JSC News

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

A Fond Farewell: Sabine Höfler-Thierfeldt Has Retired

Essential minerals are the elements on Earth and in foods that our bodies need to develop and function normally. Sabine Höfler-Thierfeldt was a truly essential mineral of the JSC for 34 years. Shortly after celebrating her 40-year anniversary at FZJ, Sabine started her well-deserved retirement. Thanks to her tasks and engagement in the areas of public relations, science communication, and publication management, she was one of the few people at the institute who knew and was known to everyone.

Applying the strict word limit she implemented for the JSC News makes it impossible to list all of her activities. So here are some of the most outstanding ones: She coordinated press releases (also in close collaboration with Corporate Communications, UK) and articles for journals and magazines such as “effzett” or “intern” or InSiDE, contributed to and organized PR campaigns and JSC activities at the FZJ’s Open Day, and was responsible for the JSC websites, project dissemination for SiVeGCS, flyers, posters, event organization, management of the JSC training course programme, and social media channels. She was also responsible for the management of JSC’s entries in the publication database JuSER and the publication workflow within the institute. Last, but not least, she was also the editor of 298 issues of JSC News (or ZAM Aktuell, as it was originally called) – which we would like to commemorate with this article in the 300th edition (which she unfortunately just missed out on editing).

Sabine will be truly missed as a colleague who is always helpful and approachable, absolutely reliable and loyal, knows everything about JSC (like the embodiment of a JSC wiki), and who delivered excellent proofreading.

A deficiency in essential minerals leads to an abnormality in the metabolic functioning of the body – and so we now have the difficult task of finding a suitable replacement for Sabine, who was an essential cornerstone at JSC. Thank you for your last 34 years of commitment to JSC, Sabine!

Contact: Your JSC Colleagues (jsc-pr@fz-juelich.de)

PASQAL To Deliver 100+ Qubit Quantum Simulator to JSC

At the SC23 conference in Denver, Grand Equipement National de Calcul Intensif (GENCI), Commissariat à l’énergie atomique et aux énergies alternatives (CEA), Forschungszentrum Jülich, and PASQAL demonstrated progress within the framework of the European project “High-Performance Computer and Quantum Simulator hybrid” (HPCQS). PASQAL will deliver two 100+ qubit quantum simulators, which are a type of analogue quantum computer, to its first customers: JSC and CEA/GENCI. At JSC, the device, which has been acquired as part of the European project HPCQS and has been co-funded by the EuroHPC Joint Undertaking (EuroHPC JU) and the German Federal Government, will be coupled with the JURECA DC supercomputer. The PASQAL quantum simulator at JSC will be accessible to a wide range of European users in 2024. The two PASQAL systems are the first building block of a European federated HPC Quantum Computing and Simulation (HPC-QCS) infrastructure that will also consist of the six quantum computers acquired by the EuroHPC JU. At JSC, HPCQS is fully integrated into the Jülich UNified Infrastructure for Quantum computing (JUNIQ).

HPCQS users are already able to validate their use cases through various entry points, such as the Pulser environment deployed on JURECA DC, as well as thanks to remote access to a 100+ qubit device hosted at PASQAL’s premises in Massy, France. Currently, some HPCQS users from JSC are performing remote simulations on this device to benchmark it and to demonstrate quantum many-body scarring, a phenomenon that has recently attracted a lot of interest in foundations of quantum statistical physics and potential quantum information processing applications. European end users will soon have access to a more scalable, tensor network-based emulator from PASQAL, called EMU-TN, which will be deployed on both French and German environments.

More information is available in the press release.

Contact: Prof. Kristel Michielsen

30th GCS Large-Scale Call – New Projects Started in November 2023

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – Hawk (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are classified as "large-scale" if they require at least 2 % of the systems' annual production in terms of estimated availability.
Since computing time on Hawk and SuperMUC-NG are specified in core hours (specifically in million core hours, Mcore-h) and on JUWELS in peak floating point operations per year (FLOP/a), projects only fall into the "large-scale" category if they require at least 100 Mcore-h on Hawk, 45 x 10^{21} FLOP/a on JUWELS, or 45 Mcore-h on SuperMUC-NG.

The GCS Peer Review Board decided to award the status of a large-scale project to over 20 proposals from various scientific fields. In total, six projects were granted about 2050 Mcore-h on Hawk, 12 projects were granted approx. 535 x 10^{21} FLOP/a on JUWELS, and six projects were granted about 590 Mcore-h on SuperMUC-NG. More details about these projects can be found on the GCS website.

Contact: **Dr. Alexander Trautmann**, **coordination-office@gauss-centre.eu**

NIC Excellence Project Awarded to Prof. Gerhard Gompper

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its October meeting, the board decided to honour Prof. Gerhard Gompper (University of Cologne and Forschungszentrum Jülich) for his project on the collective dynamics of intelligent microswimmers.

Sensing of the environment and information processing, combined with motility, is a fundamental characteristic of life – from the largest animals to the smallest single-cell organisms. Adaptive self-steering gives rise to fascinating phenomena, ranging from large-scale collective behaviours referred to as swarming, as observed in mammalian herds, flocks of birds, schools of fish, and even cell layers and tissues to the formation of bacterial biofilms. Gompper and his group study the collective behaviour of cognitive self-steering microswimmers by means of large-scale hydrodynamic simulations using a particle-based mesoscale hydrodynamics approach combined with the squirmer model (prescribed surface flows) for the swimmer. Preliminary results show the formation of self-organized swirls and jets, depending on the manoeuvrability of the swimmer and the propulsion type (puller or pusher).

More details can be found on the NIC website.

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PRACE Scientific and Innovation Case

On 20 October 2023, PRACE kick-started a new edition of its Scientific and Innovation Case with a workshop, where more than 84 leading scientists from across Europe and beyond came together to outline the future of scientific research and innovation relying on high-performance computing (HPC) and related technologies.

This workshop focused on a pivotal objective, namely to usher in a new era of computational excellence. PRACE, together with the scientific and industrial user communities, will embark on an ambitious journey to revisit and reimagine the case for the use of HPC – with artificial intelligence (AI), quantum computing (QC), and other advanced computing technologies – to support science and industry endeavours. Building on the foundation laid by "The Scientific Case for Computing in Europe 2018 – 2026", PRACE has set itself the target of publishing a new edition in 2024.

This objective is perfectly aligned with PRACE's mission to represent the interest and identify the needs of users of HPC and related technologies in Europe as an Association of Users and HPC Centres in Europe. It also aims to pursue actions that enable high-impact research and innovation across all disciplines and industrial applications, thus enhancing scientific, technological, and economic competitiveness across Europe for the benefit of society.

This document will serve as a guide for European and national funding agencies and policymakers, and will help to strengthen and expand the competitive edge of European research and innovation, harnessing emerging technology infrastructure such as HPC, QC, AI, (high-performance) data analytics, and other transformative technologies.

More details about the workshop can be found on the event website.

Contact: **Dr. Florian Berberich**, **Veronica Teodor**

PRACE-6IP Final Review Result Celebrates PRACE's Achievements

Due to the complexity of the project and the high number of partners involved, the result of the PRACE-6IP final review, that took place in January 2023, was delivered only in November. With this, the reviewers concluded that PRACE-6IP has delivered excellent results with significant immediate or potential future impact:

- Provision of Tier-0 services through calls based on scientific excellence and specific services for new users
- Tier-0 user support and preparation of their applications for pre- and exascale, through best practice guides and various technical reports
- Establishment of a functional European HPC ecosystem: support for Tier-0 and Tier-1 users through DECI, HLSTs, and Preparatory Access

- Industrial users' support through SHAPE, the PRACE IAC, and workshops
- Collaboration with FocusCoE and several CoEs
- Provision and development of tailored training and skills development programmes for different levels of expertise, including promotion for young students
- Distribution of all information through an efficient website, social networks, and the HPC in Europe portal
- Coordination with new actors: ETP4HPC, EUROHPC JU INFRAG and RIAG
- The tremendous impact of the Ada Lovelace award on the careers of female scientists

In addition, the result of the final review of PRACE-6IP celebrated the PRACE community and underlined the importance of its achievements for the European HPC ecosystem. They also stressed that the future of the ecosystem could be at severe risk if the continuity and sustainability of the excellent PRACE services, results, and tools are not guaranteed in the EuroHPC era.

Contact: Dr. Florian Berberich, Veronica Teodor

Human Brain Project and ICEI Celebrate Successful Completion

In 2013, the Human Brain Project (HBP) was selected by the European Commission as one of two Future and Emerging Technologies Flagship initiatives to receive funding over a period of 10 years in order to build a novel digital research infrastructure for neuroscience and brain-related research. Since then, HBP members have presented their scientific results in over 3000 publications, advanced medical and engineering applications, and developed over 160 freely available digital tools for neuroscience research. With 155 participating institutions from 19 countries and a total budget of € 607 million, the HBP was one of the largest research and infrastructure projects in Europe.

The interdisciplinary team of HBP technology experts worked with HBP researchers to build EBRAINS: the digital research infrastructure offering brain atlases, services for finding and sharing brain data, modelling and simulation services, and health research platforms. EBRAINS builds on the computing, cloud, and data services of the Fenix e-infrastructure, which was developed in the Interactive Computing e-Infrastructure (ICEI) project, a sister project of the HBP. The JSC contributed to the development, hosting, and operation of a multitude of the EBRAINS services, and also managed the computing-related part of the HBP. JSC also coordinated the ICEI project and managed in particular the development contracts resulting in the Fenix User and Resource Management Service (FURMS) and the Data Mover Service. The JSC looks forward to continuing the journey of EBRAINS and Fenix after the end of the HBP and ICEI, which were both successfully completed in September 2023.

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TrustLLM Project Started

The EU project TrustLLM was officially launched on 20-21 November. In the next three years, the project will create a new generation of large language models with improved accessibility, reliability, and mitigated negative effects such as hallucinations and bias. The consortium has a focus on northern Europe. For example, AI Sweden, located in Stockholm, is a project partner that has created the LLM GPT-SWE, the strongest model in the Swedish language to date. The company Miðeind has worked with OpenAI on improving their models' capacity in Icelandic, a low-resource language with only approximately 300,000 speakers for which the internet is flooded with low-quality automatic translations.

Within the project, JSC's role will be twofold: Firstly, HPC experts will ensure that resource-intensive GPU-based LLM training will take place at an ideal level of efficiency on all systems. Secondly, the team from the Simulation and Data Lab Applied Machine Learning will work on new features of LLMs for digesting longer inputs, develop methods for reducing the parameter count, and work on scaling laws that allow for predictions of LLM performance without even having to train them.

More information can be found on the website of Linköping University, the project coordinator.

Contact: Dr. Stefan Kesselheim

JSC Joins New Trillion Parameter Consortium

JSC is a member of the new international Trillion Parameter Consortium (TPC) formed by federal laboratories, research institutes, academia, and industry to create trustworthy and reliable generative, large-scale AI models for science. TPC aims to address key challenges in advancing AI for science, which include developing scalable model architectures and training strategies; organizing and curating scientific data for training models; optimizing AI libraries for current and future exascale computing platforms; and developing deep evaluation platforms to assess progress with regard to scientific task learning and reliability and trust.

TPC addresses three aspects relating to the complexity of building large-scale AI models: Identifying and preparing high-quality training data of various scientific domains and data sources; designing and evaluating model architectures, performance, training, and downstream applications; and developing cross-cutting and foundational capabilities such as innovations in model evaluation strategies with respect to bias, trustworthiness, and goal alignment. The initiative aims to provide the community with a venue in which multiple large model-building initiatives can flexibly collaborate to leverage global efforts to accommodate the diverse goals of individual initiatives.

Trillion parameter models represent the frontier of large-scale AI, with only the largest commercial AI systems currently approaching this scale. Even using the exascale

systems on the horizon, training a state-of-the-art one trillion parameter model will require months of dedicated time. Such efforts will therefore involve large, multi-disciplinary, multi-institutional teams. TPC is seen as a vehicle to support collaboration and cooperative efforts among and within such teams. By joining this initiative, JSC successfully continues to be involved in and show support for strong interdisciplinary communities like LAION, which are pushing the frontiers of research on large-scale open foundation models and datasets to enable reproducible and transparent large-scale machine learning research.

More information can be found in the TPC press release.

Contact: Dr. Jenia Jitsev

JSC Experts Win Best Paper Award at ISAV

JSC would like to congratulate Mathis Bode, Jens Henrik Göbbert, Jonathan Windgassen, and their collaborators from Argonne National Laboratory (USA) on winning the Best Paper Award for their paper entitled "Scaling Computational Fluid Dynamics: In Situ Visualization of NekRS using SENSEI". The award was presented at the "ISAV 2023: In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization" workshop, which took place in conjunction with SC23 on 13 November 2023 in Denver, Colorado, USA.

In their paper, the team writes about a novel pipeline for in situ and in transit visualization and analysis utilizing SENSEI, ADIOS2, and ParaView in Python. The aim is to solve the dilemma of having to choose between data accuracy or decreasing the resolution for computational fluid dynamics on GPU-powered HPC systems. Their approach takes more regular data snapshots directly from memory and thus bypasses the pitfalls of checkpointing. The NekRS application is a GPU-centric thermal fluid simulation, which showcases diverse in situ and in transit strategies. Experiments on the Polaris and JUWELS Booster supercomputers were conducted to demonstrate real-world implications, which offered crucial insights into how efficient data management can be achieved without compromising accuracy.

The paper is available online:
https://doi.org/10.1145/3624062.3624159

Contacts: Mathis Bode and Jens Henrik Göbbert

Sandra Diaz Gives Inspiring Talk at SC23

Sandra Diaz, head of the Simulation and Data Lab Neuroscience at JSC, was invited to give a talk about "Boosting Neuroscience Research with High-Performance Computing Infrastructure" at SC23. Under this year's tagline "I am HPC", Sandra Diaz shared her personal journey, which took her on an unconventional path before she finally joined JSC nine years ago. She then presented the journey of the neuroscience community on its path to becoming more HPC-oriented. Neuroscience has become a highly interdisciplinary research field, which involves purely experimental studies, applied technology development, mathematical theory, computational models and simulations, AI, visualization, and data analysis. However, neuroscience is relatively new to the usage of high-performance computing. Within the EU-funded, Human Brain Project, which was successfully concluded recently, scientists from all over Europe have made substantial progress in consolidating the computational requirements and usage patterns of this heterogeneous field. Alongside the evolution of the European HPC landscape, neuroscience has also helped co-design federated access to HPC, the cloud, and data resources through the ICEI project in collaboration with the Fenix Research Infrastructure – a European effort to provide federated access to some of the largest HPC centres in Europe.

In her talk, Sandra Diaz emphasized how the relationship between neuroscience and HPC has evolved in the past decade. She also gave examples of scientific highlights that have been enabled through this interaction as well as offering a perspective of how neuroscience can contribute to future technology co-design while maintaining a focus on societal impact. She concluded her talk by highlighting the importance of community, networking, and inclusivity in the adoption and future development of HPC. This very inspiring talk in the largest conference room at SC23 was well attended and well received.

Contact: Dr. Sandra Diaz

JuWinHPC Searching for New Members

Jülich Women in HPC (JuWinHPC) is the local chapter of the international "Women in High-Performance Computing" (WHPC) organization. Focusing on the issue of why there are so few women in the HPC community, JuWinHPC aims to achieve greater equality, diversity, and inclusion in the community.

Founded about one year ago, the network has organized several meetings at JSC, either online or as joint lunches. The last meeting specifically targeted male colleagues in order to obtain their view on the network's aims and activities. In summer, JuWinHPC, together with the "Female Voice" network, organized the 2nd Jülich Write'athon during which Wikipedia articles about female scientists at Forschungszentrum Jülich were written to increase the visibility of female experts on this platform. More recently, JuWinHPC also started its own Jülich Blog "JuWinHPC Voices", where women in the HPC community write about their experiences, challenges in managing work and family life, or how they got into the world of HPC.

As the name suggests, JuWinHPC is a women's network, but it remains open for anyone to join. Colleagues interested in joining events and network meetings from time to time are just as welcome as those who would like to become a bit more involved and join the JuWinHPC board and coordination team. Joining JuWinHPC is a great opportunity for meeting other women in the field and does not involve any commitments.

More information about JuWinHPC, upcoming events, and how to join the network and its communication channels are available on the website.

Contact: Dr. Ruth Schöbel

SEA Projects To Host Their Final Workshop

The SEA projects (DEEP-SEA, IO-SEA, and RED-SEA) are a family of EuroHPC-funded research initiatives dedicated to advancing software technologies and interconnect solutions for large-scale modular and heterogeneous high-performance computing (HPC) systems. After three years of intense and productive work, the SEA projects will come to an end in March 2024. To mark the success achieved and to disseminate their results within the wider HPC community, a workshop will be held on 16 January 2024 at the Leibniz Rechenzentrum (LRZ) in Garching, which is conveniently timed to take place just before the start of the HiPEAC conference in Munich.

The workshop invites anyone interested in the latest results of the SEA projects to take part and offers an opportunity to learn about the readily deployable SW results and engage in a technical dialogue with the development teams. We will take a deep dive into diverse areas of the SEA projects' HPC stack, covering performance analysis tools, I/O solutions, software deployment, and integration strategies. Key themes include the DEEP-SEA framework for continuous software integration, a toolset for mapping applications onto modular supercomputer architectures, the user-centric data access and storage interface (DASI), and the VEF interconnect traffic analysis framework.

For those eager to explore these topics, the preliminary agenda and registration details can be accessed on the event website. Join the SEA projects workshop to gain insights into the latest achievements and discover how they can improve the performance of your HPC applications and the utilization of your supercomputer systems.

Contact: Prof. Estela Suarez

AIDAS Workshop 2023 – Past, Present, and Future

The European Joint Virtual Lab AIDAS (AI, Data Analytics, and Scalable Simulation) held its annual workshop at JSC. On 11-12 October, scientists from France and Germany gathered in Jülich to present results, exchange ideas, and discuss future collaborations.

AIDAS is the European Joint Virtual lab on AI, Data Analytics and Scalable Simulation founded in 2019 by Forschungszentrum Jülich (FZJ) and the French Commissariat à l'énergie atomique et aux énergies alternatives (CEA). The cooperation is based on the partner's long-running mutual scientific activities, especially in high-performance computing (HPC) – both in HPC-supported application fields and in the development of HPC technologies towards exascale. Scientists from FZJ and CEA work together on a broad spectrum of research issues ranging from quantum computing, extreme-scale systems, and extreme-scale computing, to brain networks, materials science, and energy – all topics united by the common denominator of AI, data analytics, and scalable simulation.

The motto of this year's workshop was "Past, Present and Future". Participants gave an overview of recent achievements and ongoing subjects, interacted with fellow scientists, and talked about ways of intensifying and expanding joint actions, for example by integrating additional topics and partners.

All in all, the meeting showcased exciting research and scientific achievements whilst underlining the value of this partnership and calling for its further continuation and expansion. We are therefore looking forward to future developments and next year's workshop in Paris.

More information about AIDAS can be found on its website.

Contact: Andrea Grego

HiRSE Continuous Benchmarking Hackathon Wrap-Up

When developing research software, it is vital to track performance over time and to ensure that performance is not compromised by ongoing development. This can be automated by including benchmarking in continuous integration practices, continuous benchmarking (CB) for short. Due to its importance, the newly established Research Software Engineering for HPC (RSE4HPC) team at JSC hosted the "HiRSE Hackathon on Continuous Benchmarking" on 17-18 October, bringing together researchers from different Helmholtz institutions and universities to develop, collaborate, and discuss CB. This included CB software frameworks, data aggregation, and visualization as well as repository and user policies to cover the many aspects that need to be considered when implementing CB due to the diversity in applications, codes, algorithms, and machines. In total, 32 teams and numerous individuals joined the activity that started with short presentations of their software and their goals for the event, with some of them showcasing their ongoing efforts to tackle CB. The remaining time was open for participants to spend it according to how they saw fit, utilizing the wealth of expertise present at the event to pursue their goals. This open format programme provided a platform for spontaneous discussions as well as a time and place to work towards a specific goal. The hackathon was jointly organized with the Steinbuch Centre for Computing at the Karlsruhe Institute of Technology (KIT) and was the second HiRSE event of this kind, following on from the "Continuous Integration Hackathon" in September 2022 at KIT. Both events were very well received, suggesting that there will be more events to come in 2024.

More details are available on the workshop website.

Contact: Dr. Robert Speck