hpc.bw NEWSLETTER 2026/2

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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

Community Contributions – Share your HPC Expertist

Author: Alexander Kolling

HPC competencies are rarely acquired through formal education alone. Instead, researchers typically build their expertise gradually while working on their own projects, by solving technical problems, consulting various forms of soft- and hardware documentation, exchanging ideas with other colleagues, participating workshop formats, using online tutorials or simply through experimenting with software and learning from trial and error. Over time, this process results in highly specialized knowledge that is closely connected to discipline-specific research questions, software environments, and computational methods.

However, much of this knowledge remains personal and project specific. Solutions to recurring problems, successful workflows, software configurations or methodological insights often stay within individual research groups and are rarely documented in a way that allows other to benefit from them. As a consequence, new HPC users frequently face the same learning barriers and invest considerable time in solving problems that have already been addressed elsewhere.

From an educational perspective, sustainable competence development therefore depends not only on providing learning materials but also on creating opportunities for researchers to share, document and continuously refine their practical knowledge within the HPC community. For hpc.bw that means working towards a mentality best described as knowledge transfer becoming a collaborative process rather than an individual achievement.

To support this idea, the HPC Portal has been designed as a collaborative platform for community-driven learning resources. Members of the HPC community can contribute documentation, tutorials, software-specific guides, best practices, project reports and self-study materials, allowing valuable experience to become accessible far beyond individual research projects.

To make contributing as easy as possible, we have also created dedicated documentation pages explaining the available contribution formats, the submission workflow and practical examples:

- General Information
- Available Contribution Formats
- Contribution Workflow

To make contributions even easier for you, we are here to provide hands-on support and help you transfer your practical insights and expertise into fully developed learning materials: hpc-portal@hsu-hh.de.

Calculation of Surface Tension of Fluids in Vapour-Liquid Equilibrium

Authors: Johann A. Duffek, Philipp Neumann, Philipp Marienhagen & Karsten Meier

Our aim within the MaST project (Macro/Micro-Simulation of Phase Decomposition in the Transcritical Regime) is the development of a general workflow to accurately determine the surface tension and vapour pressure of pure substances via direct molecular simulations. We apply Metropolis-Hastings Monte Carlo simulations and utilize highly accurate ab initio pair and nonadditive three-body potentials to describe the intermolecular interactions.

We extended an inhouse Monte Carlo code for simulations of single phase liquids or gases in a cubic container, which was optimized in the BMBF funded project 3xa, to inhomogeneous simulation domains in a rectangular container. The extension was accompanied by a stronger modularization of the code and a further optimization of the subroutine for the calculation of the distances between the particles by saving more redundant algebraic operations. Furthermore, we implemented the calculation of the surface tension according to Goujon et al. [1] for pair and three-body interactions. This also required the calculation of the density profile perpendicular to the vapour-liquid interface and the direction dependent pair distribution function. We account for quantum effects semiclassically by the Feynman-Hibbs corrections to the pair potential.

A separate program has been developed to estimate the long-range corrections for interactions beyond the simulation cutoff radius that are not calculated explicitly by a Monte Carlo integration to take the inhomogeneous nature of the simulation domain into account.

First validation calculations for argon with the potentials of Jäger et al. [2, 3] yielded values for the surface tension close to experimental results. Our next steps include several simulation campaigns to study the influence of simulation parameters on the results for the surface tension, the implementation of the calculation of the vapour pressure, as well as the implementation of accurate ab initio potentials for further substances such as neon, krypton, nitrogen, and carbon dioxide.

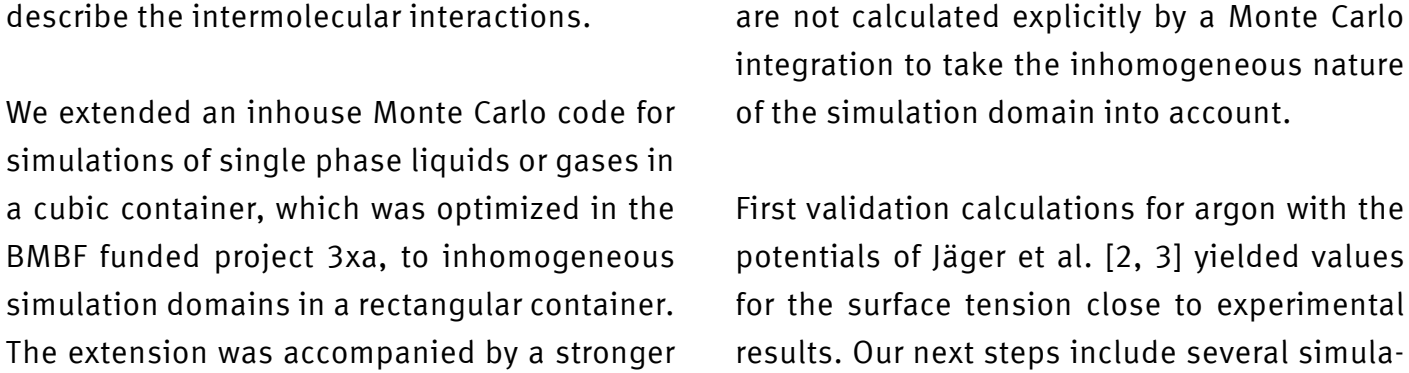

Figure 1: Average density distribution in a vapour-liquid simulation domain and particle positions in the last sampling cycle of a simulation for argon at 120 K

References

[1] Goujon, F., Malfreyt, P., & Tildesley, D. J. (2014). The gas-liquid surface tension of argon: A reconciliation between experiment and simulation. Journal of Chemical Physics, 140(24), 244710. Doi: 10.1063/1.4885351

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[3] Jäger, B., Hellmann, R., Bich, E., & Vogel, E. (2011). Ab *initio* virial equation of state for argon using a new nonadditive three-body potential. Journal of Chemical Physics, 135(8), 084308. DOI: 10.1063/1.3627151

GABLER Naval Technology Group AG meets HSU/UniBw H

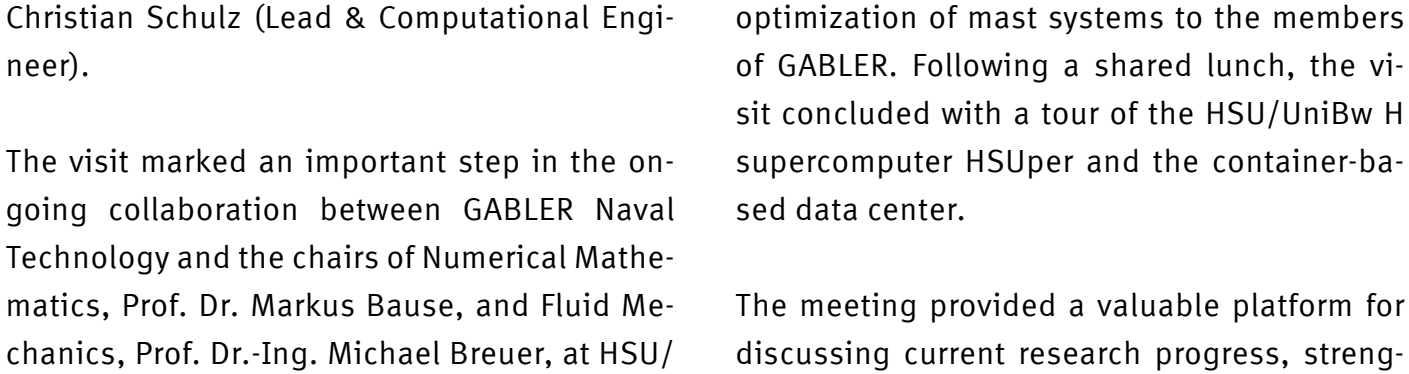
Authors: Marius P. Bruchhäuser & Markus Bause

On February 27, GABLER Naval Technology Group from Lübeck, a world market leading company for naval and submarine technology visited Helmut Schmidt University/University of the Federal Armed Forces Hamburg (HSU/UniBw H). The delegation from GABLER included Alexander Homrich (Director Subsea Drives), Bastian Boger (Head of Design), Christian Lux (Surface Treatment Inspector), and Christian Schulz (Lead & Computational Engineer).

The visit marked an important step in the ongoing collaboration between GABLER Naval Technology and the chairs of Numerical Mathematics, Prof. Dr. Markus Bause, and Fluid Mechanics, Prof. Dr.-Ing. Michael Breuer, at HSU/UniBw H, focusing on elucidation of flow phenomena and shape optimization of submarine mast systems. Research results from two Bachelor’s theses, conducted in autumn 2025 by the mechanical engineering students F. Jung and A. Korell, were presented. F. Jung analyzed flow around mast systems by advanced numerical simulation methods. A. Korrell conducted experimental studies of flow around innovative mast systems shapes in the laboratory of the Chair of Hydraulic Engineering, Prof. Dr.-Ing. Mario Oertel, who co-supervised the thesis.

The visit started with a tour in the laboratory of the Chair of Hydraulic Engineering in Glinde, guided by M. Oertel. The performance of the laboratory experimental setup, used by A. Korell for his investigations, was demonstrated to the participants. Afterwards, the group returned to HSU/UniBW H, where F. Jung and A. Korell, presented their theoretical and experimental results on the shape optimization of mast systems to the members of GABLER. Following a shared lunch, the visit concluded with a tour of the HSU/UniBw H supercomputer HSUper and the container-based data center.

The meeting provided a valuable platform for discussing current research progress, strengthening existing partnerships, and identifying promising new research directions. Particular emphasis was put on the use of high-performance computing and computational fluid dynamics to enable efficient and reliable analysis of complex flow processes. The exchange laid the groundwork for future joint projects and the further expansion of collaborative research activities.



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New Publication: Trilinos Enables Sustainable Scientific Computing on Modern Supercomputers

Author: Matthias Mayr

Researchers from Universität der Bundeswehr München and international partner institutions have published a comprehensive overview article on the open-source software framework _Trilinos_ in the journal _ACM Transactions on Mathematical Software_.

The article, “Trilinos: Enabling Scientific Computing across Diverse Hardware Architectures at Scale”, presents the current state of Trilinos, one of the world’s leading software ecosystems for large-scale scientific computing. Trilinos (https://trilinos.github.io) provides reusable building blocks for the development of simulation software and supports modern heterogeneous high-performance computing systems, including CPU- and GPU-based supercomputers. The typical use of Trilinos is on leadership-class systems with new or emerging hardware architectures, for example the currently fastest exascale machines such as _El Capitan_ at Lawrence Livermore Laboratory (USA) or _Frontier_ at Oak Ridge National Laboratory (USA) (https://top500.org).

The publication highlights how modern Trilinos builds on the Kokkos ecosystem to achieve performance portability across diverse hardware architectures. At the same time, it documents the community-driven development model that enables researchers from universities, national laboratories, and industry to collaborate on a shared software infrastructure for next-generation scientific computing.

Within the hpc.bw project, methodological developments are contributed directly to Trilinos. This strategy ensures that research results are not limited to a single application code but become available to a broad international community. By integrating algorithms and software components into a sustainable open-source framework, hpc.bw strengthens software reuse, long-term maintainability, and scientific reproducibility.

The work was carried out in collaboration with researchers from Sandia National Laboratories (USA), Delft University of Technology (Netherlands), the University of Liège (Belgium), NVIDIA, AMD, and other international partners. The article also acknowledges support from dtec.bw – Digitalization and Technology Research Center of the Bundeswehr through the project hpc.bw.

© Trilinos

Reference

Mayr, M., Heinlein, A., Glusa, C., Rajamanickam, S., et al. (2026). Trilinos: Enabling Scientific Computing across Diverse Hardware Architectures at Scale. ACM Transactions on Mathematical Software, 52(2), Article 12. DOI: 10.1145/3802822

Upcoming: HPC-Driven Decision Science @ NHR Conference ‘26

Author: Andreas Fink

The NHR Conference ’26 brings together high-performance computing users and providers. It is organized by the NHR Alliance, a national network of high-performance computing centers in Germany. This year’s main topics are “Advances in Atomistic Simulations,” “Low and Mixed-Precision Computing for Simulation and AI,” and “HPC-Driven Decision Science: Optimization, Simulation, and AI for Economics and Management”. For the latter topic, which is co-organized by the Gesellschaft für Operations Research (GOR), Andreas Fink from HSU/UniBw H and the hpc.bw project serves as a member of the scientific committee of the conference. The topic addresses computational challenges in application areas ranging from energy grids and supply chains to volatile financial markets, as well as techno-economic and environmental dynamics. It explores the frontier of high-performance decision intelligence at the intersection of large-scale data processing, complex simulation, and rigorous optimization. Envisioned submissions use high-performance computing to solve high-dimensional problems in economics and operations research, including scalable agent-based modeling, discrete-event simulation, and multi-level mathematical optimization. Contributions may also address reproducible HPC workflows that integrate simulation with machine learning, such as simulation optimization and digital twins, as well as LLM-augmented pipelines for scenario generation and policy analysis. Such contributions may also address the technical challenges of efficient execution on heterogeneous HPC architectures. Key application areas include transportation and logistics, market design, finance, risk management, macroeconomics, and public-sector resilience.

The scientific part of the NHR Conference ’26 will take place on September 14–15, 2026, at the Heinz Nixdorf MuseumsForum in Paderborn, in collaboration with PC2 (https://www.nhr-verein.de/conference).

New Publication: Supporting Competence Development and Problem Solving in High Performance Computing

Author: Alexander Kolling

In another article of this newsletter, we emphasize the importance of sharing knowledge, experiences and successful approaches within the HPC community. While community contributions enable the continuous exchange of practical expertise, we are pleased to present another step towards documenting and disseminating knowledge: the publication of our new anthology *Supporting Competence Development and Problem Solving in High Performance Computing – Insights inti Performance Engineering Projects from an Educational Perspective*.

This volume brings together final reports from Performance Engineering Projects carried out within the hpc.bw project between 2021 and 2025. It documents how researchers from different scientific disciplines addressed computational challenges with the support of HPC experts and highlight strategies for improving software performance, scalability, and the efficient use of HPC resources.

Beyond the technical solutions, the anthology also illustrates the educational dimension of these projects. Each contribution reflects how interdisciplinary knowledge transfer enabled researchers to successfully integrate HPC methods into their own scientific work. Additionally, we added an introductory chapter from an educational perspective to frame the performance engineering projects in context of HPC education in general. Finally, we would like to highlight the very well written preface by Philipp Neumann and Johann Duffek, who conceived and established the PE-projects.

We hope this publication will not only document the achievements of hpc.bw but also serves as a valuable resource and source of inspiration for future HPC users, educators, and researchers.

You can access the anthology via the following DOI: 10.24405/23823 // https://openhsu.ub.hsu-hh.de/handle/10.24405/23823.
Feel free to share the anthology with others.

Review: HSUper Workshop April 23—24, 2026

Author: Shashini Wanniarachchi

Annually, hpc.bw project organizes a variety of workshops aimed at supporting skill development among HSUper and ISCC users. Continuing this tradition, this year, the HSUper workshop took place on 23rd and 24th of April, at the Helmut Schmidt University/University of the Federal Armed Forces Hamburg (HSU/UniBw H). This year’s workshop primarily focused on encouraging students and staff at HSU to start integrating HSUper resources in their respective research work. At the same time, experienced users who had already been using HSUper were also invited to participate. In line with the main objective of the workshop, the content was designed around setting a strong foundation about HPC and HSUper for new users. For example:

- How to login to HSUper, transfer data, manage folders and storage space.
- How to interact with the system using the web interface or Linux-based terminal.
- How to load existing software modules and install required software packages.
- How to create new jobs, run them, and monitor progress.

A total of 16 participants attended the workshop, including complete beginners interested in exploring HPC systems, students planning to utilize HPC resources in their upcoming projects and theses work as well as advanced users seeking support for specific issues related to their projects. To provide on-site support and guidance, six HSUper experts from the Chair of High Performance Computing at HSU also took part in the workshop on both days.

First day of the workshop began with an introductory session conducted by the Head of HPC Lab, Piet Jarmatz. This was an interactive session with the participants and introduced the fundamental concepts of high performance computing starting with the historical background and addressing the wide range of application areas. In addition, the participants were given an overview of the container based computing centre (CBRZ) familiarizing them with HSUper and introducing the soon expected upgrade, HSUpreme. This session concluded with an ice-breaking session among the participants. The second half of day one was focused on giving the participants hands-on experience in working with HSUper through the workshop tasks, which are available on the HPC Portal (Training | HPC Portal). Following the introduction to accessing HSUper and navigating the Linux terminal, participants got to explore topics of data transfer, understanding the storage systems and the underlying hardware architecture towards the end of day one.

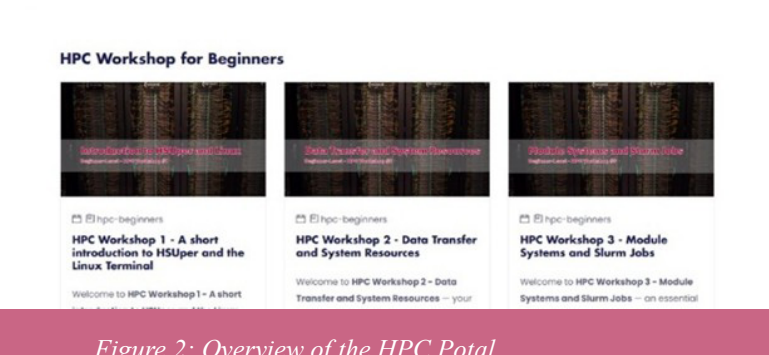


Figure 2: Overview of the HPC Potal

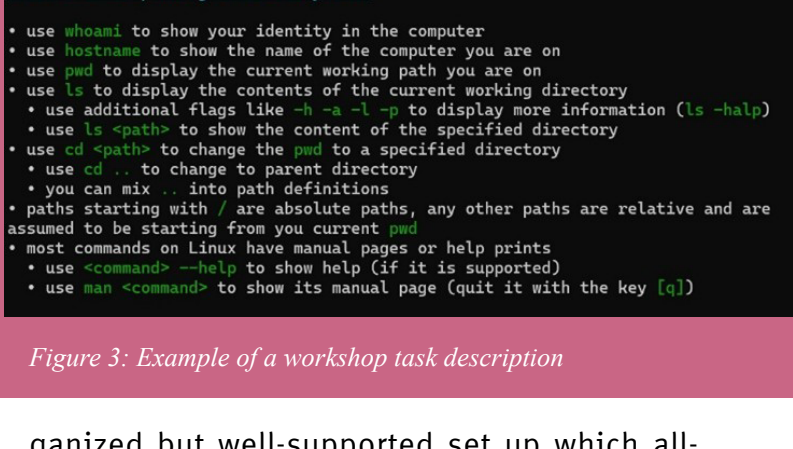


Figure 3: Example of a workshop task description

After a successful first day of the participants gaining the beginner knowledge on HSUper, the day two of the workshop transitioned towards more advanced topics through presentations delivered by HPC experts, Ruben Horn and Hauke Preuß. The sessions covered the topics of module system and Slurm job submissions along with job priorities, dependencies, checkpointing, and related concepts. These topics are highly relevant and essential for efficiently utilizing HPC resources, as they help users better understand Slurm messages, what could hinder a job from running and limitations set by HSUper.

At the end of the two-day workshop, participant feedback highlighted the value of self-organized but well-supported set up which allowed them to work through the tasks on their own pace, deepen their knowledge independently, and gain practical experience instead of passively following demonstrations. One of the most appreciated, and a new tool introduced in this year’s workshop was the workshop game. This allowed the participants to track their progress and compare it with the others while serving as a feedback mechanism for the organizers to identify topics that require additional discussion or support. This optional game was designed with a score for each completed workshop task and the participants mentioned this was highly motivating and encouraging them to actively engage with the workshop tasks.

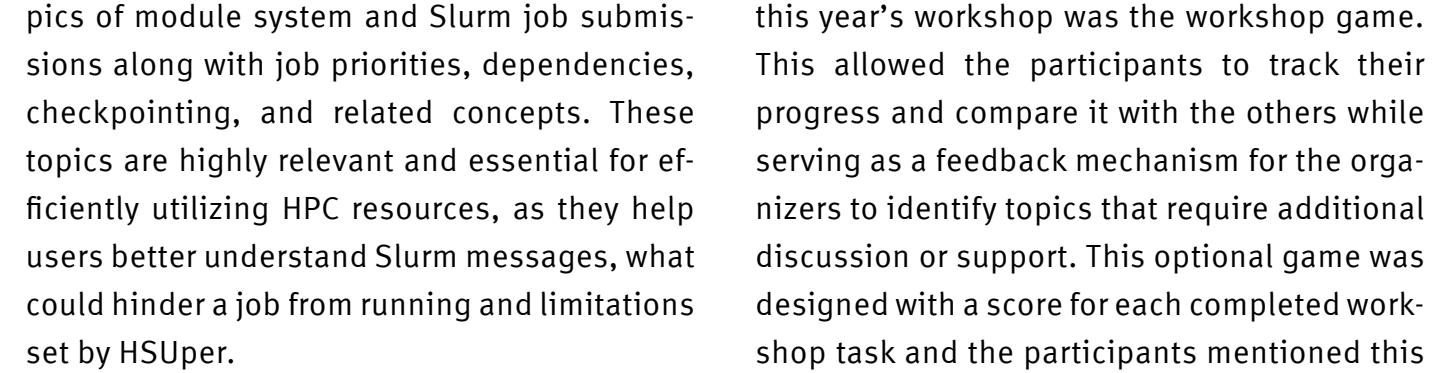


Figure 4: Workshop game demonstration

hpc.bw @ 96th Annual Meeting of the International Association of Applied Mathematics and Mechanics (Gamm 2026) in Stuttgart, Germany

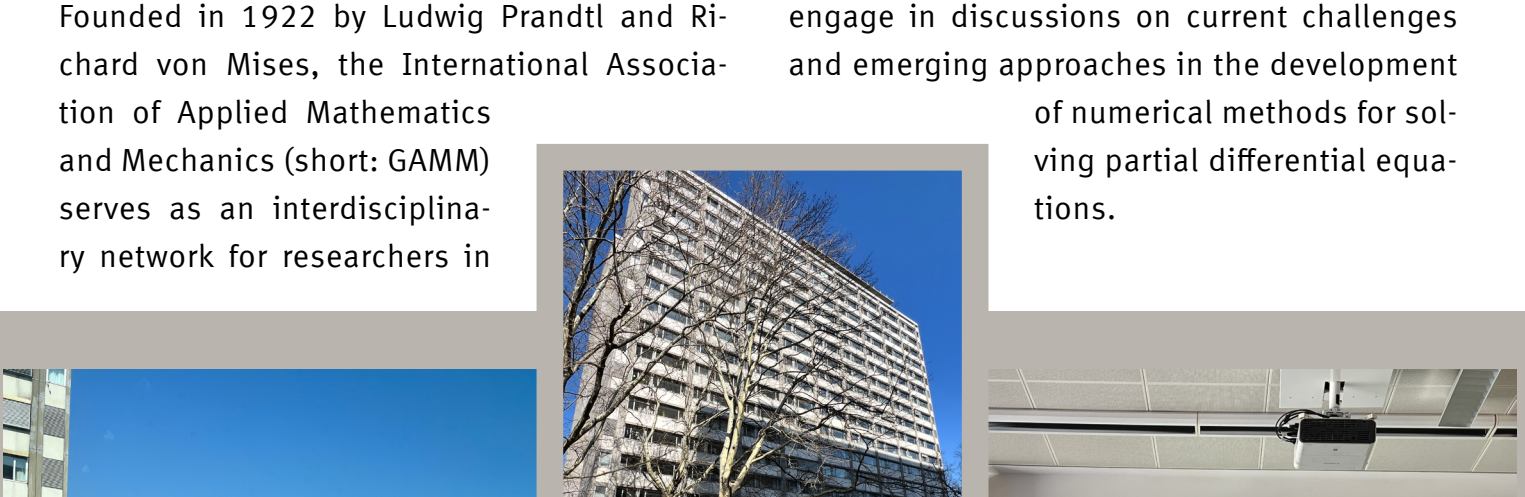
Author: Marius P. Bruchhäuser

hpc.bw made a strong appearance at the Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2026), held from March 16–20 in Stuttgart, Germany. Researchers from hpc.bw contributed three presentations, showcasing recent advances in numerical methods and scientific computing:

- Markus Bause: *On geometric multigrid convergence and its application to space-time FEM.*
- Marius Paul Bruchhäuser: *Goal-oriented adaptivity and multigrid techniques for flow problems.*
- Pavel Shamko: *Numerical approximation of the the dynamic poroelasticity equation in first order form.*

Founded in 1922 by Ludwig Prandtl and Richard von Mises, the International Association of Applied Mathematics and Mechanics (short: GAMM) serves as an interdisciplinary network for researchers in applied mathematics, mechanics, and related fields. The Annual Meeting is one of Europe’s leading scientific conferences in applied mathematics, mechanics, and computational science. With more than 1,000 participants from academia and industry, the event provides a platform for presenting cutting-edge research, exchanging ideas, and discussing the latest developments in numerical methods, simulation, and high-performance computing.

All three contributions were presented within Section 18: Numerical Methods for Differential Equations, one of 28 scientific sections featured at the conference. The session provided an excellent opportunity to present recent research results to a specialized audience and to engage in discussions on current challenges and emerging approaches in the development of numerical methods for solving partial differential equations.



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1st Stuttgart Research Software Day and 6th Conference for Research Software Engineering in Germany (deRSE26)

Author: Willi Leinen

The 1st Stuttgart Research Software Day took place on March 2, 2026, at the University of Stuttgart. Our contribution was a poster titled “xbat–An easy-to-use and universally applicable benchmarking automation tool for HPC software within the project hpc.bw (dtec.bw)”.

This event was followed by the deRSE26 conference, held from March 3 to 5, 2026. The slides of our talk, “Easy, collaborative benchmarking with the extended benchmarking automation tool xbat”, are available here. At the end of the conference, we attended a guided tour of the HLRS (High-Performance Computing Center Stuttgart), where we saw their first supercomputer, a Cray-2, as well as their current flagship supercomputer, Hunter.

© Willi Leinen
Figure 5: Cray-2 (fastest computer in 1985)

Figure 6: Hunter (Rank 61 in TOP500 List 11/2025)

German Operations Research Society (GOR) Workgroup “Practice of Mathematical Optimization” (PMO) Meeting on “High Performance Computing”

Author: Willi Leinen

The 110th meeting of the GOR workgroup PMO, held in Bad Honnef from March 12 to 13, 2026, focused on the topic High Performance Computing. We contributed a talk titled “Computational Insights into Solving Optimization Instance Sets with MIP Solvers on Multi-Core Hardware”. All talk titles and abstracts are available here.

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.

“High Performance Computing”

– Willi Leinen @1st Stuttgart Research Software Day, Stuttgart, Germany, 02 March 2026

– Willi Leinen @6th Conference for Research Software Engineering in Germany (deRSE26), Stuttgart, Germany, 03–05 March 2026

– Willi Leinen @110th meeting of the GOR working group “Practice of Mathematical Optimization” with the topic “High Performance Computing”, physics center Bad Honnef (DPG – Deutsche Physikalische Gesellschaft), Bad Honnef, Germany, 12–13 March 2026

– Guillaume De Nayer @DLES15 (ERCOFTAC workshop Direct & Large Eddy Simulation), Delft, Netherlands, 22–22 May 2026

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