JSC @ Supercomputing Conference SC22

The SC22, the leading international exhibition and conference on high-performance computing, networking, storage, and analysis, will take place from 13 to 18 November 2022 in Dallas, Texas, USA. JSC together with its partners from the Modular Supercomputing and Quantum Computing research group of the Goethe-University Frankfurt and the Jülich Aachen Research Alliance (JARA) will present their diverse range of activities at JSC's booth.

As the upcoming European exascale hosting site and operator of the D-Wave Quantum Annealer, this year's highlights at JSC's booth #1027 can best be summarized as "Towards Exascale and Quantum Computing – from the very largest to the very smallest".

We are looking forward to giving visitors to our booth the opportunity to live code our D-Wave Advantage™ System JUPSI via JUNIQ (Jülich UNified Infrastructure for Quantum computing). Our partners from the Goethe-University Frankfurt will present fundamental research and development in the area of the new architecture and programming paradigm for modular supercomputing. Colleagues from the SEA projects will highlight their solutions for exascale systems. This year's application focus will be Earth system modelling (ESM) with videos visualizing the results of multi-scale climate simulations. In addition, in-house HPC tools like LLview, SIONlib, JUBE, and Scalasca will be demonstrated and JSC's support infrastructure will be presented. The JARA Center for Simulation and Data Science (CSD) will highlight its activities and services.

As part of the conference programme, Kristel Michielsen will give an invited talk on "Integrating Quantum and High-Performance Computers for Practical Quantum Computing". JSC employees will organize the full-day tutorial "Efficient Distributed GPU Programming for Exascale", co-organize the tutorial "Hands-On Practical Hybrid Parallel Application Performance Engineering" and the workshop "Second International Symposium on Quantitative Codesign of Supercomputers", and present talks and posters. The "Scientific Visualization & Data Analytics Showcase" is also organized by JSC. And, of course, JSC colleagues will participate in multiple special interest group sessions and panel discussions.

Please visit https://go.fzj.de/sc22 for detailed information.

Contact: **Jens Henrik Göbbert**

Folding Lattice Proteins with Quantum Annealing

The recent publication "Folding lattice proteins with quantum annealing" by Anders Irbäck et al. (DOI: 10.1103/PhysRevResearch.4.043013) was chosen as an "Editor's suggestion" by the journal *Physical Review Research*. In this article, the authors – among them Sandipan Mohanty from JSC's Simulation and Data Lab Biology – explore a new way of encoding the protein folding problem for quantum computers. Using a simple HP (H = hydrophobic, P = polar) protein representation on a 2D lattice, the authors demonstrate the viability of the use of quantum annealers for bio-physical problems in the near future.

For the simple 2D HP lattice model used here, exact results are known for systems of up to 30 amino acids. This makes it an interesting test-bed for evaluating the reliability of new methods. The simulations performed on the D-Wave Advantage system JUPSI at the Jülich Supercomputing Centre show that the hybrid quantum annealer has a 100% hit rate in finding the ground state of the lattice protein model.

Crucially, the newly developed method retains its analytical simplicity as more particles are added to the system, so that larger systems can be studied with little extra effort. The authors applied the method to two systems of 48 and 64 amino acids, whose ground states were known from older classical simulations, and found that the quantum annealer identifies those ground states, once again with a 100% hit rate, costing only a small fraction of the computing time.

This study opens up exciting new possibilities regarding applications of quantum technologies in the life sciences.

The authors are currently researching ways of bringing more biophysically detailed models to quantum computers.

Contact: Dr. Sandipan Mohanty

Retrospective of the 11th NIC Symposium

The John von Neumann Institute for Computing (NIC) supports research projects from a broad scientific spectrum. On 29 and 30 September 2022, computational scientists presented their research results at the 11th NIC symposium in Jülich. The symposium was very well attended with over 160 participants – much to the satisfaction of the organizers.

Director of the Jülich Supercomputing Centre (JSC) and the NIC, Prof. Thomas Lippert, welcomed all participants at the beginning of the event. The symposium started with the very sad news of Prof. Kurt Binder passing away. Prof. Binder, former chair of the NIC Scientific Council was one of the driving forces in the high-performance computing (HPC) community in Germany and particularly in the NIC. We mourn the loss of Prof. Binder and would like to express our deepest condolences to Prof. Binder's family during this difficult time.

In his scientific talk, Prof. Lippert focused on the rise of quantum computing at JSC. He emphasized the enormous importance of quantum computing, and gave some insights into the development of this emergent, disruptive technology.

Following tradition, researchers' recent activities and results were compiled in the NIC Symposium's proceedings. The symposium and the proceedings address both computational scientists and practitioners as well as the general public with an interest in the advancement of computational science and its applications in diverse, contemporary research fields.

All accompanying materials such as the programme, talks, posters, proceedings, and photographs are available at https://go.fzj.de/nic-symposium-2022.

Contact: Dr. Alexander Trautmann

Looking Back at Workshop “Transformers for Environmental Science”

JSC, the Otto von Guericke University of Magdeburg, and the Technical University of Munich jointly organized a workshop on "Transformers for Environmental Science" from 22 to 23 September 2022. The workshop was co-sponsored by the ERC grant IntelliAQ and brought together about 40 participants in Magdeburg and up to 20 additional online attendees, who discussed the potential of this new AI technology for environmental applications. The programme included lectures on recent advances in transformer architectures and transfer learning as well as on prototype developments focusing largely on atmospheric research and remote sensing. Keynote presentations were given by Peter Düben (ECMWF), Pedram Hassanzadeh (Rice University, Houston), Duncan Watson-Parris (Oxford University), Lucas Beyer (Google Brain), and Jonathan Godwin (Google Deepmind). A poster session and panel discussion provided opportunities for an exchange of ideas. For more details, please visit https://sites.google.com/view/esstransformers/.

Large transformer models require huge amounts of data and constitute an attractive application for accelerated supercomputers such as JUWELS Booster. Within the “atmorep” compute time project, first steps towards training such a model for atmospheric research are being taken.

Contact: Dr. Martin Schultz

First MAELSTROM Boot Camp at JSC

The EuroHPC project MAELSTROM organized the first of two planned bootcamps at JSC. From 27 to 30 September 2022, 32 participants from all over the world and 16 tutors from the MAELSTROM project partners enjoyed an intensive training course on HPC-powered machine learning (ML) applications in weather and climate. The programme consisted of introductory lectures on ML methods, selected meteorological topics, and the Jülich HPC systems, more detailed lectures on the ML approaches of the six meteorological applications in MAELSTROM, and comprehensive hands-on tutorials based on the MAELSTROM applications. The tutorials were realized as Python notebooks on the Jupyter-JSC platform. Preparations for the bootcamp were supported by the Helmholtz AI team at JSC, who also provided technical support for this event. Two bootcamp participants from the African Institute for Mathematical Studies received travel support from the MAELSTROM project after they were selected in a competitive procedure from 26 high-quality applications.

Contact: Dr. Martin Schultz

Cooperation Agreement on CESOC

The University of Bonn, the University of Cologne, and Forschungszentrum Jülich signed a new cooperation agreement and Memorandum of Understanding with the European Centre for Medium-Range Weather Forecasts for their joint Centre for Earth System Observation and Computational Analysis (CESOC). CESOC brings together expertise in Earth system research, scientific computing, informatics, and mathematics at the respective sites and provides opportunities for joint research and training. The JSC is represented in CESOC primarily by the Simulation and Data Laboratories Climate Science and Terrestrial Systems as well as the Research Group Earth System Data Exploration. The first joint projects have been initiated. Further information on CESOC can be found at https://cesoc.net/.

Contact: Dr. Martin Schultz

EDITH Project Launched

The EDITH project (Ecosystem for Digital Twins in Healthcare) is a two-year European Coordination and Support Action (CSA), which aims to foster an ecosystem for digital twins in healthcare. This will be achieved by mapping and analysing the status of the fields considered crucial for the growth, uptake, and use of digital twins in healthcare, such as *in silico* medicine, managing health-related data, using cloud and high-performance computing for health-related simulations, as well as dealing with ethical and legal regulations. A vision and roadmap for the integrated human digital twin will be developed, based on standardized (meta-)data and models. A federated repository will bring together currently available resources and best practices. Building on available infrastructure, a framework for a simulation platform will be proposed, including a proof-of-concept implementation with pre-selected prototypes. User communities (healthcare professionals, patients, industry, and academia) will be actively involved to ensure their needs are built into the architecture.

The project is coordinated by the VPH Institute in Leuven (Belgium) and involves a wide range of institutions from academia and industry. Forschungszentrum Jülich is participating with two groups. The group of Prof. Katrin Amunts at INM-1 will contribute its experience with brain atlases, and the coupling of these atlases to multi-scale models. The coupling of brain models to other organ models is of high interest as well. JSC will contribute to the simulation platform and federated repository. This includes the provisioning of computational resources (HPC and cloud) for prototyping and evaluation, as well as expertise in HPC, cloud, and building federated systems. For further information, please visit https://www.edith-csa.eu/.

Contact: Dr. Bernd Schuller

Obituary Prof. Dr. Kurt Binder

On 27 September, Prof. Kurt Binder, former Chair and longstanding member of the Scientific Council of the John von Neumann Institute for Computing (NIC) at Forschungszentrum Jülich passed away at the age of 78. Prof. Binder was born 10 February 1944 in Korneuburg, Austria. He studied physics at the University of Vienna, Austria, and became one of the most renowned Austrian physicists of his generation. Between 1977 and 1983, he was head of the Theory of Soft-Matter Physics and Biophysics subinstitute (IFF-2) at Forschungszentrum Jülich. He was appointed a member of the Scientific Advisory Board at Höchstleistungsrechenzentrum (HLRZ) in Jülich in 1987. He maintained a close connection with the HLRZ and its successor, the John von Neumann Institute for Computing (NIC). In 2001, Kurt Binder and Friedel Hoßfeld, the former head of the JSC predecessor Central Institute for Applied Mathematics, chaired the international Conference on Computational Physics (CCP2001), which strengthened the ties between the computational sciences and the supercomputer facility in Jülich. Kurt Binder became Deputy Chair of the NIC Scientific Council in 2011 and was Chair of the NIC Council and Vice-Chair of the Steering Committee of the Gauss Centre for Supercomputing (GCS) between 2012 and 2017.

The Jülich Supercomputing Centre and its partner institutions in NIC and GCS mourn the loss of Prof. Kurt Binder and would like to express their deepest condolences to Prof. Binder's family.

Contact: NIC coordination office

Events

Software Development in Science
Instructors: Guido Trensch, Wouter Klijn, JSC
Date: 15–17 November 2022, 09:00–14:00
Venue: online
https://go.fzj.de/2022-sw-devel

Introduction to Supercomputing at JSC - Theory & Practice
Instructors: JSC employees, representatives of Atos, Intel, and ParTec
Date: 21–25 November 2022
Venue: online
https://go.fzj.de/2022-sc-2

Advanced Parallel Programming with MPI and OpenMP
Instructor: Dr. Rolf Rabenseifner, HLRS
Date: 28-30 November 2022, 08:45–18:00
Venue: online
https://go.fzj.de/2022-adv-mpi

Introduction to machine learning in the application area of fluid mechanics and combustion using HPC
Instructors: JSC employees, members of CoEC
Date: 8 December 2022, 08:30–17:00
Venue: online
https://go.fzj.de/2022-ml-hpc-combustion

For further events, talks, and training courses see
https://fz-juelich.de/en/ias/jsc/events