand, **tailored educational offerings must be made accessible to enable researchers from non-technical disciplines** to make meaningful use of HPC - especially in addressing the complex challenges related to the SDGs.The conference provided an excellent platform to bring this perspective into the discussion and engage in dialogue with international stakeholders from education and sustainability research.

Overall, the event featured a wide range of inspiring contributions on the role of adult learning in advancing the SDGs. We are pleased to have introduced a technological impulse into this discourse and see great potential for future collaboration at the intersection of HPC, education, and sustainable development.

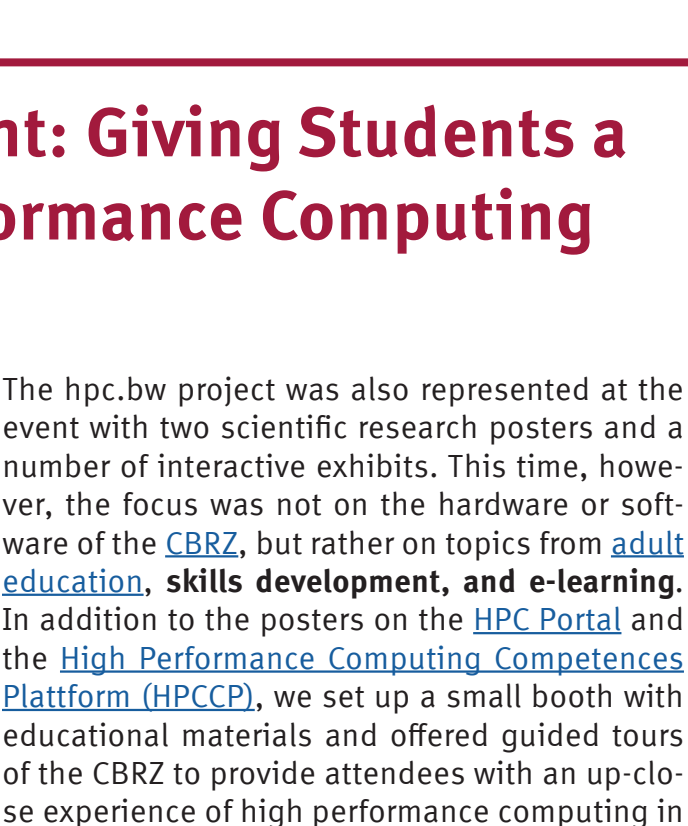


Photo: Marie Rathmann

hpc.bw at Jugend forscht: Giving Students a Glimpse into High Performance Computing

Author: Alexander Kolling

From May 29 to June 1, the 60th national finals of **Jugend forscht** (Germany's premier youth science competition[1]) took place. This anniversary event was held in collaboration with the Stiftung Jugend forscht e.V. at the Helmut Schmidt University/University of the Bundeswehr Hamburg.

At the event, **young researchers** from across Germany presented their innovative projects to a jury of experts. In addition to the competition itself, the program featured an **interactive exhibition on science, technology, and innovation** organized by the STEM Campus. The exhibition showcased current research and development across land, sea, air, and cyber domains, making scientific practices accessible and engaging for all visitors.

[1] https://www.jugend-forscht.de/information-in-english.html

The hpc.bw project was also represented at the event with two scientific research posters and a number of interactive exhibits. This time, however, the focus was not on the hardware or software of the CBRZ, but rather on topics from adult education, **skills development, and e-learning**. In addition to the posters on the HPC Portal and the High Performance Computing Competences Plattform (HPCCP), we set up a small booth with educational materials and offered guided tours of the CBRZ to provide attendees with an up-close experience of high performance computing in action.

We would like to extend our **heartfelt congratulations to all participants** for their inspiring projects, and especially to the award winners for their outstanding achievements.

HPC.BW@CONFERENCES

Author: Markus Bause

Members of hpc.bw and associated fellows attended several international conferences and presented research results of hpc.bw in different formats (oral presentations, poster contributions and organization of minisymposia or special seesions). The list of conferences includes in particular:

- 95th Annual Meeting of the International Association of Applied Mathematics and Mechanics, Poznan, Poland
- XI International Conference on Coupled Problems in Science and Engineering, Villasimius, Sardinia
- International Supercomputing Conference High Performance, Hamburg, Germany
- 15th International Conference on Large Scale Scientifc Computations, Sozopol, Bulgaria
- 14th ESREA Network 'Between Global and Local – Adult Learning and Communities' Conference, Wrocław, Pola

OUTLOOK/DISSEMINATION

Save the Date: HSUper Workshop, October 16-17, 2025 @HSU/UniBw H

Author: Alexander Kolling

Over the past two years, the HSUper Workshop has become a recurring opportunity for both HPC newcomers and advanced users at HSU to build skills and competencies in using HPC resources—particularly the HSUper. This year's edition will take place **October 16–17, 2025**, featuring a combination of hybrid and on-site formats.

Unlike previous years, the focus will not be solely on knowledge transfer. Instead, **the workshop emphasizes peer-group-based collaboration**, problem-solving, and the practical implementation of individual solutions.

On **Thursday, October 16**, participants will join a hybrid tutorial format designed to help them refresh their skills and close knowledge gaps using self-guided materials available on the HPC Portal.

On Friday, October 17, attendees will work in small groups tailored to their specific needs, experience levels, and application areas. Each group will be supported by one or more HPC experts and receive access to resources on the HSUper system. The goal is to collaboratively address research-specific challenges and implement working solutions, fostering both individual autonomy and mutual support within the groups.

To enable this tailored experience, a **detailed registration process will begin shortly**. It will collect information on participants' prior experience, relevant topics, and areas of interest to support group formation and resource planning.

We look forward to another productive and collaborative HSUper Workshop!

Contact:
hpc.bw – Competence Platform for Software Efficiency and Supercomputing
Project Management at HSU/UniBw H:
Prof. Dr. Markus Bause
Prof. Dr.-Ing. Michael Breuer
Project Coordination: Marie Rathmann
E-Mail: info-hpc-bw@hsu-hh.de

Imprint:
Helmut-Schmidt-Universität/Universität der Bundeswehr Hamburg
Holstenhofweg 85, 22043 Hamburg
Published by Marie Rathmann (info-hpc-bw@hsu-hh.de)
Layout: HSU/MZ/Grafikstudio/KS

Helmut Schmidt Universität
Universität der Bundeswehr Hamburg