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The bwHPC Symposium promotes a successful cross-university collaboration includes an ongoing dialogue between operators and users.

Flashback of the 10th bwHPC Symposium

The 10th bwHPC Symposium, the premier event for High Performance Computing (HPC) in Baden-Württemberg, was hosted at the University of Freiburg on September 25 and 26, 2024.



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The symposium brought together more than 80 experts, researchers, and enthusiasts to explore the latest advancements and innovations in high-performance computing.

The two-day symposium commenced on Wednesday, September 25, 2024, featuring a diverse program of 23 scientific presentations, workshops and tutorials led by top experts in the field. Highlights of the first day included an introductory HPC tutorial and a workshop on scientific programming with Python using Jupyter notebooks.

In the evening, attendees enjoyed an enlightening lecture titled "Keep calm and carry on - Cancer Research in Turbulent Times" by Marek Dynowski from the Cancer Research UK Manchester Institute at the Peterhofkeller, followed by a conference dinner and networking session.

The second day of the symposium commenced with a keynote by Joachim Ankerhold from the University of Ulm on "High Performance and Quantum Computing." The day's agenda included scientific presentations, poster sessions, the inauguration of the bwForCluster NEMO2 and concluded with a panel discussion and the presentation of poster and paper awards.

The symposium was free of charge and open to researchers from all scientific fields.

Some more impression from the Symposium

Two main topics stood out at the 10th Symposium: the convergence of HPC power with larger user groups and the importance of Green IT. Among the notable presentations were:

- Galaxy goes HPC (Björn Grüning) showcasing how the open-source platform Galaxy leverages HPC power for data-intensive biomedical research. For more information, visit usegalaxy.org.
- KI-Morph - User-friendly large-scale image analysis & AI on bwHPC systems (Alexander Zeilmann) focusing on efficient processing of X-ray-generated 3D tomographic images to empower researchers with tools that enhance scientific insights. KI-Morph was also the recipient of our Poster Award. Visit ki-morph.de for an impressive demo.

The Symposium also featured discussions on Green IT, including presentations on the necessity of efficient and sustainable IT in research environments, energy efficiency analysis of server components, and promoting sustainability in university settings and cooperative services.

The presentations in detail were

- Why efficient IT is also necessary (costs) and mandatory (EnEfG/RZReg) in the research environment (Peter Radgen)
- Thermographic and Energy Efficiency Analysis of Server Components under Variable Load Conditions (Benjamin Ott et al.)
- Green IT in the university environment: promoting sustainability through transparency (Lena Ritzinger)
- GreenIT in cooperative services (Jan Münchenberg)
- And the Panel discussion.

Special thanks to:

Special thanks were extended to participants who shared valuable insights, including presentations by David Eriksson: „Deepnetworks for reviving and accumulating experimental animal data: From Matlab to Python“ with the hint of code rewriting using ChatGPT as well as the presentation by Hanna-Friederike Poggemann: „Theoretical investigations on the catalytic pathway of unspecific peroxygenases in the context of biocatalysis“ with an alternate calculation solution for GROMACS + CP2K or ORCA. Ms. Poggemann was also the recipient of our Talk Award.

Collaboration partners bwCloud and SDS@hd as well as HLRS were acknowledged for their support at the Symposium 2024.

We hope all attendees enjoyed their time in Freiburg and look forward to welcoming them back for the next bwHPC Symposium in 2025.



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Lunch break, posters and discussions



© Bernd Wiebelt

Prof. Dr. Joachim Ankerhold presenting his keynote



© Bernd Wiebelt

Hanna-Friederike Poggemann receiving the Talk Award



© Michael Janczyk

Marek Dynowski giving his lecture at the Peterhofkeller



© Sandra Meyndt

The panel discussion rounded off the two-day event

ISC 2024 Flashback

The ISC 2024 exhibition in Hamburg served as a hub for engaging with leading HPC software and hardware providers, as well as the dynamic HPC community in Europe.



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Part of the bwHPC-Team

On May 12th, 2024, Hamburg hosted the prestigious International Supercomputing Conference (ISC) 2024, renowned as the premier event for High Performance Computing, Machine Learning, Data Analytics, and Quantum Computing in Europe. This year's conference underscored the growing importance of Machine Learning and the rising impact of Quantum Computing in the technological landscape. High Performance Computing (HPC) continues to play a pivotal role in meeting the increasing performance requirements of machine learning applications.

The ISC exhibition served as a hub for engaging with leading HPC software and hardware providers, as well as the dynamic HPC community in Europe. Notable participants included ISC platinum-level exhibitors such as Eviden, Hewlett Packard Enterprise, Intel, Lenovo, Microsoft Azure, WEKA, and xFusion, alongside prominent data center operators like MareNostrum 5, Gauss Centre for Supercomputing, as well as the NHR Alliance. The event also attracted HPC communities from England, Korea, and Japan, showcasing a global presence.

Quantum computing companies like Quix Quantum were prominently featured, reflecting the increasing interest and advancements in this cutting-edge technology. With a total of 159 exhibitors from 30 countries, ISC provided a diverse and vibrant platform for networking and collaboration.

Throughout the three-day event, numerous bwHPC teams seized the opportunity to collaborate with partners, explore potential HPC system suppliers, and participate in insightful conference sessions. bwHPC stood out alongside industry leaders ASUS and Huawei, drawing over 3,000 international attendees from 51 countries to the event.

The ISC 2024 once again solidified its position as Europe's leading conference for showcasing the latest innovations in high-performance computing and related technologies.

For more information, visit <https://www.isc-hpc.com>.

SOME MORE IMPRESSIONS FROM ISC 2024

Destination Earth: Digital Twins for weather and climate

We are frequently asked about the calculations we perform on our High-Performance Computing (HPC) systems. Explaining these calculations can be challenging due to the specialized knowledge and software involved. However, one project that showcases the power of HPC and offers intuitive handling is Destination Earth.

Destination Earth (DestinE) is an ambitious initiative aimed at creating a digital twin of our planet. With extreme weather events becoming more frequent and climate changes growing more pronounced, there is an urgent need for accurate forecasting to predict their impact on the environment, life, and property. This groundbreaking project commenced in 2022 and was transferred into operation in June 2024, with a „full“ digital replica of the Earth scheduled for 2030. Ioan Hadade, Senior Analyst at ECMWF, recently shared a stunning 60-day video rendering that provides a glimpse into the project's capabilities.

To learn more about Destination Earth and witness its innovative approach to weather and climate forecasting, please visit <https://destination-earth.eu>.

MareNostrum 5: Pre-Exascale HPC-system

Sometimes it is necessary to see the bigger picture and look at Tier-0 systems. Sergi Giróna, Operations Director of the Barcelona Supercomputing Center, presented some slides of the new MareNostrum 5. MareNostrum 5 is one of the pre-exascale EuroHPC systems hosted at the Barcelona Supercomputing Center. The system was tendered in 2022 and, following its inauguration in December 2023, is now in production mode and open to researchers from universities and public research centres. We look forward to seeing the first results at ISC25! MareNostrum 5 has a total peak computational power of 314 PFlops. In Germany, the first exascale HPC system called Jupiter is being installed at the Forschungszentrum Jülich. Kristel Michielsen presented the timeline and construction progress. The installation of Jupiter is planned for 2024, with full production expected in 2025. Hopefully, more details will be available at ISC 2025. Both HPC systems are partially funded by EuroHPC.

If you would like to learn more, please visit the following links: <https://www.bsc.es/mare-nostrum/marenostrum-5> and <https://www.fz-juelich.de/en/ias/jsc/jupiter>.

Green 500

Sustainability is becoming increasingly crucial for HPC systems, including Tier-3 systems. The Green500 competition specifically focuses on the energy efficiency of HPC systems listed in the TOP500. This year, the JEDI system in Jülich, Germany, has taken the lead with an impressive energy efficiency rating of 72.73 GFlops/Watt, utilizing 19,584 cores.

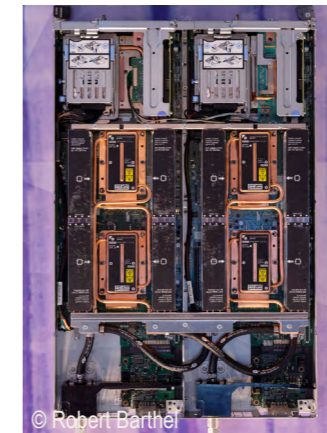
To learn more about this development, please visit the [Green500 website](#).



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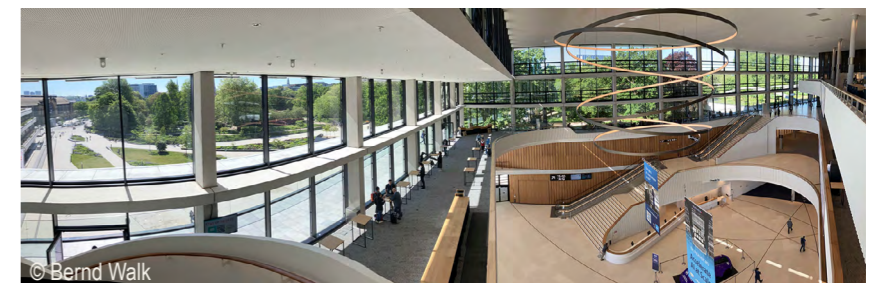
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AI Expansion

Baden-Württemberg provides over three million euros in funding for bwHPC AI research.

In a move to strengthen research in Artificial Intelligence (AI), the Ministry of Science, Research, and Arts of Baden-Württemberg has approved a funding exceeding three million euros. The „Strengthening of AI Infrastructure“ (SKII) initiative aims to enhance AI research capabilities through the procurement of hardware and software as well as services to support innovative AI research projects with the aim to improve the AI capabilities of central HPC infrastructure accessible to all researchers in the state. The funding has started in January 2024 and will continue until June 30, 2025.



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All bwHPC cluster sites will profit from this funding and invest in the GPU-capabilities of existing or future clusters, namely in Freiburg (NEMO 2), Tübingen (BinAC 2), Heidelberg (Helix) and Ulm (JUSTUS 3), as well as Karlsruhe (bwUniCluster2.0).



The images above are generated with Adobe Firefly, a generative machine learning model. Generative machine learning models like Adobe Firefly harness vast datasets and complex algorithms to create new images, text, or audio from simple prompts, enabling users to generate highly customized, photorealistic visuals, compelling artwork, or dynamic content with just a few inputs, transforming creative processes with speed and ease.

„Whether in medicine, quantum technology, or at the intersection of humanities and computer science, AI applications are indispensable in the research and teaching at our state universities,“ stated Minister of Science Petra Olschowski (Green Party). „To remain internationally competitive, we are expanding the computing capacity for AI research.“ [1] Michael Weber, Chairman of the State Rectors' Conference and President of the University of Ulm, welcomed the initiative, stating, „With the expansion of the AI infrastructure, young researchers can conduct their research projects faster and more effectively, which will also accelerate the technology transfer to the economy - this new program is a win for the entire state.“ [1]

Especially young researchers applying Artificial Intelligence methods will profit from these new resources.

References:

[1] https://www.baden-wuerttemberg.de/de/service/presse/pressemitteilung/pid/ausbau-der-rechenkapazitaet-in-der-ki-forschung?pk_medium=newsletter&pk_campaign=240517_newsletter_weekly&pk_source=newsletter_weekly, last edited 14.05.2024, last visited 27.05.2024

For further information:

- [Baden-Württemberg](#)
- [The Ministry of Science, Research and Arts of Baden-Württemberg](#)
- [Universität Ulm](#)
- [Südwest-Presse, 12.05.2024](#)



JUSTUS 3: Funding Approval

Ulm University is set to welcome an advanced high-performance computer, JUSTUS 3, with the help of a generous funding of 2.1 million euros from the German Research Foundation (DFG).



© Elvira Eberhardt

The predecessor: JUSTUS 2

Ulm University is set to welcome an advanced high-performance computer, JUSTUS 3, with the help of a generous funding of 2.1 million euros from the German Research Foundation (DFG). This Major Research Instrument Proposal, approved by the university, has cleared the path for the establishment of JUSTUS 3, with a total funding amount of 4.2 million euros. The DFG's contribution of half the funding, alongside counter-financing from the state and investment contributions from the universities of Ulm and Stuttgart, underscores the collaborative effort to advance research capabilities in the region beyond 2025.

Designed to support over 100 research projects from state universities and universities of applied sciences, JUSTUS 3 will primarily focus on innovative fields such as battery research and quantum sciences. With a total record of supporting more than 1300 scientific publications, the supercomputer is ready to surpass its predecessor in both computing power and energy efficiency.

Acknowledging the significance of this development, Minister of Science Petra Olschowski (Green Party) said “Baden-Württemberg is an European leader in supercomputing. The Ulm University makes a significant contribution to high-performance computing in theoretical chemistry, quantum physics and solid-state physics in particular. The new high-performance computer JUSTUS 3 will take supercomputing to the next level, and not only at Ulm University. In the future fields of quantum technology and battery research, the computing capacity will be available to all state

universities - thereby strengthening our QuantumBW innovation campus and Baden-Württemberg as a research location.”

Professor Joachim Ankerhold, Vice President for Research at Ulm University, who is responsible for the application, emphasizes the incorporation of the latest technology trends in high-performance computing within JUSTUS 3: „The new high-performance computer will also be more sustainable to operate“ with features such as hot water cooling and the utilization of waste heat for building heating.

Jürgen Salk, who heads the Scientific Software & Computer Services department at Ulm University, underscores the collaborative effort involving over 40 scientific working groups from seven state universities in shaping the funding application.

The technical specifications of JUSTUS 3 will be finalized through an EU-wide tender process, ensuring customization to user requirements and future needs, including AI-supported methods.

For further information:

- [Ulm University](#)
- [DFG, German Research Foundation](#)
- [Ministry of Science, Research and Arts](#)
- [Stuttgart University](#)

New Type of Friction Discovered in Ligand-Protein Systems

A team from the University of Freiburg and the Max Planck Institute of Biophysics in Frankfurt-am-Main identifies anisotropic friction.

An interdisciplinary research team of the Institutes of Physical Chemistry and Physics of the University of Freiburg and the Max Planck Institute of Biophysics in Frankfurt-am-Main has discovered a new, direction-dependent friction in proteins called anisotropic friction. "Until now, nobody had observed that friction in biomolecules was dependent on direction," says physicist Dr. Steffen Wolf of the University of Freiburg. The results have been published as cover story in the scientific journal "Nano Letters."

Experiments on model complex of protein-ligands

Proteins constitute the microscopic machinery of cells. They perform work during their functional cycles. Accordingly, they follow the laws of thermodynamics, exhibit an energy conversion efficiency, and lose energy during their functional cycle due to dissipation. From a macroscopic perspective, the latter effect corresponds to apparent friction. On the microscopic scale of single proteins, a known source of friction is internal friction of proteins that results from the excitation of protein-internal vibrations. A further source is solvent friction, which arises from the acceleration of surrounding solvent molecules. These sources of friction lead to heating of both protein and solvent. Here, the researchers discovered the novel type of friction by carrying out single molecule experiments and simulations on a model complex of a protein and a ligand.

In their single molecule experiments, the team used a new method applying stereographic single molecule force spectroscopy, which is based on atomic force microscopy (AFM). This technique allowed them to study the unbinding of a ligand from a protein bound to a surface not only along a single coordinate, but along all three Cartesian coordinates. During their experiments, Dr. Wanhao Cai, Prof. Dr. Thorsten Hugel and Dr. Bizan N. Balzer of the Institute of Physical Chemistry of the University of Freiburg as well as

BinAC, located in Tübingen, is one of the five statewide bwForClusters. It's available to all academic scientists in Baden-Württemberg in the fields of astrophysics, bioinformatics, medical informatics, geoscience and pharmaceutical science. To date, BinAC and its bwHPC Competence Center has contributed to the publication of over 300 research papers by providing computational power and dedicated user support. Currently the successor BinAC 2 is being installed. The commissioning is scheduled for 2024.

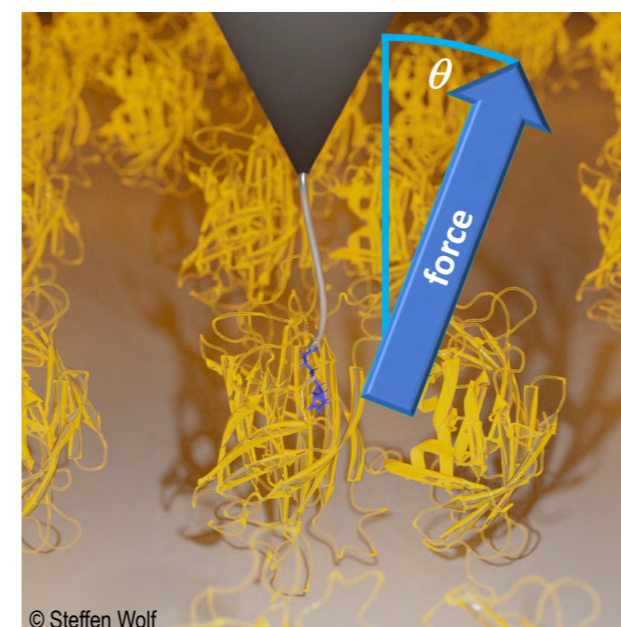
Dr. Jakob T. Bullerjahn of the Max Planck Institute, made the surprising discovery that friction during ligand unbinding increases with the pulling angle applied.

Combining experiment and computer simulations

Miriam Jäger and Dr. Steffen Wolf of the University of Freiburg's Institute of Physics subsequently recreated the experiment using computer simulations. They used the high performance computing (HPC) resources of the BinAC-HPC-Cluster in Tübingen. During the simulations they determined that the work of detaching a ligand from its binding site depends on the exact direction of application of the pulling force. By combining results from the experiment and simulations, the researchers recognized that the source of the angle-dependent friction is the undefinable and random orientation of the proteins along their rotational axes bound to the surface in the experiment. The team repeated the single molecule pulling experiments by binding and unbinding a ligand to and from a protein many times in order to achieve statistically significant results. There, the ligand binds to a different protein for each measurement. Consequently, in each measurement, a ligand was pulled at the same angle with respect to the surface, but over different regions of the randomly-oriented protein. This orientation cannot be defined, both in the experimental setup and in the real world, and each measurement cannot be exactly and reversibly repeated. Therefore, each time different amounts of energy were deposited into the biomolecule. The irreversible part of this energy was lost as heat to the system. The corresponding effect is a source of friction, which the researchers call anisotropic friction.

A fundamental type of friction

"We assume that this previously unknown and fundamental type of friction is present in every bioassembly in which randomness in protein orientation appears together with directionality of force application," says Dr. Bizan N. Balzer, a biophysicist. He explains that this is the case in biomolecular motors or force-sensitive membrane proteins, as well as for processes such as blood flow, where forces are exerted on randomly oriented proteins. Balzer concludes, "Anisotropic friction is thus another important piece of the puzzle for understanding friction in both technical applications and in biological complexes in general."



© Steffen Wolf

Pulling experiments on a biotin-streptavidin complex. Biotin (blue lines) is pulled out of a streptavidin protein (yellow) via a polymer linker (gray line), which is bound to a cantilever tip of an atomic force microscope (gray triangle).

Factual overview:

Original publication: Cai, W., Jäger, M., Bullerjahn, J. T., Hugel, T., Wolf, S., Balzer, B. N.: Anisotropic Friction in a Ligand-Protein Complex. In: Nano Letters 2023. DOI: <http://doi.org/10.1021/acs.nanolett.2c04632>.

Thorsten Hugel is a professor, Bizan N. Balzer a lecturer and Wanhao Cai a post-doctoral researcher at the Institute of Physical Chemistry of the University of Freiburg. Hugel and Balzer are members of the Excellence Cluster "Living Adaptive and Energy-autonomous Materials Systems" (liv-MatS) of the University of Freiburg. Balzer is a member of the Freiburg Materials Research Center (FMF). Steffen

Wolf is a lecturer, and Miriam Jäger a doctoral candidate, at the Institute of Physics at the University of Freiburg. They are members of the Research Unit FOR5099 of the German Research Foundation (DFG) "Reducing complexity of nonequilibrium systems." Jakob T. Bullerjahn is a staff researcher at the Max Planck Institute of Biophysics in Frankfurt-am-Main.

The German Research Foundation (DFG) is supporting their research through the project HU 997/13-1, the excellence initiative – EXC-2193/1 – 390951807 and the project WO 2410/2-1 within the Research Unit FOR5099 "Reducing complexity of nonequilibrium systems" (project no. 431 945 604) and the project INST 37/935-1 FUGG, as well as the Max Planck Society. Furthermore, the work is being supported by the bwUniCluster-Computing-Initiative, the High Performance/Cloud Computing Group at the Center for Data Processing at the University of Tübingen as well as the state of Baden-Württemberg through bwHPC.

The article was first published at Universität Freiburg on March, 31 2023. https://kommunikation.uni-freiburg.de/pm-en/press-releases-2023/new-type-of-friction-discovered-in-ligand-protein-systems?set_language=en

2024 User Survey

Insights and Findings

We would like to extend our thanks to all users who participated in our recent survey. Your feedback is invaluable to us in improving our services to better meet your needs.

We appreciate your feedback and look forward to implementing these improvements to better serve our community.

Thank you!

One of the most frequently mentioned requests in the survey was for more GPUs. We are pleased to inform you that we are currently in the process of renewing or extending all clusters in the bwHPC network. This renewal includes a significant upgrade to the GPUs, providing you with access to more powerful computing resources.

Key findings from the survey have also highlighted concerns regarding the presence of inconsistent or outdated information in the Wiki and training materials. In response, we will be taking a more proactive approach in the future by ensuring a clearer separation between the Wiki and Training materials. This will involve offering additional exercises in the Training section and providing guidelines and other resources in the Wiki to reduce redundancies.

We encourage users to report any discrepancies via the bwSupport portal as described at: <https://wiki.bwhpc.de/e/Feedback>.

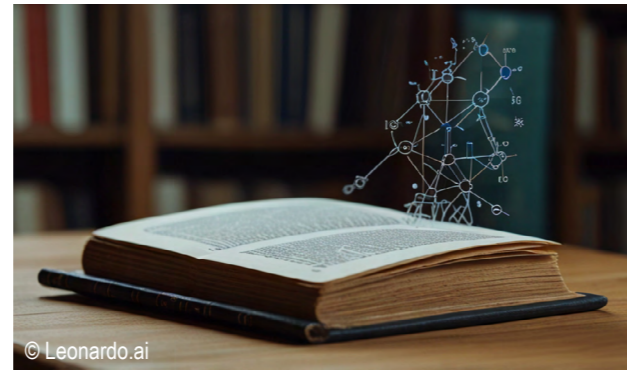


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Proceedings of the 8th Symposium

Foreword of the Proceedings for the 8th Symposium

Digital research infrastructures are important tools for enabling groundbreaking research results and thus finding answers to social challenges. The state's aim is to provide all scientists in Baden-Württemberg with high-performance research infrastructures and optimal conditions for innovative and excellent research. The state's high-performance computing strategy is also based on this claim, which is to build the necessary first-class infrastructures in dialogue with top-level research, to design them reliably and to support them with suitable support and training structures.



The bwHPC symposium is an important format for this exchange. Strong involvement of users in the conception and design of infrastructure services is essential to fully exploit the potential of digital tools. With regard to the existing digital infrastructures in the state, this results in further requirements, such as the integration of tools for data analysis, the management and archiving of research data, and the consideration of new methodological approaches. The continuous further development of the digital research infrastructure remains essential in order to set the appropriate framework for an excellent, internationally competitive research landscape.

In order to cover the entire range of services and ensure optimal support for users, our computer centers are based on a culture of cooperation. This culture of cooperation is the result of the joint efforts of many dedicated people. On behalf of the Ministry of Science, Research and Arts, I would like to thank all those involved for their extraordinary commitment and their efforts to find the best solutions.

Let us continue to successfully pursue this path together with nationwide collaborations. Only through trusting cooperation and self-determined organization can we optimally utilize the opportunities of the digital future.

A key factor for success is that the cross-university collaboration also includes an ongoing dialogue between operators and users, which raises awareness on both sides of the possibilities and needs of the other.

Dr. Raphael Dorn
Ministry of Science, Research and Arts of the State of Baden-Württemberg

We would like to express our gratitude to all those who contributed to these proceedings.

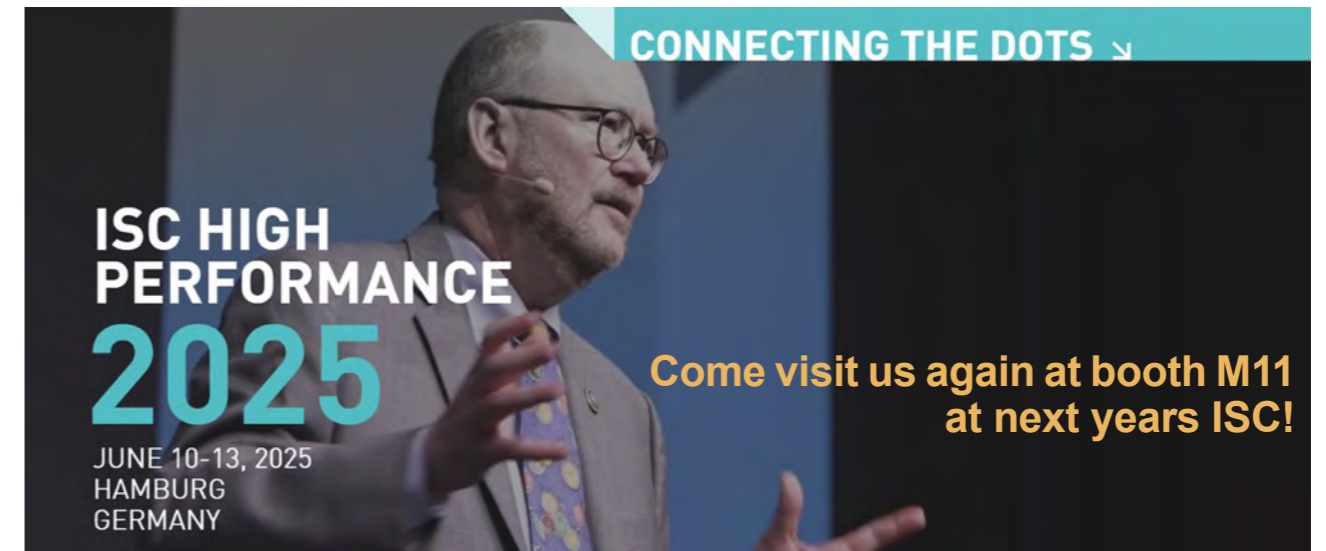
Lectures in detail:

- *Using BinAC to analyze microbiome samples*, Anupam Gautam and Daniel H. Huson, Institute for Bioinformatics and Medical Informatics and Max Planck Institute for Biology, University of Tübingen
- *A Proof of Concept for High Energy Physics Data Archival of PhD and Master Theses at the University of Freiburg*, Michael Böhrer, Institute of Physics, University Freiburg
- *Climate sensitivity and convective parameterization in the Earth system model of intermediate complexity PlaSim*, Felix Pollak, Elisa Ziegler, Olga Erokhina, and Kira Rehfeld, Institute of Environmental Physics, Heidelberg University and Department of Geosciences and Department of Physics, Tübingen University
- *The Dynamics of Adult Neurogenesis in the Dentate Gyrus of the Hippocampus*, Aadhar Sharma and Stefan Rotter, Bernstein Center Freiburg & Faculty of Biology, University of Freiburg
- *Planned Missing Data in Social Surveys: Evaluating Strategies Regarding Their Design and Imputation*, Deutsche Institut für Wirtschaftsforschung (DIW) Berlin
- *Smallholder adaptation through agroforestry: Agent-based simulation of climate variability in Ethiopia*, Habtamu Yismaw, Christian Troost and Thomas Berger, Department of Land Use Economics (490d), University of Hohenheim
- *Universal Dynamics at the Lowest Temperature*, Ido Siovitz, Philipp Heinen, Niklas Rasch, Stefan Lannig, Yannick Deller, Helmut Strobel, Markus Oberthaler, and Thomas Gasenzer, Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, Universität Heidelberg

Further information:

- The Proceedings of the 8th bwHPC Symposium have been published and are available [online](#).
- [Höchstleistungsrechenzentrum Stuttgart](#)
- You can access the flashback of the 8th bwHPC Symposium 2022, featuring a link to the collection of posters [here](#).

Upcoming Events



The next bwHPC-Newsletter will be published in spring 2025. We wish you a nice autumn and calm winter holidays!

Greetings from the bwHPC-Team

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