hpc.bw NEWSLETTER 2026/3

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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 „Computation & Data" and HPC Café, HT2026

Time		Speakers	Title of Lecture
28.10.2026; Seminar Room H1 - 0308			
16:00-17:00	Scientific Talk	Piet Jarmatz (HSU/UniBw H)	Parallel in Time Molecular-continuum Flow Simulation
17:00-18:00	HPC Café	Ruben Horn (HSU/UniBw H)	Energy Efficiency
25.11.2026; Seminar Room H1 - 0308			
16:00-17:00	Scientific Talk	Alexander Kolling (HSU/UniBw H)	Learning through Communities of Practice in interdisciplinary High Performance Computing: An Adult Education Perspective
17:00-18:00	HPC Café	Willi Leinen (HSU/UniBw H)	Mathematical Optimization Software
16.12.2026; Seminar Room H1 - 0308			
16:00-17:00	Scientific Talk	Piet Jarmatz (HSU/UniBw H	HSUper goes SUPREME!
17:00-18:00	HPC Café	Hauke Preuß (HSU/UniBw H)	System Administration

Six Months in Perth: Robots That Need to Know What to Do

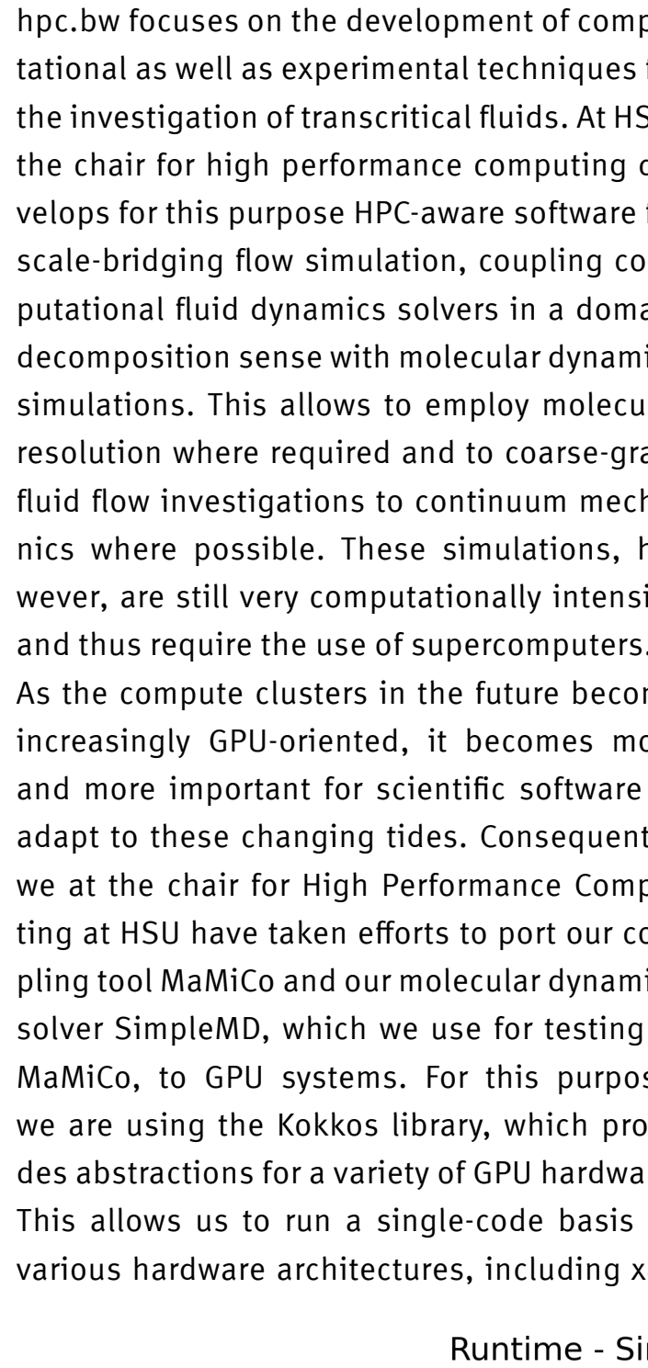
Research Stay at the University of Western Australia, July 2026 to January 2027

Author: Fabian Deuser

Since July 2026 I have been spending six months at the University of Western Australia in Perth, in Prof. Thomas Bräunl's Robotics and Automation Lab. The stay is funded through the Young Researcher Program of the hpc.bw project (dtec.bw), which supports research stays abroad for academic staff at UniBw M and HSU/UniBw H. The Thomas lab has two strands. The older one is autonomous driving: the group develops the control system of a driverless shuttle bus that operates on campus. The newer one is humanoid robots, since recently two Unitree G1 units of roughly child height. I work on the second strand, together with PhD and master's students from the group.

Robots have been executing fixed, pre-programmed routines reliably for decades. An industrial arm repeats the same motion millions of times, as long as its environment does not change. What is new is that neural networks, so-called vision-language-action models, are slowly making robots useful for general tasks, meaning tasks that nobody programmed in advance. The difficult part is transferring these models to real hardware, and that is where my work sits. Three questions guide it. Which motions can a robot perform at all, given a body plan that differs from a human one? What data does it need in order to learn them? And how do we present its surroundings so that the model can derive a sensible action from them?

What interests us at the moment is reaction: how a robot copes when its surroundings change while it is acting, instead of following a plan fixed in advance. Someone steps into its path, or an object it was about to reach for is moved. People handle this without thinking about it, and recordings of human movement are one of the few sources that capture how. That is why we collect motion data in the first place.



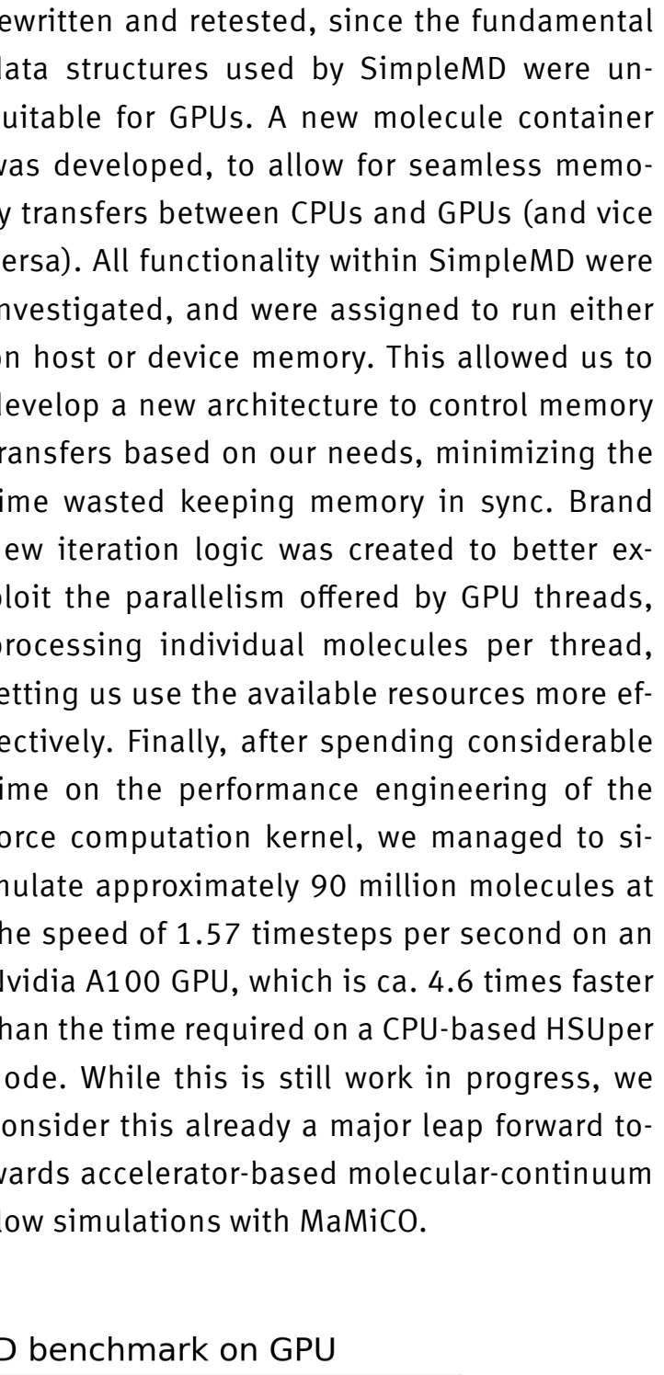
© Fabian Deuser

Fabian Deuser with the two Unitree G1 humanoids in the Robotics and Automation Lab at UWA.

We collect it in two ways. The first is a motion capture suit, borrowed for this purpose, which records a person's posture continuously while they move. Those recordings cannot be sent to the robot directly, because its limb lengths, joint limits and mass distribution differ from ours. A retargeting step maps the human posture onto the robot's joint structure, and a physics simulation then shows which of the resulting motions the machine could execute without losing its balance. The second way avoids that gap: an operator wears a VR headset and teleoperates the robot, so the recorded motion already belongs to the robot's own body. To evaluate what we get, we compare the executed motion against the reference and note where and why the two drift apart. The systematic failures are the interesting ones, because they usually point to something missing in the data rather than in the model.

Training is the step at which computing power becomes the binding constraint. Vision-language-action models carry billions of parameters, and adapting one to our recorded motion data takes days of GPU time on hardware well beyond a single workstation. That is the direct link to hpc.bw: without high-performance computing resources, the data collected here could not be turned into a working model.

Perth lies a good 2,000 kilometres from the next comparably large city, and that shapes daily life more than I had expected, without a car you get almost nowhere. A first trip therefore took me to the Pinnacles in Nambung National Park, two and a half hours of driving during which, after a while, you see nothing but the road and the landscape. In the city itself I was surprised by the size of the local Magic: The Gathering scene, a collectible card game with an organised tournament circuit, which I now play regularly.



© Fabian Deuser

The Pinnacles in Nambung National Park, about two and a half hours' drive north of Perth.

GPU-Driven Molecular Dynamics Using SimpleMD

Author: Amartya Das Sharma

The MaST work package (work package 6) in hpc.bw focuses on the development of computational as well as experimental techniques for the investigation of transcritical fluids. At HSU, the chair for high performance computing develops for this purpose HPC-aware software for scale-bridging flow simulation, coupling computational fluid dynamics solvers in a domain decomposition sense with molecular dynamics simulations. This allows to employ molecular dynamics for detailed investigations of the fluid flow investigations to continuum mechanics where possible. These simulations, however, are still very computationally intensive and thus require the use of supercomputers. As the compute clusters in the future become increasingly GPU-oriented, it becomes more and more important for scientific software to adapt to these changing tides. Consequently, we at the chair for High Performance Computing at HSU have taken efforts to port our coupling tool MaMiCo and our molecular dynamics solver SimpleMD, which we use for testing in MaMiCo, to GPU systems. For this purpose, we are using the Kokkos library, which provides abstractions for a variety of GPU hardware. This allows us to run a single-code basis on various hardware architectures, including x86 and GPUs. Most of the functionality had to be rewritten and retested, since the fundamental data structures used by SimpleMD were unsuitable for GPUs. A new molecule container was developed, to allow for seamless memory transfers based on needs, minimizing the transfers between CPUs and GPUs (and vice versa). All functionality within SimpleMD were investigated, and were assigned to run either on host or device memory. This allowed us to develop a new architecture to control memory transfers based on needs, minimizing the time wasted keeping memory in sync. Brand new iteration logic was created to better exploit the parallelism offered by GPU threads, processing individual molecules per thread, letting us use the available resources more effectively. Finally, after spending considerable time on the performance engineering of the force computation kernel, we managed to simulate approximately 90 million molecules at the speed of 1.57 timesteps per second on an Nvidia A100 GPU, which is ca. 4.6 times faster than the time required on a CPU-based HSUper node. While this is still work in progress, we consider this already a major leap forward towards accelerator-based molecular-continuum flow simulations with MaMiCo.

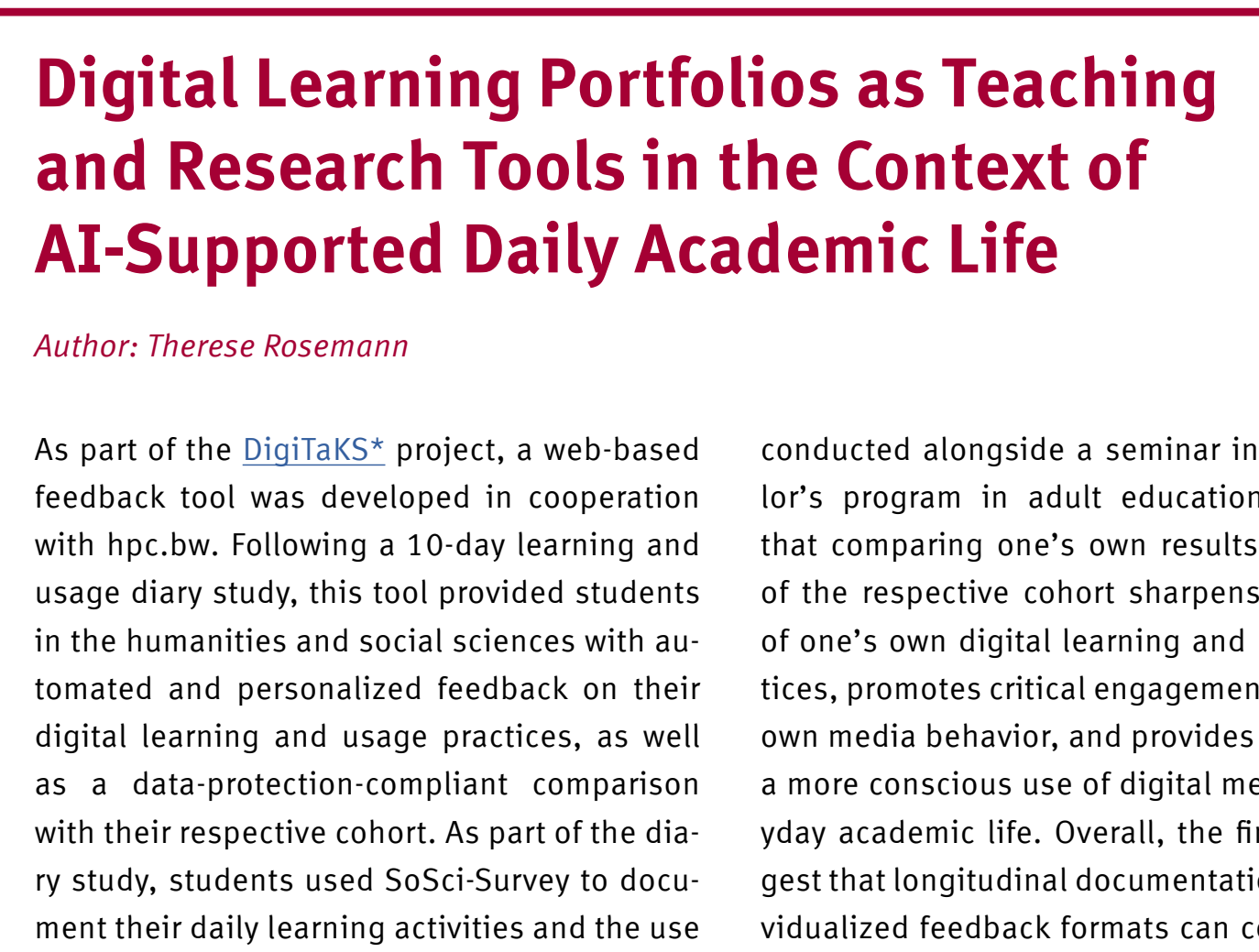


Figure 1: Runtime – SimpleMD benchmark on GPU

Scaling performance of the SimpleMD simulation on GPU, with ideal scaling normalized versus a setup with approx. 1.4 million molecules in a 120 x 120 x 120 cubical domain.

Digital Learning Portfolios as Teaching and Research Tools in the Context of AI-Supported Daily Academic Life

Author: Therese Rosemann

As part of the DigiTaKS* project, a web-based feedback tool was developed in cooperation with hpc.bw. Following a 10-day learning and usage diary study, this tool provided students in the humanities and social sciences with automated and personalized feedback on their digital learning and usage practices, as well as a data-protection-compliant comparison with their respective cohort. As part of the diary study, students used SoSci-Survey to document their daily learning activities and the use of digital media in their everyday academic life [1].

The longitudinal study's results show that digital competencies do not arise solely from access to digital technologies, but primarily through their reflective integration into specific teaching and learning contexts. Crucial to this are reflective, critical, and productive forms of media use that empower students to employ digital tools in a purposeful and self-directed manner [2]. Against the backdrop of the increasing prevalence of generative AI, this insight takes on even greater significance. Generative AI is an integral part of students' daily academic lives: Findings from DigiTaKS* show that 94% of students in the humanities and social sciences at HSU use AI tools for study-related purposes [3]. This gives rise to new requirements for teaching and assessment formats designed to promote students' critical and reflective practices in their use of digital media. The personalized feedback proved not only to be an incentive for participation in the longitudinal study but also an effective starting point for reflecting on one's own digital learning and usage practices [3, 4]. Furthermore, an evaluation of individual learning and usage profiles conducted alongside a seminar in the bachelor's program in adult education illustrates that comparing one's own results with those of the respective cohort sharpens awareness of one's own digital learning and usage practices, promotes critical engagement with one's own media behavior, and provides impetus for a more conscious use of digital media in everyday academic life. Overall, the findings suggest that longitudinal documentation and individualized feedback formats can contribute to the promotion of transformative digital competencies [5] in a higher education context.

The currently ongoing teaching and research project in the Master's program in Adult Education builds on these findings. The seminar focuses on the use of digital learning portfolios in ILIAS, which help document, visualize, and provide didactic support for students' learning, development, and reflection processes—particularly in their engagement with generative AI. The goal is to help students understand and critically reflect on the use of generative AI. Digital learning portfolios play a key role here by not only documenting the final exam performance (e.g., a term paper) but also focusing on the students' entire individual development process. Students document their work steps, justify their decisions, and reflect on the use of AI tools within the context of their research projects. Over the course of three trimesters, they complete various portfolio assignments that accompany key steps in academic work—from developing research questions through research and analysis processes to reflecting on their own decisions. Regular feedback from the instructor supports the further development of the projects.

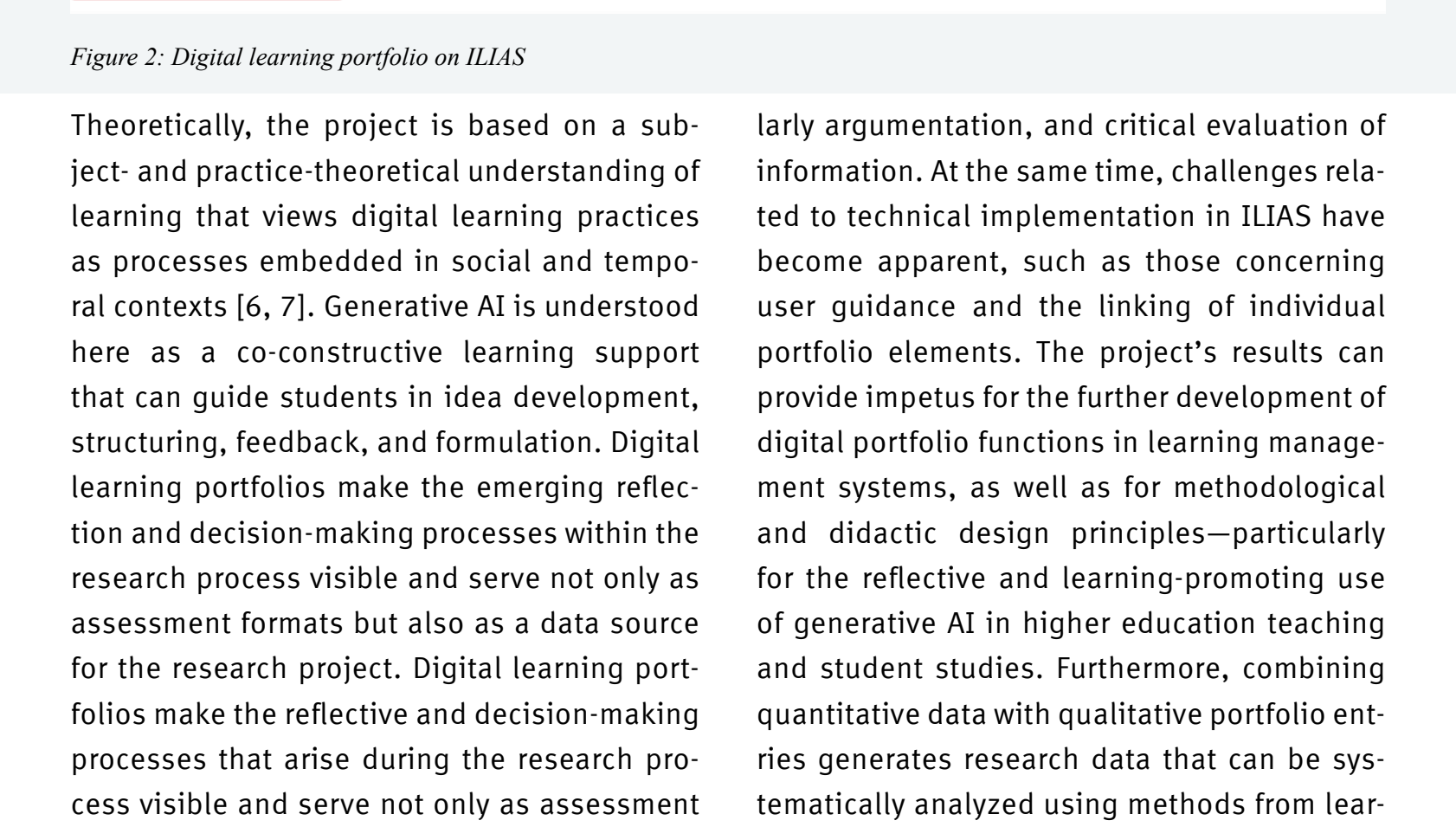


Figure 2: Digital learning portfolio on ILIAS

Theoretically, the project is based on a subject- and practice-theoretical understanding of learning that views digital learning practices as processes embedded in social and temporal contexts [6, 7]. Generative AI is understood here as a co-constructive learning support that can guide students in idea development, structuring, feedback, and formulation. Digital learning portfolios make the emerging reflection and decision-making processes within the research process visible and serve not only as assessment formats but also as a data source for the research project. Digital learning portfolios make the reflective and decision-making processes that arise during the research process visible and serve not only as assessment tools but also as a data source for the research project. This makes it possible to integrate research, teaching, and practice in a way that is both critically reflective and innovative. larly argumentation, and critical evaluation of information. At the same time, challenges related to technical implementation in ILIAS have become apparent, such as those concerning user guidance and the linking of individual portfolio elements. The project's results can provide impetus for the further development of digital portfolio functions in learning management systems, as well as for methodological and didactic design principles—particularly for the reflective and learning-promoting use of generative AI in higher education teaching and student studies. Furthermore, combining quantitative data with qualitative portfolio entries generates research data that can be systematically analyzed using methods from learning analytics, natural language processing (NLP), and statistical modeling. Looking ahead, this opens up opportunities for integration with high-performance computing (HPC), for example, for analyzing large volumes of text-based portfolios or simulating learning and development trajectories [8].

Initial experiences in teaching reveal potential, particularly for fostering independence, scho-

Would you like to learn more about the project or discuss digital learning portfolios? I look forward to hearing from you.

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hpc.bw @ECER 2026 in Tampere

Author: Alexander Kolling

From 18 to 22 August 2026, Marie Rathmann and I (Alexander Kolling) had the opportunity to attend at the European Conference on Educational Research (ECER) in Tampere, Finland, organised by the European Educational Research Association (EERA). The conference followed the Theme "*Knowing and Acting: The changing conditions and potentials of education research*", bringing together researchers from a remarkably range of educational research fields.

To get a better feeling of what large means: 6.619 participants from 83 countries attended the ECER 2026, making it the largest ECER in EERA's history and also the largest academic conference we've ever attended. With around 1.050 sessions, the conference offered an enormous variety of opportunities to present research, discuss current developments and connect across disciplinary and national boundaries. Of course, Marie Rathmann and I were among the 6.800 applications for a presentation, and we were fortunate enough to be accepted (out of the total of 915 reviewers) with the topic *Learning through Communities of Practice in Interdisciplinary High Performance Computing: An Adult Education Perspective*".

The presentation focused on how learning and educational processes emerge within HPC communities. Using first insights from surveys and problem centred interviews, we explored how HPC competences are acquired though research practice, problem solving and community based knowledge sharing. The interviews also provided first empirical indications that can be related to the theoretical framework of Communities of Practice (by Etienne Wenger). In particular, shared problem solving, the exchange of experiential knowledge, and the gradual development of expertise through participation point towards learning as a social and practice based process. The main finding of our research by this point can be summarised as followed:

1. HPC is an emerging and dynamic field with considerable potential, yet it remains largely unexplored from an adult education perspective.
2. HPC Education remains weakly grounded pedagogically. Adult Education could provide systematic frameworks for understanding, structuring, and supporting learning processes in HPC.
3. The research potential remains open: How can HPC resources benefit adult education research, and which new research questions might they be enable?

While HPC was new to many participants, other topics were not. Themes surrounding *Communities of Practice* had featured prominently in several previous sessions, creating strong continuity here.

Besides substantive presentations, conferences thrive on international exchange, cultural events and the encounters we had. For that, we would like to share some impressions with you.

The Conference started with a particularly impressive keynote by Pigga Keskitalo about "*Ecologies of Knowledge and the Future of Teaching: Sámi Education in Times of Transition.*" Keskitalo, among others Professor of Education at the University of Lapland, explored Sámi education through Indigenous knowledge systems, land based learning, language, community and intergenerational responsibility. The keynote was particularly impressive in its challenge to standardized understandings of knowledge and education and its emphasis on knowledge as contextual, relational and co-produced.

I also had the opportunity to participate in a session by Maria Kontradjuk, which took more hands on approach to qualitative research methods. Instead of simply discussing methods theoretically, participants were able to try out approaches from *Situational Analysis* (by Adele Clarke) themselves and *mapped* factors in context of the anticipated influence and impact the conference has on its participants. This provided a fascinating opportunity to explore how complex social phenomena can be visualised, related and analysed through different forms of mapping.

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Last but not least we had some time to explore Tampere between our conference sessions. The city offered plenty of opportunities to explore Finnish culture and everyday life. One particularly memorable discovery was the worlds only Moomin Museum, located in Tampere Hall. The museum features original illustrations by Tove Jansson and dioramas representing the story of the Moomins, made by Tove Jansson herself.

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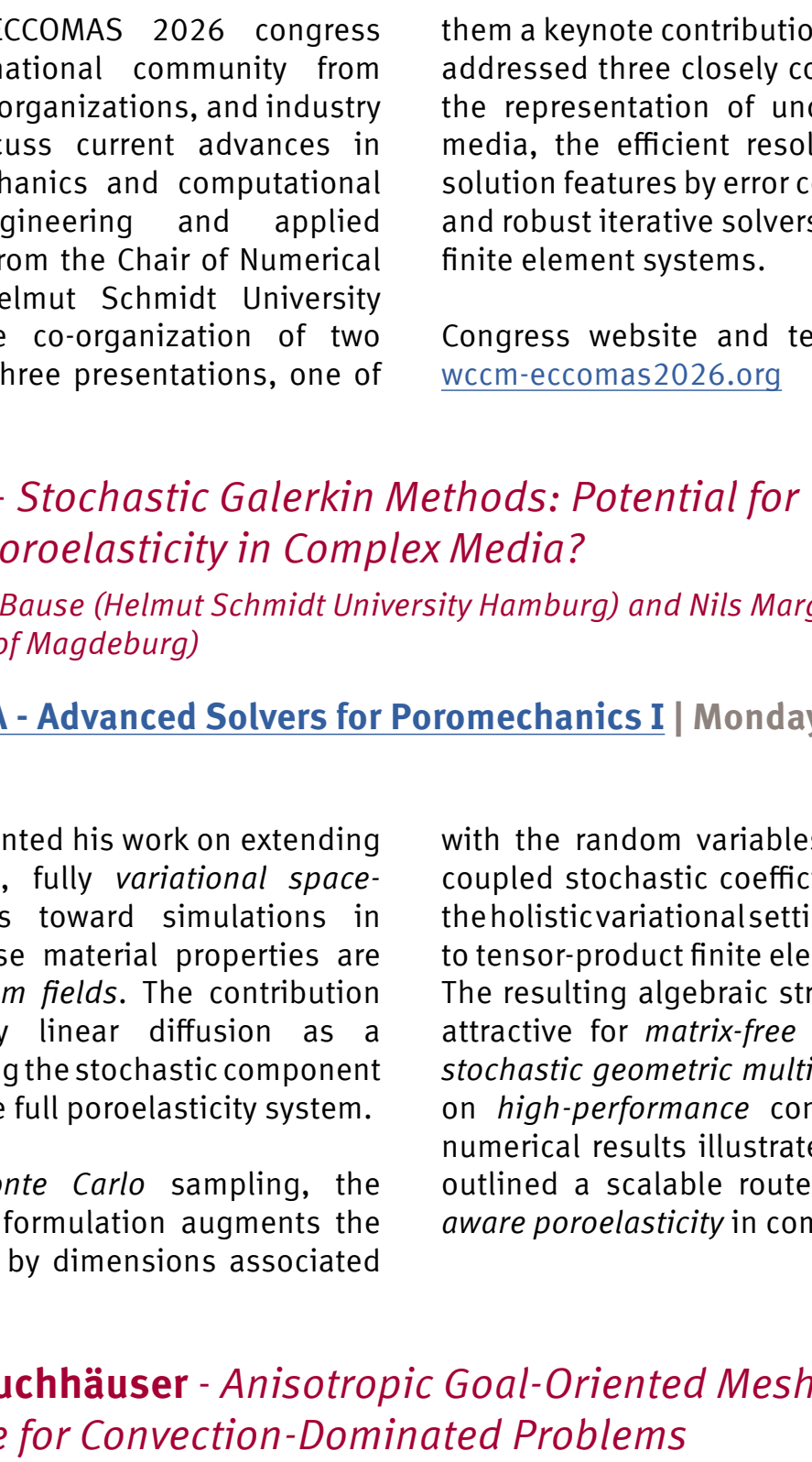
Overall, ECER 2026 was an impressive combination of international exchange, methodological inspiration and opportunities to position the HPC research at HSU within the broader field of educational research. It was especially valuable to see how questions around learning, technology, knowledge and research are being discussed from such different perspectives, and to bring the rather specialised topics of HPC Education into that conversation.

hpc.bw @WCCM-ECOMAS 2026 in Munich

17th World Congress on Computational Mechanics & 10th European Congress on Computational Methods in Applied Sciences and Engineering

ICM International Congress Center Messe München | 19–24 July 2026

Authors: Moataz Dawor, Marius Paul Bruchhäuser and Markus Bause



Marius Paul Bruchhäuser, Markus Bause, Moataz Dawor (from the left to the right)
© unknown

The joint WCCM-ECCOMAS 2026 congress brought an international community from academia, research organizations, and industry to Munich to discuss current advances in computational mechanics and computational methods for engineering and applied science. The team from the Chair of Numerical Mathematics of Helmut Schmidt University contributed by the co-organization of two minisymposia and three presentations, one of them a keynote contribution. Together, the talks addressed three closely connected challenges: the representation of uncertainty in complex media, the efficient resolution of anisotropic solution features by error control and adaptivity, and robust iterative solvers for large space-time finite element systems.

Congress website and technical programme: wccm-eccomas2026.org

Moataz Dawor - *Stochastic Galerkin Methods: Potential for Simulation of Poroelasticity in Complex Media?*

Co-authors: Markus Bause (Helmut Schmidt University Hamburg) and Nils Margenberg (Otto von Guericke University of Magdeburg)

Session: MS034A - Advanced Solvers for Poromechanics I | Monday, 20 July 2026, 15:00-16:30

Moataz Dawor presented his work on extending structure-preserving, fully *variational space-time* discretizations toward simulations in porous media whose material properties are described by *random fields*. The contribution used nonstationary linear diffusion as a prototype for studying the stochastic component before moving to the full poroelasticity system.

In contrast to *Monte Carlo* sampling, the *stochastic Galerkin* formulation augments the variational problem by dimensions associated with the random variables and solves for the coupled stochastic coefficients. This preserves the holistic variational setting and leads naturally to tensor-product finite element discretizations. The resulting algebraic structure is particularly attractive for *matrix-free* implementation and *stochastic geometric multigrid* preconditioning on *high-performance* computers. Preliminary numerical results illustrated the approach and outlined a scalable route toward *uncertainty-aware poroelasticity* in complex random media.

Marius Paul Bruchhäuser - *Anisotropic Goal-Oriented Mesh Adaptivity in Space and Time for Convection-Dominated Problems*

Co-authors: Markus Bause (Helmut Schmidt University Hamburg), Bernhard Endtmayer (Leibniz University Hannover), Nils Margenberg (Otto von Guericke University of Magdeburg), Ioannis Toulopoulos (University of Western Macedonia), and Thomas Wick (Leibniz University Hannover)

Session: MS051A - Anisotropic Meshes and Adaptive Refinement for Simulations of PDEs Within Complex Anisotropic Materials I | Tuesday, 21 July 2026, 15:00-16:30

Marius Paul Bruchhäuser presented an anisotropic goal-oriented error estimator for time-dependent convection-diffusion-reaction equations. Based on the Dual Weighted Residual method and anisotropic interpolation operators, the estimator decomposes the local error contribution into individual spatial directions and by time. These directional indicators identify where refinement is important for a selected quantity of interest and whether the mesh should be refined isotropically or preferentially along particular directions.

For convection-dominated regimes, the underlying discretization is stabilized with the Streamline Upwind Petrov-Galerkin method to suppress nonphysical oscillations at high Péclet numbers. Benchmark computations with different goal functionals showed that the directional strategy resolves sharp layers efficiently and can outperform isotropic adaptive space-time mesh adaptivity.

Sustainable Research Software @ WCCM & ECCOMAS

Author: Matthias Mayr

With open-source software being a central pillar of sustainable research software, this topic simply could not be left out at the joint 17th World Congress on Computational Mechanics (WCCM) and the 10th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), the largest WCCM so far, held in Munich in July 2026.

Consequently, open-source research software played a prominent role in the scientific program of the WCCM–ECCOMAS Congress 2026. To this end, PD Dr.-Ing. habil. Matthias Mayr (Universität der Bundeswehr München, project lead for sustainable research software development within hpc.bw) co-organized the minisymposium "Open-Source Software in Mechanics" (MS031) together with Łukasz Kaczmarczyk (University of Glasgow), Tzanio Kolev (Lawrence Livermore National Laboratory), Francesc Verdugo (Vrije Universiteit Amsterdam), Garth Wells (University of Cambridge), and Vladislav Yastrebov (Mines Paris – PSL).

With 44 contributions spread over three days, it was the largest minisymposium of the congress. The presentations covered a broad spectrum of open-source scientific computing, ranging from software design, numerical algorithms, and scalable high-performance computing to testing, performance profiling, development infrastructures, and community building. The minisymposium brought together developers and users of established as well as emerging open-source software for solid and fluid mechanics and multiphysics, providing a forum to exchange both scientific results and practical experience in developing sustainable research software.

hpc.bw Conference Contributions on Space-Time Methods and Efficient Solvers

Author: Michael Reichelt

In spring 2026, Michael Reichelt presented recent research on space-time formulations and their implications for efficient numerical solvers at two scientific events in Austria.

The first contribution was given on April 29, 2026, during the thematic programme "*Differential Complexes: Theory, Discretization, and Applications*" at the Erwin Schrödinger International Institute for Mathematics and Physics in Vienna. The programme brought together researchers from differential geometry, mathematical modelling, and numerical analysis to study differential and Hilbert complexes and their role in structure-preserving discretizations.

- **Michael Reichelt: Towards a de Rham-like Complex for Hyperbolic Problems**

The presentation discussed a space-time Hilbert-complex framework for hyperbolic partial differential equations. The central point was that identifying the appropriate complex structure is not merely a theoretical question. It also reveals the relevant operators, function spaces, and stability properties that must be respected by the discretization. This structural understanding provides a foundation for designing robust preconditioners and, consequently, fast iterative solvers for large-scale space-time systems.

The second contribution was presented on May 7, 2026, at the *20th Austrian Numerical Analysis Day* at Graz University of Technology. The annual workshop provides a forum for Austrian research institutions to exchange recent results in numerical analysis and applied mathematics and to initiate new scientific collaborations.

- **Michael Reichelt: An Elliptic Space-Time Variational Formulation for Parabolic Problems**

The presentation addressed parabolic equations formulated simultaneously in space and time. By using the polar decomposition of operators in Hilbert spaces, the evolution problem can be transformed into an elliptic formulation involving fractional Sobolev spaces. This perspective permits the construction of efficient and operator-adapted preconditioners. Moreover, the matrices associated with the fractional temporal operators can be applied efficiently using fast Fourier transform techniques, making the approach particularly relevant for large-scale and parallel space-time computations.

Both contributions demonstrated how a detailed analysis of the underlying functional-analytic structure can be translated directly into scalable numerical algorithms. Suitable Hilbert-space formulations do not only establish stability and well-posedness; they also guide the development of efficient preconditioners and high-performance solvers for time-dependent partial differential equations.

Event information: ESI thematic programme | Austrian Numerical Analysis Day 2026

Project Activities

Michael Reichelt @20th Austrian Numerical Analysis Day, Graz, Austria, 7–8 May 2026

Willi Leinen @RSE Day 2026, Hamburg, Germany, 25 June 2026

Min Son, Lars Zigan & Tobias Sander @22nd International Symposium on Applications of Laser and Imaging Techniques to Fluid Mechanics, Lisbon, Portugal, 29 June–2 July 2026

Willi Leinen @24th Conference of the International Federation of Operational Research Societies (IFORS 2026), Vienna, Austria, 12–17 July 2026

Markus Bause, Marius P. Bruchhäuser & Moataz Dawor @17th World Congress on Computational Mechanics and 10th European Congress on Computational Methods in Applied Sciences and Engineering (WCCM-ECCOMAS 2026), Munich, Germany, 19–24 July 2026

Min Son, Lars Zigan & Tobias Sander @Europe-Korea Conference on Science and Technology (EKC2026), Toulouse, France, 20–23 July 2026

Michael Reichelt @Computational Methods in Applied Mathematics (CMAM 2026), Vienna, Austria, 20–24 July 2026

Alexander Kolling & Marie Rathmann @European Educational Research Association (ECER), Tampere, Finnland, 17–21 August 2026

Min Son, Max Wenderoth, Moritz Drost, Tobias Sander & Lars Zigan @34th Conference on Liquid Atomization & Spray Systems, Lisbon, Portugal, 6–9 September 2026

Min Son, Lars Zigan & Tobias Sander @34th Conference on Liquid Atomization & Spray Systems, Lisbon, Portugal, 6–9 September 2026

Markus Bause @DMV Annual Meeting (DMV 2026), Konstanz, Germany, 7–10 September 2026

Moataz Dawor @Chemnitz Finite Element Symposium (CSAM 2026), Chemnitz, Germany, 7–9 September 2026

Johann A. Duffek, Philipp Marienhagen, Philipp Neumann & Karsten Meier @Thermodynamik-Kolloquium, Dortmund, Germany, 30 September–2 October 2026

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