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NEWSLETTER 2026/1

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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 „Computation & Data“ and HPC Café – FT 2026

Date	Speaker & Moderator	Title of Lecture & HPC Café
29.04.2026		
16:00–17:00 (hybrid)	Zhen Li (Clemson University)	Neural Operator Learning Applied to Multiscale Complex Fluids
17:00–18:00 (on-site)	HPC Café with HPC Expert (HSU/UniBw H)	Peer Guidance & User Collaboration
27.05.2026		
16:00–17:00 (hybrid)	Andreas Martin (DIE Bonn)	Using natural language processing in adult education research
17:00–18:00 (on-site)	HPC Café with HPC Expert (HSU/UniBw H)	Peer Guidance & User Collaboration
25.06.2026		
16:00–17:00 (hybrid)	Alexander Kolling (HSU/UniBw H)	Community Based Learning Approaches for HPC Education
17:00–18:00 (on-site)	HPC Café with HPC Expert (HSU/UniBw H)	Peer Guidance & User Collaboration

Cyclopentane Sprays in a Transcritical Environment

Authors: Min Son, Alexander Döhring, Isabelle Veith, Markus Klein, Lars Zigan and Tobias Sander

Within the frame of the MaST (Macro/Micro-Simulation of Phase Decomposition in the Transcritical Regime) project, a collaborative experimental and numerical investigation was conducted to study cyclopentane sprays injected into a high-pressure, high-temperature nitrogen environment. The experiments were conducted in an optically accessible injection chamber that is able to simulate IC engine and rocket-like conditions. The work aimed to clarify how spray structure, phase transition, and mixing behavior vary as conditions change from subcritical to transcritical regimes relevant to high-pressure combustion systems.

On the experimental side, three optical diagnostic techniques were applied; shadowgraphy, Mie scattering, and infrared imaging. Shadowgraphy captured the overall spray structure and spray penetration, while Mie scattering enabled identification of liquid-phase regions and droplet behavior. Infrared imaging provided additional qualitative information on spray evolution after evaporation. Together, these diagnostics allowed the liquid phase, two-phase region, and gas-like spray to be distinguished under varying chamber pressures and temperatures.

In parallel, large-eddy simulations (LES) were performed to numerically investigate the same transcritical spray conditions. The LES employed a real-fluid thermodynamic model based on vapor–liquid equilibrium and compared several subgrid-scale turbulence models; Smagorinsky, Vreman, SES, and WALE. The numerical results provide detailed information on mixing processes, vapor mass fraction evolution, and the extent of the two-phase region, offering further insight into the phase change mechanisms.

Experiments reveal that increasing chamber pressure and temperature shortens the liquid jet penetration and accelerates phase transition. LES predicts similar axial developments of vapor mass fraction and confirms that mixing and evaporative cooling prevent the spray from reaching the critical temperature, even under supercritical ambient conditions.

Current numerical development within the MaST project focuses on transitioning from on-the-fly iterative thermodynamic calculations to a tabulated equation of state methodology. This approach performs complex phase equilibrium calculations once during preprocessing and stores the results in lookup tables, enabling the flow solver to retrieve properties via constant time interpolation during runtime. The method achieves order-of-magnitude computational speedups while simultaneously improving thermodynamic accuracy through the use of high-fidelity equations of state such as GERG-2008 or PC-SAFT, making high-resolution direct numerical simulations of transcritical flows significantly more feasible on HPC systems.

In consequence, this collaboration demonstrates how closely coupled experiments and simulations can enhance the understanding of transcritical spray physics and support the improvement of modern combustion systems.

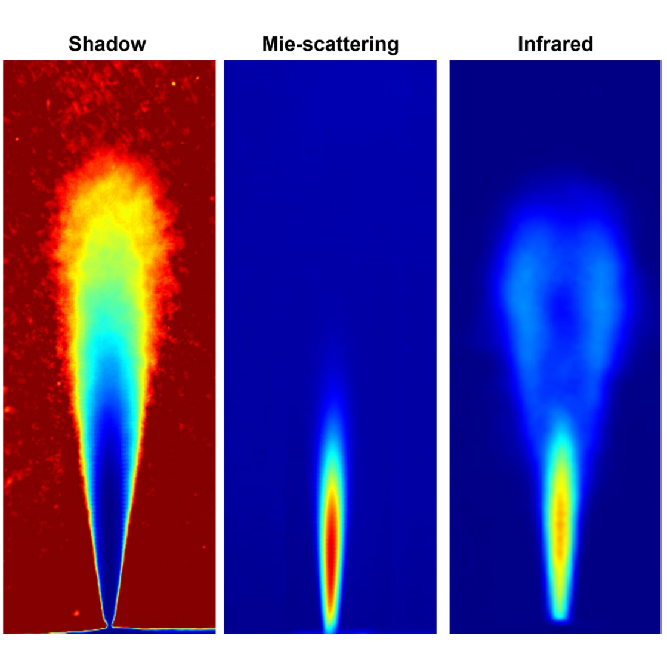


Figure 1: LED illuminator with lens array and diffusive LEDs

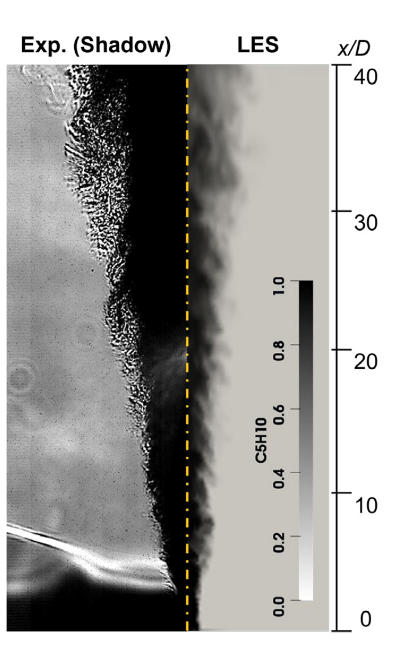


Figure 2: 3.4 µm bandpass filter

Advancing Multigrid Methods for Complex Materials: New Preprint and Collaboration with Sandia National Laboratories

Author: Max Firmbach and Matthias Mayr

Research at the Institute for Mathematics and Computer-Based Simulation (IMCS) of the University of the Bundeswehr Munich continues to advance scalable numerical methods for challenging material simulations. Funded through hpc.bw, our recent preprint entitled “Smoothed aggregation algebraic multigrid for problems with heterogeneous and anisotropic materials” by Max Firmbach, Malachi Phillips, Christian Glusa, Alexander Popp, Christopher Siefert, and Matthias Mayr documents significant progress in the development of robust and efficient solvers for demanding high-performance computing (HPC) applications.

The work addresses a long-standing challenge in smoothed aggregation algebraic multigrid (SA-AMG) methods: the reliable treatment of highly heterogeneous and anisotropic materials. In many large-scale simulations, material parameters vary over several orders of magnitude or exhibit pronounced directional behavior. Conventional multigrid approaches often lack mechanisms to consistently incorporate such detailed material information into the coarsening process, which can lead to severe performance degradation and reduced robustness.

The newly proposed approach introduces a material-aware strength-of-connection measure that explicitly integrates material tensor information into the construction of coarse levels. By embedding physical characteristics directly into the algebraic framework, the approach significantly improves robustness, scalability, and applicability across a broad range of problem classes. Extensive numerical experiments, including both academic benchmark problems and real-world applications such as solar cells or thermally activated batteries, demonstrate reliable convergence behavior even in large-scale simulations.

This work is closely connected to Max Firmbach’s research visit to the Computer Science Research Institute (CSRI) at Sandia National Laboratories in Albuquerque, New Mexico, from September to December 2024. During his stay, he collaborated with leading scientists on high-performance computing projects focusing on multigrid methods for highly anisotropic and heterogeneous materials. The exchange provided an ideal setting to refine methodological ideas, discuss implementation strategies, and further develop the concepts that are now presented in the preprint.

The visit strengthened the collaboration between IMCS and Sandia National Laboratories, one of the United States’ premier research institutions in computational science. Such international partnerships play a crucial role in advancing solver technologies for next-generation scientific computing and in addressing computational challenges at scale. Together, the new preprint and the intensified collaboration with Sandia National Laboratories highlight IMCS’s continued commitment to methodological innovation in multigrid methods, the advancement of high-performance computing within hpc.bw, and the cultivation of strong international research partnerships.

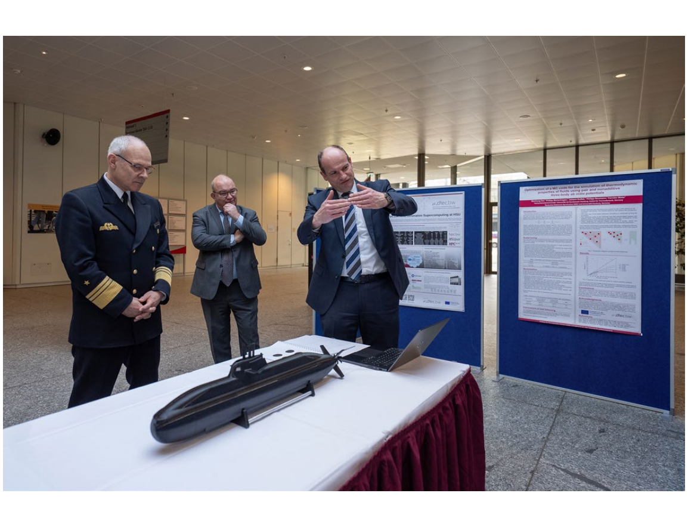
Link to the preprint: https://arxiv.org/abs/2602.05686

Vice Admiral’s Visit to HSU/UniBw H: Insights into hpc.bw Research and SubDesHyHPC

Author: Marie Rathmann

On Thursday, 26 February 2026, Vice Admiral Jan C. Kaack, Inspector of the Navy, visited HSU/UniBw H. During his visit, various research topics and activities at HSU were presented to him, particularly those related to the Navy.

Markus Bause also presented the research activities surrounding hpc.bw. Particular focus was placed on the research activities related to “Submarine Design by Hybrid SciML and FEM HPC,” in which insights are gained through high-resolution 3D HPC simulations of the flow around a submarine’s velocity measurement systems and the subsequent optimization of the height of the velocity measurement system using scientific machine learning.



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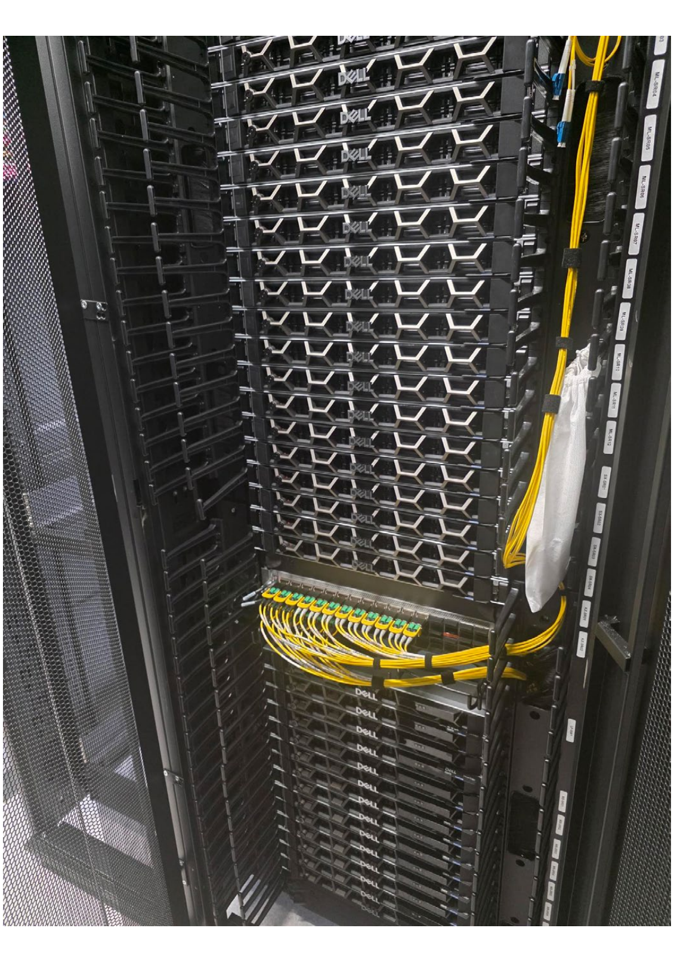
Installation Process: Cerebras CS-3

Author: Piet Jarmatz

Helmut Schmidt University has acquired a two-node Cerebras CS-3 system. This is a cutting-edge AI-focused supercomputer, designed among other HPC applications also for training and using large language models. This system is powered by Cerebras‘ third-generation Wafer Scale Engines, delivering an FP16 peak performance of 125 PFLOP/s through 900 000 for sparse linear algebra optimized compute cores and utilizing 44 GB on-chip SRAM per CS-3. The two-node system supports models with up to 240 billion parameters. For more information, see Cerebras‘ official website: https://www.cerebras.ai

Unlike traditional HPC clusters that employ multiple chips from a single wafer, the CS-3 uses the entire wafer to create one large chip. Although designed with ML applications in mind, the system can also be used for traditional HPC workloads such as computational fluid dynamics (CFD) simulations. However, keep in mind that existing HPC software projects require a re-design run efficiently on the new hardware and software stack (e.g. Cerebras Software Language (CSL) and CSL compilers). In contrast, ML frameworks such as PyTorch and TensorFlow are already supported, making it significantly easier to transition to the CS-3.

In the last week of February, two Cerebras racks were moved into our Container-Based Computing Center (CBRZ), marking the beginning of the installation process. Over the next weeks, more work will be performed on the hydraulic systems to ensure a stable environment and sufficient cooling for the CS-3 supercomputer. This work will result in a temporary shutdown of HSUper. We aim to have the CS-3 units up and running for beta testers in May 2026.



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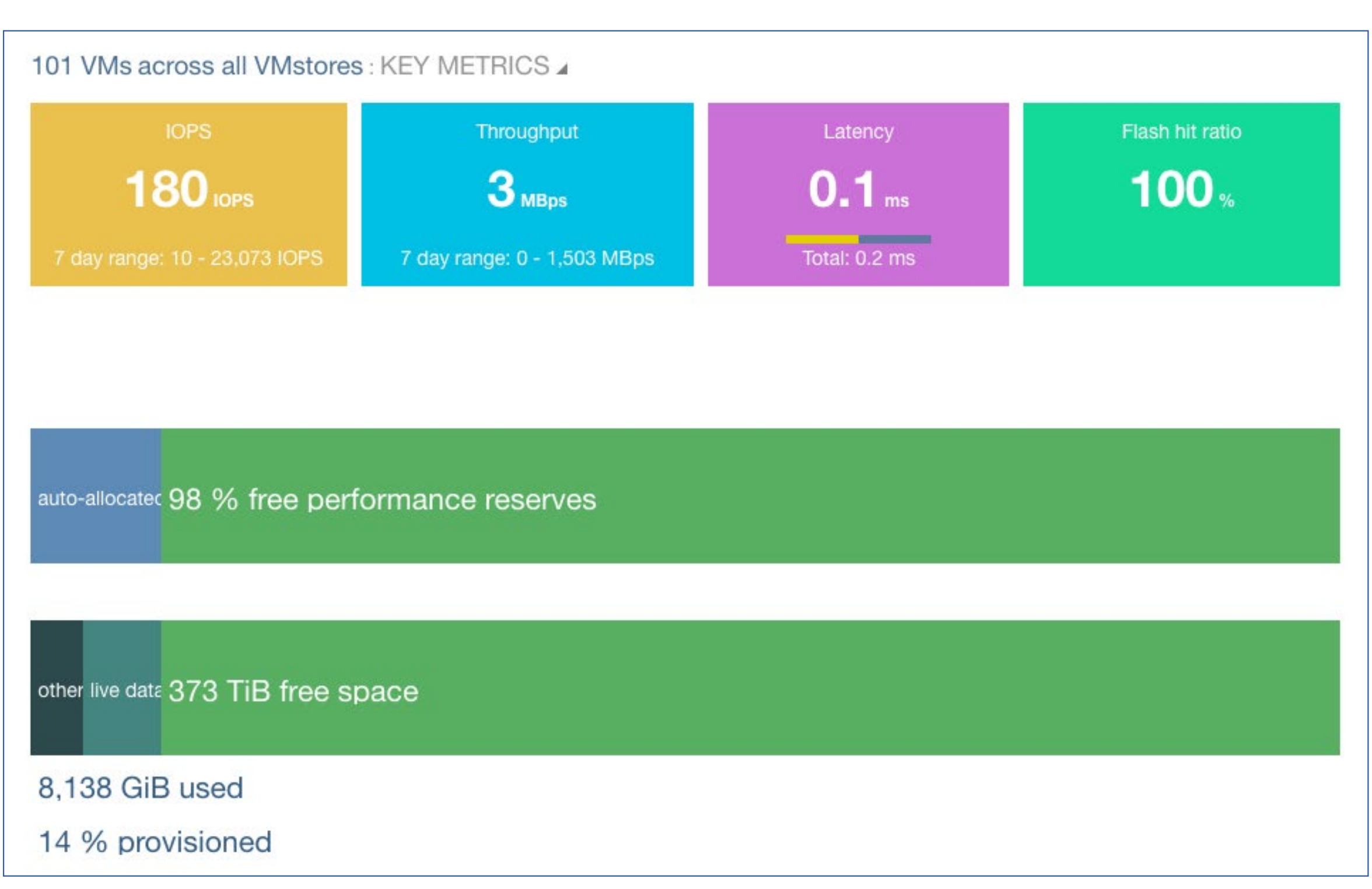
New Storage Systems: HSUper Backup and Fast Flash ISCC Storage now online

Author: Piet Jarmatz

We are happy to announce that two new storage systems went into operation!

All HSUper users have now access to an additional file system designed specifically for backups. This new storage system, which can be found using the $BACKUP environment variable, built on top of ZFS, provides excellent data resilience and automatic snapshots of stored files. A key feature of this backup storage configuration is its ability to retain deleted data for a period of 30 days, from once per night created snapshots. For the past two years, monthly snapshots are kept. This provides an additional layer of protection for research data. Note that HSUper users are responsible for backup of their own data. The backup storage must be used manually, no automatic backup service is provided for other file systems. The backup storage has a netto capacity of 1300 TB on the hard disk drives. Thanks to automatic compression, we expect to be able to store up to 2000 TB of data.

Users of the Interactive Scientific Computing Cloud (ISCC) can now enjoy improved performance, thanks to our new flash-based dedicated storage system. This upgrade is designed for running a very large number of virtual machines (VMs) in parallel. It significantly accelerates virtualization management, making tasks such as cloning a VM remarkably faster and more efficient. Cloning a VM now takes only seconds, instead of several hours or even days. The hardware is based on fast solid-state drives and provides a usable raw capacity of ca. 380 TB, plus compression and deduplication. Our benchmarks measure an 11.5x times increased R/W-bandwidth for file operations inside VMs, compared to the previous storage system.



101 VMs across all VMstores : KEY METRICS

IOPS	Throughput	Latency	Flash hit ratio
180 IOPS	3 MBps	0.1 ms	100 %
7 day range: 10 - 23,073 IOPS	7 day range: 0 - 1,503 MBps	Total: 0.2 ms	

auto-allocated 98 % free performance reserves

other live data 373 TiB free space

8,138 GiB used

14 % provisioned

Figure 3: Overview of live performance data from new ISCC storage. A throughput of up to 1503 MByte/s has been reached here.

Review: Driving Interdisciplinary HPC Research Forward – hpc.bw Annual Meeting 2026

Author: Marie Rathmann

On 24–25 February 2026, the annual Full Project Meeting of the hpc.bw project took place at HSU/UniBw H. The event was hosted in the Thomas-Ellwein-Saal.

The first day focused on computational science with a strong emphasis on modeling and HPC. Philipp Neumann and Karsten Meier presented the current status of MaST; Markus Bause and Michael Breuer provided insights into Multiscale & Multiphysics; Andreas Fink introduced the Logistics work package; and Matthias Mayr reported on recent developments in Research Software Engineering.

In the afternoon, a poster session created space for professional exchange, in-depth discussions of current research questions, and an intensive dialogue on future research perspectives. The day concluded with a joint dinner in a collegial atmosphere, offering opportunities for informal networking.

The second day highlighted key aspects of the sustainable and high-performance operation of high-performance computing ecosystems. Shashini Wanniarachchi and Ruben Horn presented progress within the Energy Efficiency work package, while Piet Jarmatz reported on Infrastructure. Sabine Schmidt-Lauff outlined perspectives on a learning-oriented and competence-based approach to working with these systems within the HPC Competence Platform work package. Marie Rathmann provided insights into the ongoing Project Activities and an outlook on the project’s planned research activities for 2026.

Once again, the meeting demonstrated how diverse, dynamic, and interdisciplinary hpc.bw is – and how valuable personal exchange remains for the project’s collective success.

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HPSF Community Summit 2026 at TU Braunschweig

Author: Matthias Mayr

© Matthias Mayr

The first edition of the HPSF Community Summit brought together 28 participants from Europe and the United States for a focused exchange on high-performance simulation frameworks and their evolving ecosystem. The workshop provided a platform for developers and users to discuss recent advances, strategic directions, and emerging challenges in scientific computing. The event took place at TU Braunschweig on Feb 25 - 27, 2026. It was organized under the umbrella of the High Performance Software Foundation (HPSF, https://hpsf.io). HPSF supports projects that advance portable software for diverse hardware by increasing adoption, aiding community growth, and enabling development efforts. HPSF is lowering barriers to productive use of today’s and future high-performance computing systems. It is part of the nonprofit Linux Foundation. The workshop has been co-organized by Dr. Matthias Mayr, highlighting hpc.bw‘s commitment to sustainable research software development for high-performance computing.

A central component of the workshop program was a series of project updates from key initiatives within the HPSF landscape: Trilinos, Spack, Kokkos, AMReX & WarpX. Core developers presented recent technical developments, ongoing refactoring efforts, performance portability strategies, and roadmap perspectives. These updates stimulated in-depth discussions on interoperability, sustainability, and community governance.

In addition to the project overviews, the workshop featured numerous developer and user talks. These contributions highlighted practical experiences, integration strategies, application case studies, and lessons learned in deploying modern simulation software on contemporary HPC architectures. The diversity of perspectives ranging from framework design to domain-specific applications fostered constructive exchanges between software architects and end users.

A particular highlight of the summit was the keynote lecture by Prof. Hartwig Anzt (TU Munich) entitled “Hardware is Changing – Do We Need to Change the Way We Design Simulation Software?” The keynote addressed the rapidly evolving hardware landscape, including heterogeneous architectures and accelerator-based systems. It particularly shed light on the recent trend of increasing lower-precision GPU architectures designed for AI / ML workloads and explored their impact on software development for high-performance scientific computing.

Overall, the HPSF Community Summit successfully strengthened connections within the community, encouraged cross-project dialogue, and reinforced the importance of collaborative development in sustaining high-performance simulation software. The discussions underscored both the technical progress achieved and the strategic challenges that lie ahead as hardware architectures and scientific demands continue to evolve.

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