hpc.bw NEWSLETTER 2025/3

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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

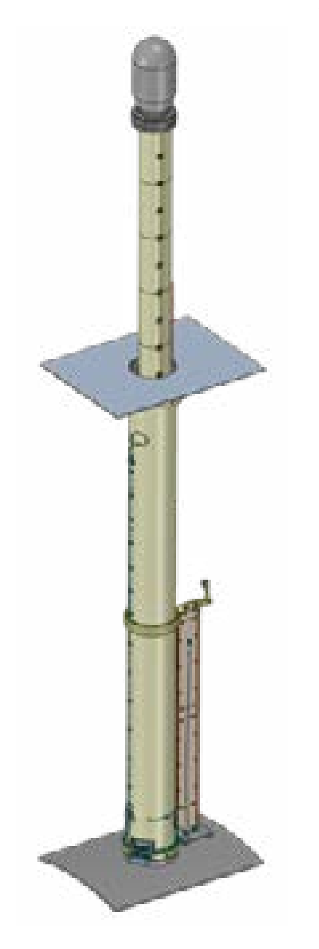
Seminar Series and HPC Café “Computation & Data”, HT2025

Date / Room	Speaker & Moderator	Title of Lecture & HPC Café
29.10.2025 **Seminar Room 0308**		
16:00-17:00	Philipp Marienhagen (HSU/UniBw H)	Thermodynamic properties of quantum fluids: Path integral Monte Carlo simulations of helium and neon using ab initio potentials
17:00-18:00	HPC Café with Ruben Horn	Peer Guidance & User Collaboration
26.11.2025 **Aulagebäude A1, Seminar Room 002**		
16:00-17:00	Kevin Lüdemann (GDWG Göttingen)	The HPC Skill Tree, design, current content, and how to work with it
17:00-18:00	HPC Café with Jose Escobar	Peer Guidance & User Collaboration
17.12.2025 **Building H7, lecture hall 32**		
16:00-17:00	Laura Linder (HSU/UniBw H)	FEM Simulation of TPMS Gyroid under multiaxial-loading: a comparison of solids and different shell elements
17:00-18:00	HPC Café with Vahid Jafari	Peer Guidance & User Collaboration

CFD Design Optimization of Submarine Velocity Log. Initiation of satellite project in submarine HPC simulation with new industrial project partner GABLER, Naval Technology, Lübeck

Author: Nils Margenberger und Markus Bause

On July 16 and September 15, two meetings were held at HSU/UniBw H and at the head office and production site of GABLER Naval Technology (NT), Lübeck. M. Bause, M. Breuer, M. P. Bruchhäuser and two students (in the second meeting) evaluated together with representatives from Gabler NT the potential of cooperation and joint research in the HPC simulation based elucidation of flow phenomena related to mast systems of submarines with the overall goal of optimizing the design of the systems. The contact between HSU/UniBw H and Gabler was initiated by BAAINBw (Bundesamt für Ausrüstung, Informationstechnik und Nutzung der Bundeswehr) and KKpt. Kevin Hostombe, Scientific Coworker at the Chair of Mechatronics, HSU/UniBw H.


© GABLER NT, C. Schulz

GABLER NT was founded in 1962 by Prof. Ulrich Gabler. Since then, they provide international navies with innovative, reliable submarine mast systems as well as key components and enable submarines to safely perform high value maneuvers. The development and production of submarine mast system is their core business. As opposed to the mast, limited to the lowering and lifting mechanism of a sensor, the mast system comprises the hydraulic control block, the hoistable mast control and the sensor. In periscope depth, hoistable mast systems generate water turbulances and in particular behind the submarine. This facilitates its detection and identification by hostile forces. Design optimization addresses the minimization of submarine's signature by innovative shapes of the mast systems and/or new materials, for instance, based on bionic concepts and structures. Modelling of the mast systems leads to complex flow systems. Their numerical simulation argues for advanced simulation techniques on modern HPC architectures which can be provided by hpc.bw.

As a first step of the colloboration, a Bachelor thesis, supervised by M. Bause and M. Breuer, has been arranged. The Bachelor thesis will be conducted by HSU/UniBw H Mechanical Engineering student F. Jung. The collaboration with GABLER NT will be extended further.

Algorithm Selection for High Performance Molecular Dynamics

Author: Samuel Newcome

In the hpc.bw work package on Transcritical Fluids, we investigate the thermodynamics of fluids in a scale-bridging approach, from molecular to continuum scales. A key component for molecular considerations in this endeavor is the HPC-capable molecular simulation software ls1 mardyn and the particle simulation library AutoPas, that is used within ls1 mardyn. AutoPas employs automated algorithm selection to always use the fastest numerical scheme, in particular for the force calculations between molecules. We developed several methods for improving the algorithm selection process inside AutoPas, which use simulation statistics, such as density or metrics for fluid homogeneity, to determine potentially optimal algorithms. One of these methods was an Expert fuzzy-logic-based algorithm selector, which would use expert-written fuzzy-logic rules, of the form “If the particle density is low, then algorithm A is good” (illustrative example only). Another method used was Random Forests, trained on data gathered from physically incorrect, but cheap to mass produce, scenarios, to predict which algorithm would perform optimally given some simulation statistics. These methods were compared against an existing Predictive method, based on linear extrapolations of past performances of algorithms, and a naive Full Search method that trails all algorithms periodically. The new methods were found to perform far better, especially in dramatically changing scenarios. In figure 1, the speedup of the three methods is presented, as well as a Full Search method that naively trials all algorithms, with speedup calculated relative to the optimal single algorithm for the simulation. A speedup above one represents advantage from AutoPas being able to change the algorithm during the simulation but a speedup below one is not necessarily a failure of the method, as this optimal single algorithm is likely not know in advance. Both new methods performed similar, but the Random Forest approach was deemed more accessible, as well as more maintainable, since the library changes over time, to adapt to the latest systems environments. One disadvantage of the method is the requirement for suitable data. This work, as well as an outline of a potential solution to the above problem, is presented by Newcome et al. [1].

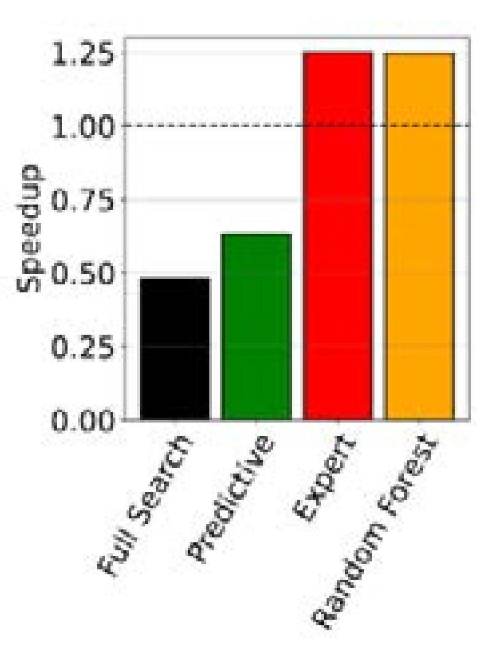


Figure 1:Speedup achieved, relative to picking the optimal single algorithm, for a simulation of a heated sphere for the Full Search, Predictive, Expert fuzzy logic-based, and Random Forest methods. See [1] for more details. Figure from submitted manuscript of Newcome et al. [2].

References

[1] Samuel James Newcome et al. “Algorithm Selection in Short-Range Molecular Dynamics Simulations”.
In: International Conference on Computational Science. Springer. 2025, pp. 292–299.

[2] Samuel James Newcome et al. “Algorithm Selection in Short-Range Molecular Dynamics Simulations”.
In: arXiv preprint arXiv:2505.03438 (2025).

preCICE at Helmut-Schmidt-University: Efficient Fluid-Structure Interaction Computational Framework

Authors: Guillaume De Nayer (HSU/UniBw H), N. Lesquoy (ISAE-SUPAERO, France), M. Breuer (HSU/UniBw H)

preCICE is an open-source coupling library for partitioned multi-physics simulations, ***specifically designed for high-performance computing***. It enables users to combine specialized solvers from different physical domains. Within the **dtec.bw project** hpc.bw, researchers at HSU are already making extensive use of **preCICE**. In the Department of Fluid Mechanics, preCICE plays a central role in efficiently studying fluid-structure interaction (FSI) problems with the help of HPC techniques.

The in-house fluid solver **FASTEST-3D** is used to compute the fluid dynamics and the resulting forces acting on one or more deformable structures applying high-fidelity methods such as large-eddy simulation (LES). These forces are mapped and transferred to the open-source structural solver **CalculiX** via preCICE, which then returns the structural displacements to the fluid solver. This FSI framework enables the investigation of real-world problems. For instance, the Department of Fluid Mechanics at HSU has wide experiences in studying civil engineering applications such as large-scale, thin membrane roofs or tents exposed to turbulent wind flows and strong gusts.

Why preCICE?

We are carrying out advanced FSI simulations for more than one decade using the coupling tool EMPIRE. Due to several restrictions with this software, we now switched to preCICE for FSI coupling. This measure is motivated by the fact that it is open source and supported by an active, responsive developer community, but also because it is explicitly designed for HPC. This aligns perfectly with the objectives of the DTEC **hpc.bw** project, which aims to improve the scalability of our FSI framework on supercomputers. Moreover, preCICE requires only minimal modifications to the coupled solvers, reducing the implementation effort.

Once the fluid solver had been adapted to use preCICE, the next step was to validate the framework against state-of-the-art FSI benchmarks (see Fig. 2 & 3). The first test case selected was the well-known **FSI3 benchmark** by Hron and Turek, which features laminar flow around a flapping plate mounted behind a rigid cylinder. This setup is very challenging in terms of coupling stability. As a second test case, we chose the **lid-driven cavity with a flexible bottom** proposed by Wall, as its configuration is particularly suitable for investigating HPC scalability.

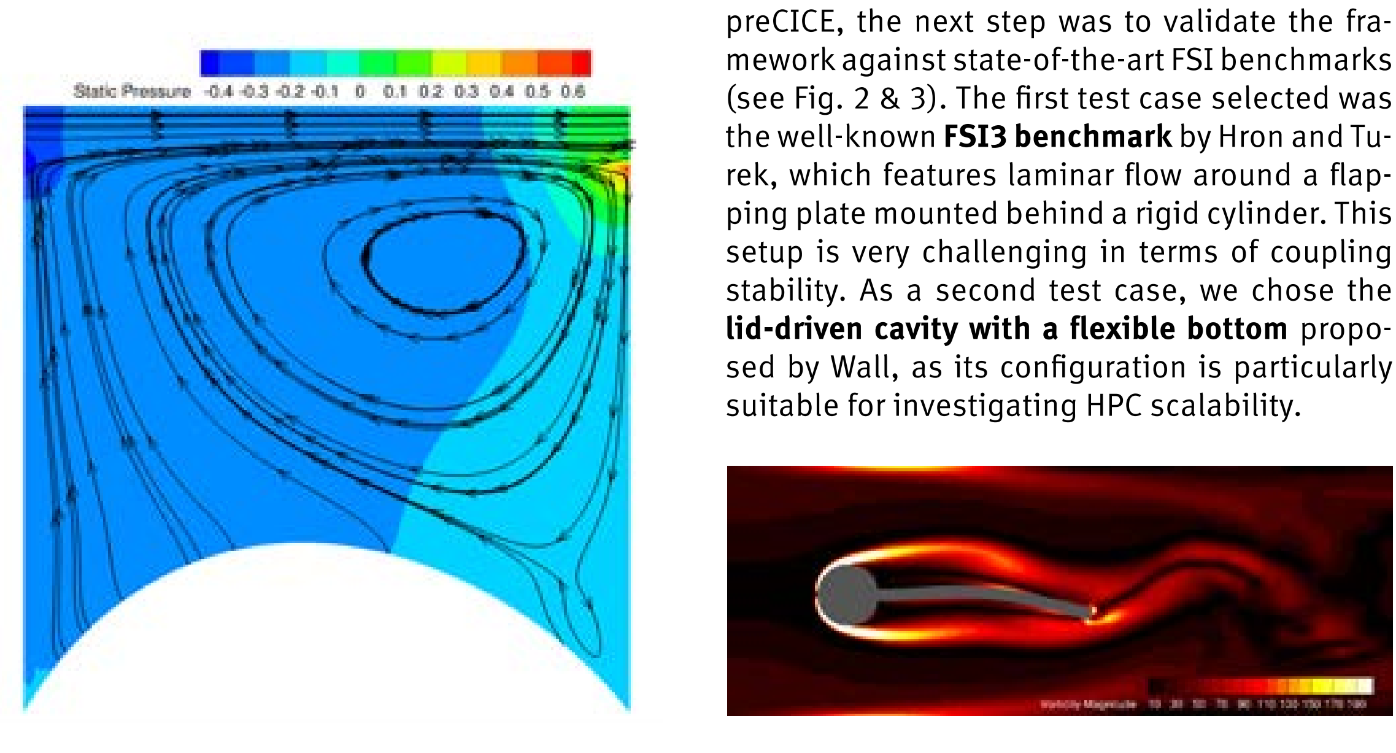

Static Pressure -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5 0.6
Velocity Magnitude

Figure 2 & 3: Examples of FSI test cases: Laminar flow around a flapping plate attached behind a rigid cylinder (left). Recirculating flow in a fixed cavity with a flexible bottom (right). N. Lesquoy (2025)

In a second step, the accuracy and efficiency of the different preCICE data mapping techniques were evaluated in this FSI context. In addition, the acceleration methods provided by preCICE to improve coupling performance and convergence between solvers were also thoroughly investigated. In particular, the **Quasi-Newton acceleration techniques** were analyzed in detail. Applying these methods to the aforementioned test cases resulted in a simulation speedup of more than a factor of 20 on HSUper, the supercomputer of the Helmut-Schmidt University, reducing the runtime from about 570 min. to approximately 25 min.

This FSI work was presented by N. Lesquoy during the poster session of the preCICE workshop 2025. We strongly acknowledge the ressources provided by **HSUper**, funded by dtec.bw - Digitalization and Technology Research Center of the Bundeswehr. dtec.bw is funded by the European Union - NextGenerationEU.

Bringing the Community Together: The preCICE User Workshop

Author: Guillaume de Nayer

In September 2025, the 6th preCICE User Workshop) took place at Helmut-Schmidt-University (HSU/UniBw H) in Hamburg, supported financially by the Zentrum für Digitalisierungs- und Technologieforschung der Bundeswehr (*dtec.bw*). **Over the course of five days, 50 participants from around the world came together to exchange knowledge, share experiences, and strengthen the preCICE community**. During the first three days dedicated training sessions were offered to beginner users to help them become familiar with the functionalities and wide range of applications of the preCICE coupling tool. The workshop also welcomed experienced users and experts, who had the opportunity to share their work through scientific talks and poster sessions on the fourth day. On this day, there was also a joint dinner by the Alster in Hamburg to strengthen the network among preCICE users – rounded off by a sunset over the water. Moreover, the preCICE Workshop was enriched by the keynote from Daniel J. Bodony from the University of Illinois Urbana-Champaign (USA) on fluid–structure interaction in high-enthalpy flows. On the final day, the workshop concluded with an extended user session, where participants presented their issues and received direct support from the preCICE developer team.

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

HPC Workshop @ HSU/UniBw H, October 16–17, 2025

Author: Alexander Kolling

Over the past two year, hpc.bw has organized and implemented different workshop formats to ensure the development of skills for using HSUper and the ISCC.

This year, we will once again be offering a workshop to which we would like to invite you. The HPC Workshop will take place at HSU on October 16—17, 2025. October 16 will take place in a self-learning format with support from our experts if needed; October 17 will take place in small groups at HSU each with an expert on site. The program will take place on both days between 9 a.m. and 5 p.m.

The workshop will focus on problem-solving strategies, active on-site support from our experts and peer-to-peer groups. The aim is to build small groups that can work together with experts on similar problems, challenges and topics and – in addition to networking – make direct progress in their research projects. Access to HSUper or ISCC is necessary. If you do not have an access yet, please register here or contact us.

In order to plan the assignment in advance, we need sufficient information about the level of competence and research focus of all participants. For this, we have designed a self-assessment questionnaire based on the HPC Skill Tree, which is mandatory registration.

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hpc.bw @EURO 2025 Leeds

Author: Willi Leinen

hpc.bw was presenting its research in the field of logistics and optimization at the 34th European Conference on Operational Research (EURO 2025), which took place 22.06.—25.06.2025 in Leeds at the University of Leeds, UK. Our presentation “**Balancing energy and performance: efficient allocation of solver jobs on high-performance computing systems**” was part of the session “Deployment & Execution” in the stream “Software for Optimization”. The corresponding slides are here.

LIKE-MINDS SEE THE DOTS
UNLIKE-MINDS CONNECT THEM
BE UNLIKE-MINDED
LEEDS BECKETT UNIVERSITY

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hpc.bw @RSE Day 2025

Author: Willi Leinen

hpc.bw attended the RSE (research software engineering) day 2025 which took place on 16.07.2025 in the Science City Bahrenfeld. It was organized by the University of Hamburg's Hub of Computing & Data Science (HCDS) and aimed to map the variety of RSE efforts in Hamburg. hpc.bw gave a lightning talk about the hpc.bw project and the extended benchmarking automation tool xbat and presented the poster **xbat – An Easy-to-Use and Universally Applicable Benchmarking Automation Tool for HPC Software within the Project hpc.bw (dtec.bw)**. Many people were interested in xbat and we had several fruitful discussions. The book of abstracts is here.

hpc.bw @dtec.bw Annual Meeting 2025

Author: Lars Zigan und Markus Bause

From September 1—3, 2025, the second dtec.bw annual conference was held at Helmut-Schmidt-Universität/Universität der Bundeswehr Hamburg in Hamburg.

Exciting insights were provided into the range of funded research in selected projects on digitization concepts covering the research dimensions of land, sea, human, cyber, space, and air.

On the one hand, we were represented with the subproject “MaST – Macro/Micro-Simulation of Phase Decomposition in the Transcritical Regime.”

Mixture formation in the transcritical regime is very complex, which happens under very high pressure but at moderate temperatures. This is especially relevant for fuel injection processes in rocket chambers. The analysis of the underlying flow processes requires detailed multiscale considerations, ranging from molecular properties to large-scale continuum flow field simulation and analysis. In an interdisciplinary effort, MaST bundles expertise from high performance computing, scientific computing, computational fluid dynamics and thermodynamics to investigate such systems.

For this purpose, we use, develop and combine high-performance simulation techniques, such as molecular dynamics simulation (MD), Monte Carlo simulations (MC), classical density functional theory (cDFT), computational fluid dynamics (CFD), molecular-continuum approaches and experimental studies. Visitors had the opportunity to learn more about this topic through presentations, exhibits at the booth, and guided tours of laboratories and the HPC „HSUper“.

On the other hand, our work was represented in research connected to High Performance Computing (HPC). In the context of dual use research, HPC simulation of flow around a submarine of class U212 A is being conducted in collaboration between the Chair of Numerical Mathematics and the 1st Submarine Squadrone of the naval base in Eckernförde. The goal of this simulation is to elucidate boundary layer effects and compute the depth of this flow region.

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This knowledge is demanded for optimizing the design of velocity logs that are mounted on the submarine's bow during testing its performance characteristics and calibrating weapon systems and related ones. Velocity measurement has to be done outside the boundary layer due to the complex and turbulent flow phenomena arising therein, thus bounding the log's height from below. On the other hand, the velocity log's height has to be reduced to its minimum in order to reduce effects of fluid-structure interaction and perturbations of the measurement quality. For this research goal, high-resolution 3D HPC simulation of the flow problem is used, complemented by scientific machine learning techniques for the subsequent velocity log design optimization process. The calculations require solving large algebraic systems of equations with the number of unknowns in each time step being in the order of magnitude of 10^8 or even higher. Geometric multigrid methods are employed as efficient preconditioners for the solution of the algebraic systems resulting from higher order self-adaptive space-time finite element approximations of the Navier-Stokes flow model.

We would like to thank the organizers, speakers, exhibitors, and visitors for making this impressive event possible.

Submarine Symposium 2025, Eckernförde

Author: Markus Bause

Symposium
Uboote 2025
17.09. - 18.09.2025
Marinestützpunkt Eckernförde
BWEVENTS

On September 17—19, 2025 the 1st Submarine Squadron organized the Symposium Uboote 2025. The 1st Submarine Squadron is based in Eckernförde and operates six Type 212 A submarines. More than 120 participants from different institutions participated in the meeting at the naval base in Eckernförde. In particular, members from the 1st Submarine Squadron, representatives from HSU/UniBw H, BAAINBw (Bundesamt für Ausrüstung, Informationstechnik und Nutzung der Bundeswehr), Marinearsenal (naval arsenal), Military Technical Center for Ships and Naval Weapons (Wehrtechnische Dienststelle 71, tasked with supporting the German Navy in maritime issues of military technology and military science), industry experts and students of HSU/UniBw H joined the meeting. The symposium provided an excellent platform for exchange of experiences, operation issues and update/regeneration strategies, technical and future innovations related to submarines as well as discussions regarding human ressources and education. The submarine class U212 A of the Bundmarine as well as the next generation U212 C/D that is under current development were focused in the presentations, exchange and discussions. From hpc.bw, M. Bause joined the meeting.

Conference Activities in the hpc.bw community

- Markus Klein and Isabelle Veith @ETMM 15 Conference (Engineering Turbulence Modelling and Measurements), Dubrovnik, Croatia, 22—24 September 2025
- Min Son, Lars Zigan, Michael Pfitzner & Tobias Sander @Europe-Korea Conference on Science and Technology 2025, Vienna, Austria, 25—28 August 2025
- Min Son, Lars Zigan, Michael Pfitzner & Tobias Sander @32. Deutscher Flammentag für nachhaltige Verbrennung, Paderborn, Germany, Sep.15—17, 2025
- Joachim Groß, Michael Pfitzner, Tobias Sander, Min Son, Rolf Stierle & Lars Zigan @Thermodynamik-Kolloquium, Hamburg, Germany, 22—24 September, 2025
- Jadran Vrabec & Bertalan Polgar @EMLG/JMLG 2025, Hévíz, Ungarn, 1—5 September 2025

Contact:

hpc.bw – Competence Platform for Software Efficiency and Supercomputing

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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