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Helmut Schmidt Universität – Universität der Bundeswehr Hamburg

hpc.bw NEWSLETTER 2025/4

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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”, WT2026

Date	Speaker & Moderator	Title of Lecture & HPC Café
28.01.2026		
16:00–17:00	Mihail Miller (InfAI e.V. Leipzig)	Disentangling the Black Box: Transparent and Structured On-Premises Knowledge Engineering and Retrieval with AI Models – Insights from LiquidInfo (URZ, Leipzig) and DigiTaKS
17:00–18:00	HPC Café with Amartya Das Sharma	Peer Guidance & User Collaboration
25.02.2026		
16:00–17:00	Surya Kiran Peravali (HSU/UniBw H)	A Multiscale Simulation Framework for Particle-Beam Experiments: From Navier–Stokes to Boltzmann
17:00–18:00	HPC Café with Hauke Preuß	Peer Guidance & User Collaboration
25.03.2026		
16:00–17:00	Shashini Wanniarachch (HSU/UniBw H)	Co-Scheduling- Towards energy efficient HPC
17:00–18:00	HPC Café with Johan Duffek	Peer Guidance & User Collaboration

Bridging the Gap for Interface Analysis in Injection Systems

Author: Rolf Stierle

Methods that bridge the gap between length scales are necessary for analyzing transcritical injection in systems ranging from the molecular to the macroscopic continuum. To describe dynamic processes on molecular length scales, we developed a set of balance equations, which we call hydrodynamic density functional theory. These equations take molecular correlations on small length scales into account and degenerate into the macroscopic Navier-Stokes equations for macroscopic systems. Thus, they unify the modeling of molecular and macroscopic continuum systems. Using molecular models from classical density functional theory, we account for effects that are considered macroscopically as surface tension and fluid-wall interactions.

We tested our hydrodynamic density functional theory against non-equilibrium molecular dynamics simulations of a microscopic droplet on an atomistically rough surface, analyzing the effects of the vapor-liquid and fluid-solid interfaces [2].

We observed good agreement in the shape of the rolling droplet, the advancing and receding dynamic contact angles, and the velocity vectors inside the droplet (see Fig. 1). This strengthens our confidence in applying continuum methods to molecular length scales. Ultimately, this will enable us to describe dynamic processes across length scales, from molecular to macroscopic, using the same method.

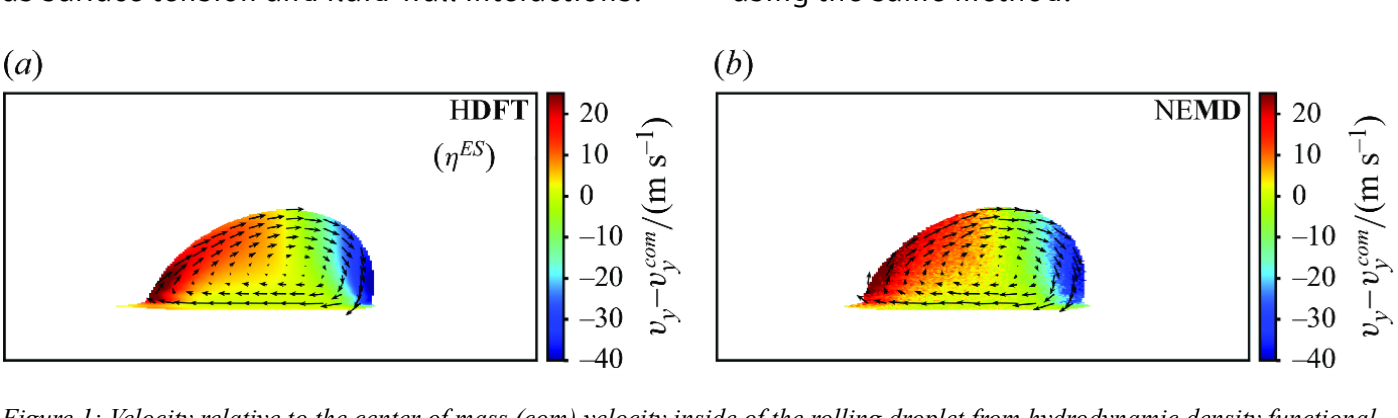


Figure 1: Velocity relative to the center of mass (com) velocity inside of the rolling droplet from hydrodynamic density functional theory (left) and non-equilibrium molecular dynamics (right).

References:

[1] Rolf Stierle, Joachim Gross: Hydrodynamic density functional theory for mixtures from a variational principle and its application to droplet coalescence. *The Journal of Chemical Physics*, 155(13), 2021.

[2] Benjamin Bursik, Rolf Stierle, Hamzah Oukili, Martin Schneider, Gernot Bauer, Joachim Gross: Modelling interfacial dynamics using hydrodynamic density functional theory: dynamic contact angles and the role of local viscosity. *Journal of Fluid Mechanics*, 1016, 2025.

Co-Scheduling for Energy Efficient HPC Operations

Author: Shashini Wanniarachchi

While high performance computing (HPC) has become an essential tool in numerous application domains, it comes with a cost that is increasingly impossible to ignore, which is energy consumption. Due to this, strategies for making the HPC system more energy efficient have become a highly relevant topic now.

Among other energy saving mechanisms, one option is co-scheduling also referred to as oversubscription. This refers to assigning more computational tasks to the system than physical capacity. Nodes of an HPC system contain many cores and shared memory channels. While some HPC workloads are memory bound, there are other applications that saturate compute units with low memory usage. These two kinds of applications thus create the opportunity to run them simultaneously, sharing the available resources on the same node. In the hpc.bw project under energy efficiency, we try to achieve such a co-scheduling scenario leading to improved energy efficiency of the HSUper system.

Two of the main concerns here are L3 cache workload and memory bandwidth [1]. Usually, memory-bound applications come with a high cache miss rate and saturate memory channels, while compute bound applications have a high compute to memory ratio. This makes memory bound jobs spending more energy on retrieving data and compute bound jobs spending more energy on computational operations. Therefore, running these together brings a better balance between resource utilization and energy consumption.

As a primary test scenario, Stream, a memory bound benchmark and Linpack, a computation bound benchmark were chosen. Running both on a single node is considered and finding a suitable co-scheduling configuration is the initial goal. Pinning each application to a certain set of cores of the node with likwid pin was carried out. Configurations range from one application occupying a limited number of cores while the other use the entire node to sharing the number of cores between the applications in a non-overlapping manner. This results in applications saturating only certain memory channels as well. Accordingly, the best results are seen when both applications are occupying 36 cores each in a non-overlapping manner. While this is a sub-optimal scenario, this is still considered as oversubscription. This is because the memory channels are oversubscribed by the two applications, as both hit all the memory channels under this allocation. This pinning configuration is depicted in Figure 2.

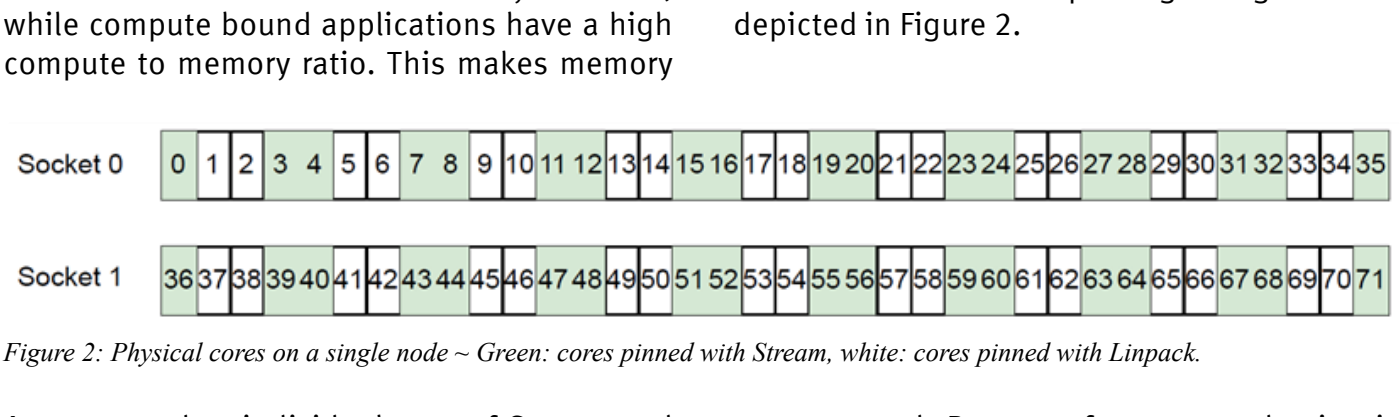


Figure 2: Physical cores on a single node ~ Green: cores pinned with Stream, white: cores pinned with Linpack.

As compared to individual runs of Stream and Linpack, the co-scheduling scenario delivered the following performance:

- Performance degradation in Stream: 3.13%
- Performance degradation in Linpack: 26%
- Reduction in energy consumption: 3.7%
- Reduction in runtime: 4.62%

In co-scheduling, a certain performance degradation is expected as a compromise on the energy saved. But a performance reduction in the range obtained is tolerable in the considered applications for the gain we have in terms of energy consumption. This initial result shows that through co-scheduling energy efficiency of HPC systems can be improved. Further experiments are now underway with applications from hpc.bw group to generalize a scenario where this can be applied in job scheduling and reach better energy efficiency on HSUper.

References:

[1] J. Breitbart, J. Weidendorfer and C. Trinitis, „Case Study on Co-scheduling for HPC Applications,“ 2015 *44th International Conference on Parallel Processing Workshops*, Beijing, China, 2015, pp. 277-285, doi: 10.1109/ICPPW.2015.38.

HPC@HSU – A short review of the latest HPC Workshop

Authors: Alexander Kolling

From October 16 to October 17, 2025, the HPC@HSU Workshop took place at the Helmut-Schmidt-University/University of the Federal Armed Forces Hamburg (HSU/UniBw H), organized by the hpc.bw project. The event represents the third part of HSUper workshop series for knowledge and competence transfer in the field of HPC. While the first two workshops strongly focused on the transfer of knowledge between HPC experts within the hpc.bw project and researchers in the field of HPC, this year’s workshop centered on networking and exchange about similar research challenges resp. questions through peer groups. Moreover, the workshop HPC@HSU conceptually combined offerings for self-organized learning with direct support from experts for joint problem-solving within the research projects. A total of 19 participants and 9 experts took part in the workshop.

Self-organized learning and Peer-to-Peer concept

The first day began with a short joint introduction to the workshop concept, including welcome remarks by Head of HPC Lab Piet Jarmatz, followed by an introduction to the new self-learning offers (E-trainings) on the digital HPC Portal. In addition to the E-trainings already available on topics such as *A short introduction to HSUper and the Linux Terminal*, *Data Transfer and System Resources*, or *Module Systems and Slurm Jobs*, the following topics were newly added onto the HPC Portal:

- Advanced Slurm,
- Loading and installing Software with Spack,
- Running Graphical Applications with X-Forwarding,
- Best Practices for HPC and
- Performance Engineering for Pythin and Deep Learning.

Participants on site were accompanied by experts who could support them while working on the E-Trainings individually selected to their own need. The goal was to provide participants with access to an offer suited to their respective competence level, including appropriate support. During the last block on the first day, all participants then had the opportunity to prepare their own research projects and, with the help of a profile sheet, structure them in a way that enabled shared exchange in small groups and active work on their own project.

The second day began with the group formation. We assigned the groups based on a self-assessment of HPC competences completed during registration, as well as the goals, methods, and discipline specific background of the participants’ research projects. The groups were clustered with regards to the following thematic categories:

- Machine Learning,
- FEM,
- Advanced Coding Problems,
- HPC Basics,
- Gurobi

The self-assessment combined with the information about the participants’ individual research projects helped the experts on the hand to adapt to the individual and various needs of the group members and on the other hand, to provide support where the researchers were currently facing challenges. The goal of this procedure was to support the researchers in such a way that they would be able to continue working independently on their projects after the workshop.

However, during the workshop, a shared structure was also created based on the learning management system MS Teams, which aims to provide new users of the HSUper and generally interested researchers with a long-term opportunity for exchange within the peer group. The day ended with a joint reflection and evaluation of the workshop. The participants clearly expressed their need for a regular workshop with the same setting and gave the workshop positive feedback.

Insights into the workshop evaluation

Of all participants who took part in the evaluation (n = 13 / N = 19), 75% stated that they agreed or strongly agreed with the statement *“The workshop helped me deepen my understanding of HPC.”* Another 82% agreed with the statement *“The workshop helped me make progress in my own project,”* and 92% would agree with *“I will use the offers on the HPC Portal in the future.”* While these ratings only provide an indication of the participants’ satisfaction with the workshop concept, they are already an important indicator that the goals we set for the workshop have been achieved. The exploratory setting, with alternating phases of self-organized learning processes and peer-to-peer group formation, seems to have been well received and offers potential for providing direct support in the implementation of research projects, rather than merely transferring knowledge. Additionally, the evaluation identified further topics that could be made available as E-trainings on the HPC Portal, e.g. working with the programming languages *R* and *Julia*. Furthermore, the feedback collected will help to further optimize the concept for the next event. Based on this feedback, we will change the first day from an overall open to a slightly more scheduled and guided concept with small inputs to support the self-organized learning experience. We will also focus on ensuring more opportunities for exchange between the groups and experts, to identify challenges and the resources to tackle them efficiently. A full evaluation will be published on the HPC Portal.

Save the date: 2nd HPC@HSU Workshop in April 2026

Author: Alexander Kolling

Based on the evaluation, it became clear that the need for further workshop concepts still exists. The participants’ feedback also indicated that the corresponding concept with self-organized but supported learning phases and group formation should be maintained. For this reason, we are already announcing the next workshop on April 23–24, 2026.

HSUper Usage Update – November 2025

Author: Piet Jarmatz

Our HPC cluster HSUper continues to grow in both user base and activity. As of November, 239 users are registered, up from 222 in August, with 117 active users submitting jobs. External users account for 3% of the submitted jobs and 1% of the used walltime. Most users originate from MB (63%), followed by WiSo (14%) and ET (9%).

Storage utilization shows steady growth: BeeGFS is at 43% (up from 41%), Ceph at 5.36%, and CephFS usage has reached 18.6 TiB. ISCC storage stands at 16.29 TiB.

Cluster utilization remains high. Between May and November, CPU nodes were allocated 52% of the time, while GPUs saw 32% allocation. However, GPU wait times have increased significantly: the average wait for small_gpu jobs is now 8.77 hours (previously 1.47h), and many jobs still run without using GPUs. For medium and large jobs, wait times improved to 22 minutes from nearly 4 hours.

Job statistics reveal that most workloads run on single-node jobs (95% of job count). 79% of total wallclock hours are spent in the small partition, highlighting strong demand, while multi-node jobs (>5 nodes) remain steady at around 21% of all wallclock hours.

Looking ahead, we expect several new hardware systems to become available in 2026, stay tuned for this. Users should also prepare for upcoming maintenance downtimes due to construction works (date TBD) and remember to backup their data!

Stay connected via the HSUper Users Teams Channel and join our regular HPC Café. The next user meeting will be on February 6, 2026 (10:30 in H11 R218).

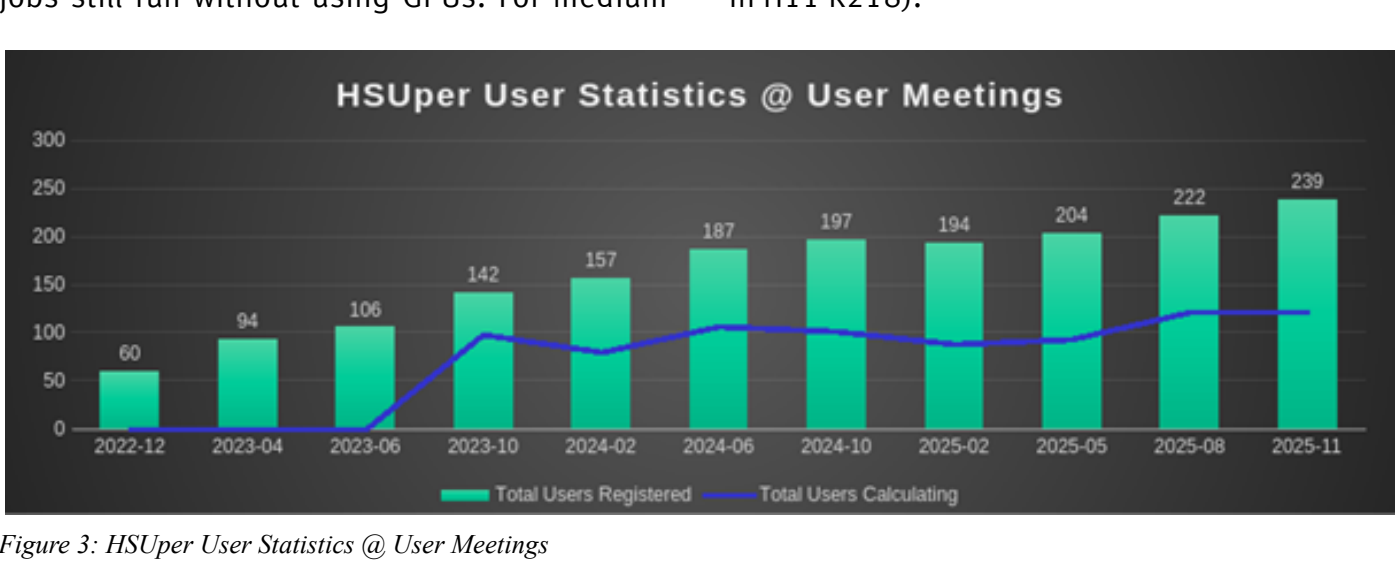


Figure 3: HSUper User Statistics @ User Meetings

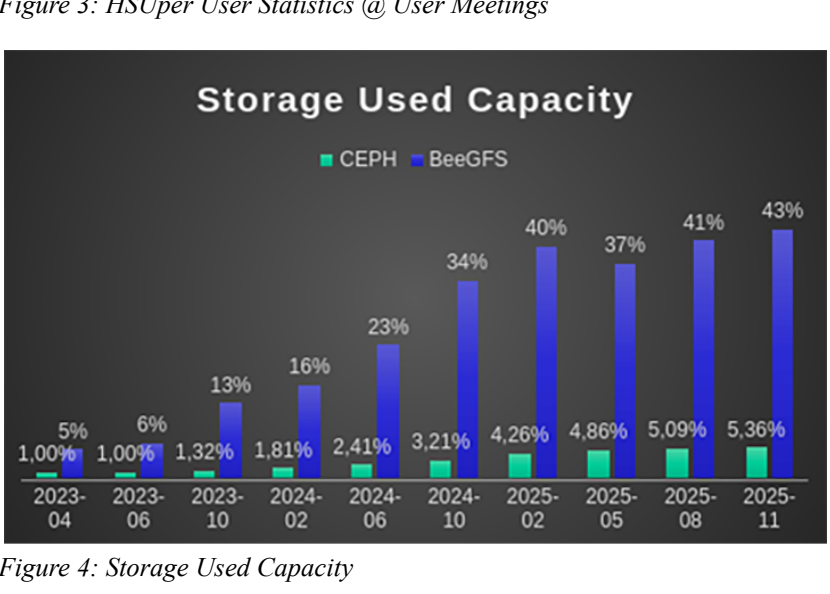


Figure 4: Storage Used Capacity

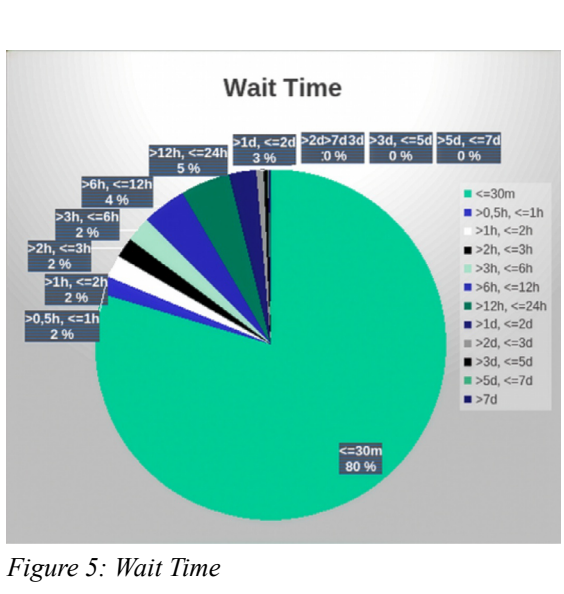
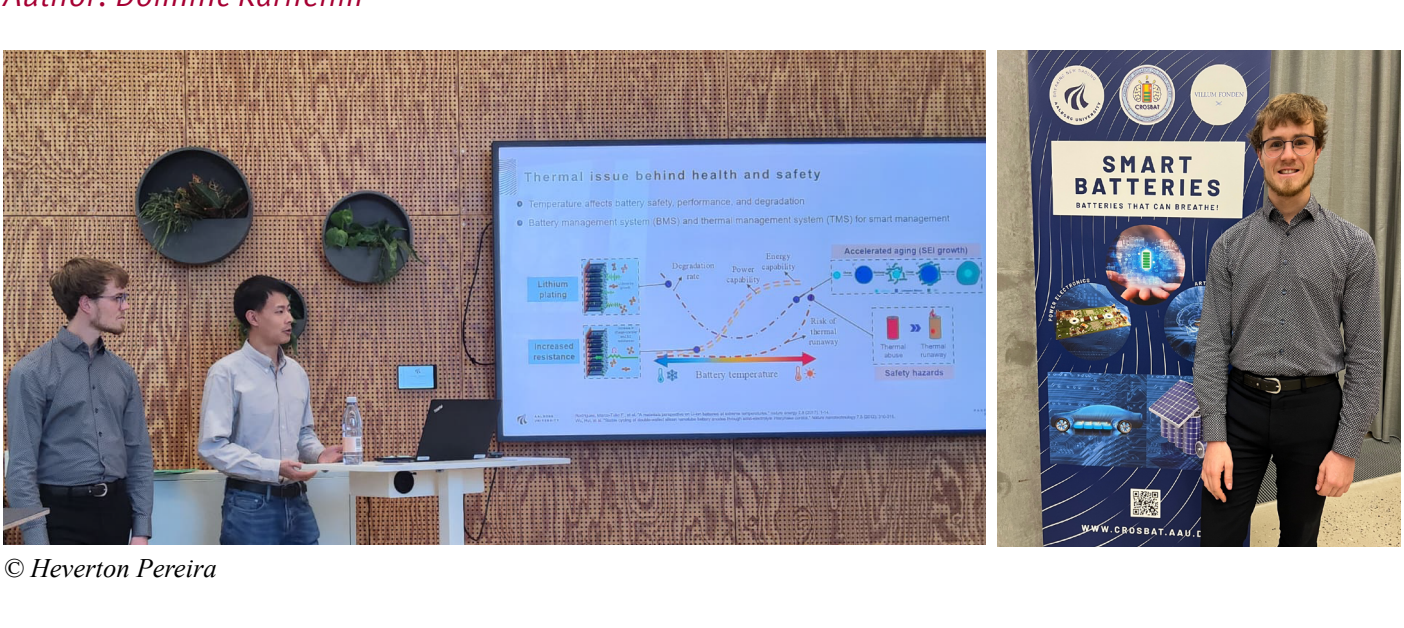


Figure 5: Wait Time

Young Researcher Program: Insights into the Activities During Dominic Karnehm’s Research Stay

Author: Dominic Karnehm



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Dominic Karnehm participated in the Third Annual Workshop of the Centre for Research on Smart Batteries (CROSBAT AIX) at Aalborg University on 10 November. He gave a presentation entitled ‘Battery State Estimation and Prediction’ together with Yusheng Zheng. The presentation showcased the results of Dominic Karnehm‘s research stay at Aalborg University, which was made possible by hpc.bw.

The workshop is organised annually under the auspices of the Villum Investigator Grant ‘Smart Battery’ by Prof. Remus Teodorescu and his team. The grant aims to research the future of intelligent battery systems, focusing on innovative methods to improve performance, safety, and sustainability through artificial intelligence.

In their presentation, Dominic Karnehm and Yusheng Zheng showcased their AI-based method, Parameter-Embedded Fourier Neural Operator (PE-FNO), for monitoring temperature distribution in lithiumion batteries. The technique uses neural operators to predict the temperature gradient within battery cells without solving the underlying partial differential equations (PDEs) numerically. Neural operators enable changing the spatial and temporal resolution of their predictions even after training, which fundamentally distinguishes them from classic deep learning methods such as LSTMs. Furthermore, unlike classical AI approaches, parameter embedding enables the integration of parameters related to physical material properties – such as density and heat capacity – directly into the learning and prediction process as model inputs. This means that temperature curves for different batteries can be predicted using the same model even after training. Thanks to their flexibility and generalisability, both properties open up new perspectives for efficient battery management and accelerated design processes in electromobility.

hpc.bw @ The 9th international conference on Advanced COmputational Methods in ENgineering and Applied Mathematics (ACOMEN2025)

Author: Marius Paul Bruchhäuser

Photo: https://cage.ugent.be/acomen2025/

The conference on Advanced Computational Methods in Engineering and Applied Mathematics (ACOMEN2025) took place in Ghent, Belgium, from 15 to 19 September 2025. The ninth edition of this conference aimed to provide an international forum to present and discuss the latest developments in computational and applied mathematics in various emerging engineering and mathematical fields.

hpc.bw was presented by means of a minisymposium regarding *Advanced Numerical Methods for Flow and Related Problems*, organized by Marius Paul Bruchhäuser, Nils Margenberg (both Helmut Schmidt University Hamburg) and Richard Schussnig (Ruhr University Bochum). With 16 contributions distributed into four sessions, this minisymposium was the largest of all in all nine minisymposia within the conference, aiming to mathematical and computational innovations in the complex simulations associated with flow problems. The focus was on the development and rigorous analysis of state-of-the-art numerical methods and solvers using high performance and extreme scale computing techniques. Two of the three organizers were represented by giving an own presentation. Nils Margenberg talked about *An hp Multigrid Approach for Tensor-Product Space-Time Finite Element Discretizations of the Stokes Equations*, whereas Marius Paul Bruchhäuser gave a talk about *Goal-Oriented Space-Time Adaptivity for Nonstationary Incompressible Flow Problems*.

All in all, the presentations and the conference as a whole offered a great framework for fruitful discussions and exchange about the latest results in using high performance computing hardware for the efficient and reliable solution of mathematically challenging problems.

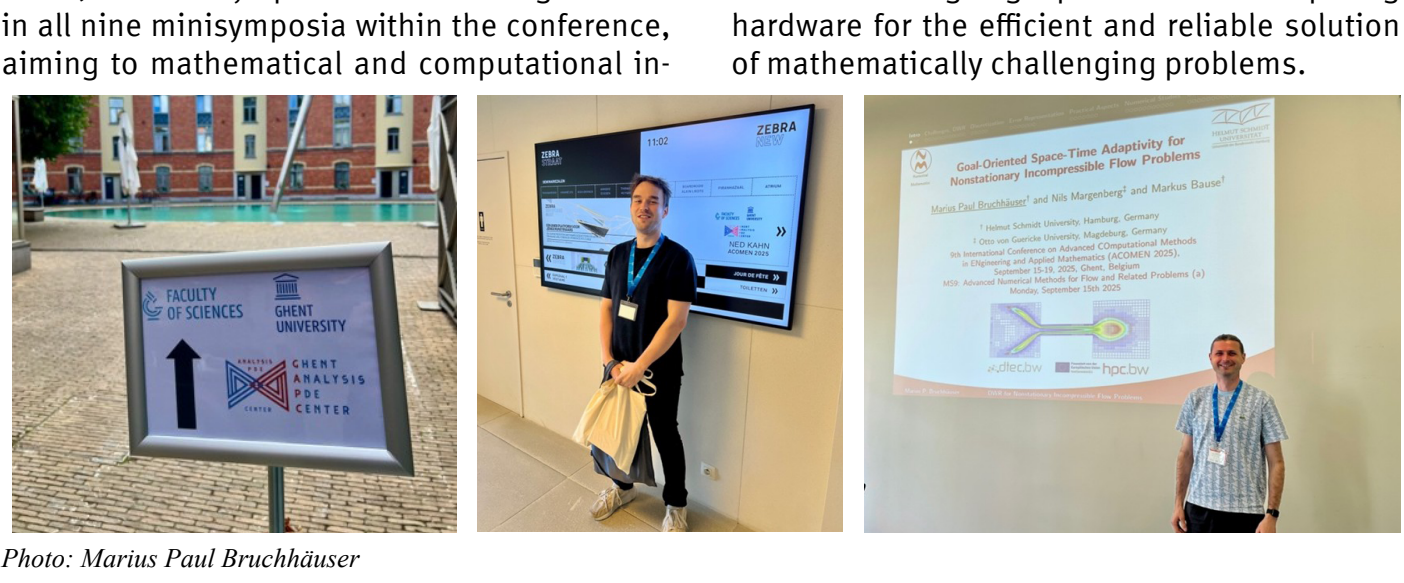

Photo: Marius Paul Bruchhäuser

hpc.bw @ The European Conference on Numerical Mathematics and Advanced Applications (ENUMATH) 2025 in Heidelberg, Germany

Author: Marius Paul Bruchhäuser

Photo: Marius Paul Bruchhäuser

At this year’s European Conference on Numerical Mathematics and Advanced Applications (ENUMATH), taking place on September 1–5, 2025, in Heidelberg, hpc.bw was represented equally several times acting in the following positions:

- Nils Margenberg: *An hp Multigrid Approach for Tensor-Product Space-Time Finite Element Discretizations of the Stokes Equations* (Presentation)
- Pavel Shamko: *Numerical Approximation of Coupled Hyperbolic-Parabolic Systems in First-Order Form* (Presentation)
- Imane Bechelaoui: *Lower Order Vanka Smoother in Geometric Multigrid Preconditioning for Space-Time FEM to the Stokes System* (Poster)
- Marius Paul Bruchhäuser: *Goal-Oriented Space-Time Adaptivity for Nonstationary Flow Problems* (Poster)

Started in 1995, the ENUMATH conference offers every two years a well-known and established forum for presenting and discussing novel and fundamental advances in numerical mathematics and challenging scientific and industrial applications on the highest level of international expertise. The two poster sessions as well as the presentations within topic related minisymposia found high appeal among the audience and offered a platform for fruitful discussions among academic colleagues.

Furthermore, a minisymposium related to Adaptivity in Space and Time was organized by Marius Paul Bruchhäuser, Nils Margenberg and Bernhard Endtmayer. Within 12 contributions current results with respect to mathematical and computational challenges associated with adaptive numerical methods were presented and discussed in-depth. Moreover, latest developments in efficient solver technologies and optimal resource allocation designed for high performance computing were introduced. All in all, this minisymposium afford a great opportunity for scientific research and future collaborations using the power of high performance computing.

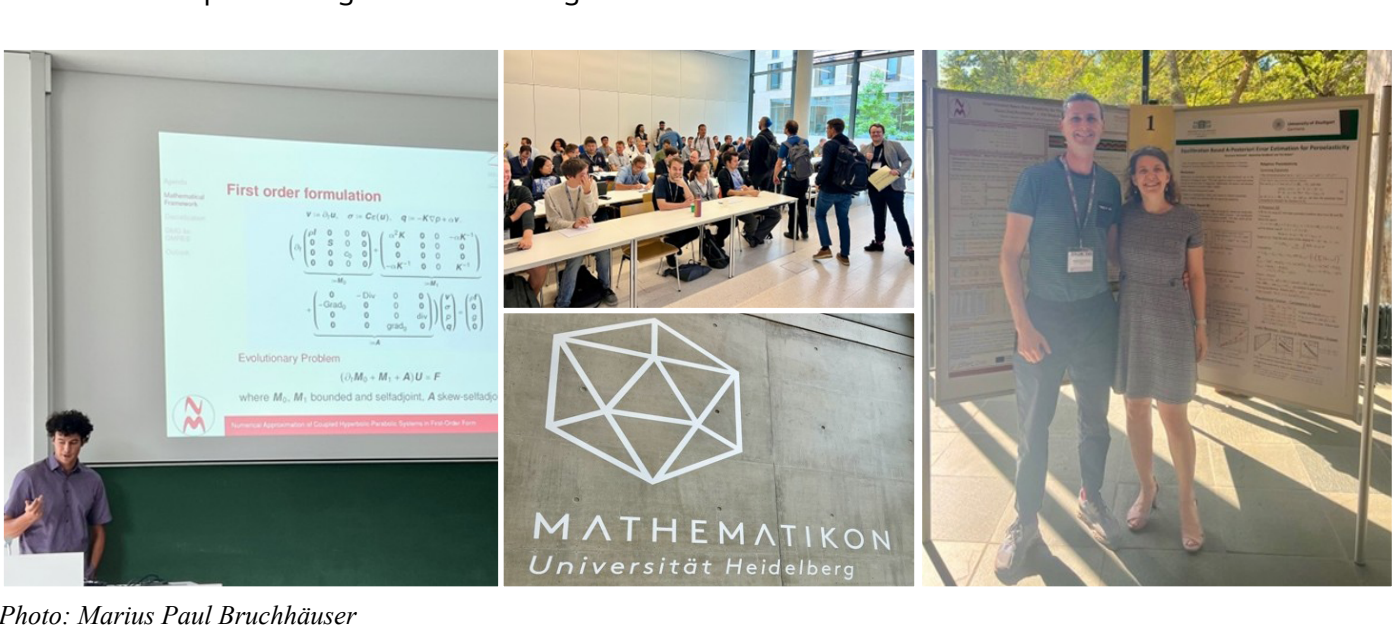

Photo: Marius Paul Bruchhäuser

NEW: hpc.bw Publication List

Author: Alexander Kolling

The hpc.bw project now includes more than 200 publications that were created within the framework of hpc.bw or produced through the resources made available by the project. These originate from various disciplines, promote knowledge transfer across many subject areas, and exist in a wide range of formats. Including academic articles in journals, Anthologies or openHSU publications, research posters from conferences and symposia, monographs, project reports, scientific presentation slides, and others.

The aim is to provide a bibliography for all interested parties to promote the exchange between disciplines and research projects and to offer orientation for everyone entering the field, exploring it, and seeking to acquire expertise.

The publication lists are now available on the HPCCP and the HPC Portal.

Closing Words 2025

Author: Marie Rathmann

As 2025 draws to a close, we also reach the end of the year in which hpc.bw entered its extension phase. With the second funding phase, we not only strengthened the dual-use aspect and aligned research results with the needs of the German Armed Forces, but the two previously separate projects, *hpc.bw* and *MaST*, have also grown together into a single joint hpc.bw project. In 2025, we have therefore expanded into a large collaborative project with partners from HSU/UniBw Hamburg, UniBw Munich, TUM, the Berlin University of Technology, and the University of Stuttgart.

What is also new in the second funding phase? The Young Researcher Program was launched in 2025! This initiative enables early-career scientists to gain international research experience. Our first doctoral candidate, Dominic Karnehm, traveled to Aalborg University in Denmark to conduct research on battery state measurements.

However, we were able to support three Performance Engineering Projects starting in April. We are supporting one project developing an automatic system for indexing and comparing German-language court decisions using unsupervised NLP methods; another project focused on the improvement of the Branch-and-Bound (B&B) method used in combinatorial optimization by enhancing its branching strategies and parallelization, with a focus on self-learning approaches; as well as a Performance Engineering Project aiming to develop a numerical model to predict sedimentation processes affecting objects on the seabed, enhancing maritime safety and detection capabilities in the North Sea.

Alongside our research activities, we were once again highly engaged in the conference landscape—both as participants and as organizers. Below is a brief overview of selected activities from 2025: The year began with our Wrap-Up & Kick-Off Project Meeting in March 2025 at HSU. The event provided an opportunity for our consortium to meet in person, present the results of the first funding phase, and introduce plans for the second phase. In May 2025, Matthias Mayr attended the HPSF Conference and delivered a presentation on the High Performance Software Ecosystem. In July 2025, we offered students from the “Jugend forscht” program an introduction to the world of High Performance Computing. Additionally, Alexander Kolling and Marie Rathmann presented on teaching HPC competencies in adult education at ESREA in Wrocław. In the same month, Willi Leinen and Hauke Preuß attended ISC High Performance 2025 in Hamburg, where they presented both the hpc.bw project and the Extended Benchmarking Automation Tool (xBAT).

In early September, the dtec.bw Annual Conference took place at HSU/UniBw H. Our project was represented with an exhibition booth, where visitors could learn more about our activities, explore our offerings, and participate in CBRZ tours. We also hosted the preCICE Workshop at HSU, welcoming more than 50 participants from around the world. The workshop allowed researchers to learn how to use the software hands-on, while user presentations provided insights into current research projects involving preCICE.

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Furthermore, we once again organized an in-person HPC workshop to support CBRZ users. Over two days, participants received guidance in expert groups to help advance their research activities and address specific challenges in the use of HPC methods and applications. In addition to our quarterly User Meetings, we held nine inspiring talks in our “Computation & Data” seminar series, covering methods and applications in HPC and related fields. We also launched the HPC Café, offering a low-threshold opportunity for researchers to exchange ideas after the seminar while providing peer-to-peer support.

We would like to take this opportunity to sincerely thank all of you for your support in so many different ways and for your continued interest in our project. We wish you a wonderful end to the year and look forward to continuing our exchange with you in 2026.

Conference Activities in the hpc.bw Community

- Amartya Das Sharma @28th Results and Review Workshop of the HLRS, Stuttgart, Germany, 09–10 October 2025
- Samuel Newcome @PARTICLES 2025 Conference & Course, Barcelona, Spain, 18–22 October 2025
- Marius P. Bruchhäuser @GAMM Fachausschuss „Numerische Analysis“, Magdeburg, Germany, 20–21 November 2025

Contact:

hpc.bw – Competence Platform for Software Efficiency and Supercomputing

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