## NIC 25th Anniversary

For the last 25 years, the John von Neumann Institute for Computing (NIC) has provided supercomputer resources for projects in science, research, and industry in the fields of modelling and computer simulation. As a joint foundation of the three Helmholtz Centres Forschungszentrum Jülich, Deutsches Elektronensynchrotron DESY, and GSI Helmholtzzentrum für Schwerionenforschung, it supports computational science in Germany and Europe.

We are delighted to invite you to the celebration of the 25th anniversary of the NIC in Cologne on 21 April 2023. Please register for the event before 14 April using the link: https://indico3-jsc.fz-juelich.de/event/95/. The event will be opened by Prof. Astrid Lambrecht, Member of the Board of Directors of Forschungszentrum Jülich, followed by presentations and a podium discussion, covering the history of the NIC, current research, technologies, and innovations. Keynote presentations will be given by Prof. Hidetoshi Nishimori on Quantum Annealing and Prof. Steve Furber on Neuromorphic Computing.

To our great sorrow, Prof. Kurt Binder, former chair of the Scientific Council of the NIC, passed away last autumn. Prof. Binder was one of the driving forces in the HPC community in Germany, and particularly in the NIC. We deeply mourn his loss. In honour of Prof. Binder's inspiring and creative scientific contributions, we are organizing a special session and have invited several of his former colleagues and friends to speak about recent advances in simulations of condensed matter.

**Contact:** **Dr. Alexander Trautmann**

## JSC to Participate in the Jülich Summer Academy

From March to September 2023, Forschungszentrum Jülich is organizing the first Jülich Summer Academy (JSA) on "Future Computing Technologies: Hardware, Software and Algorithms for Scalable Simulation and Data Science". The JSA will offer numerous interesting workshops, lectures, summer schools, etc. The academy is open to young scientists, including students, doctoral researchers, and postdocs, as well as to other interested parties. The events will deal with quantum computing, neuromorphic computing, big data, and other topics. The JSA, which is designed as an ongoing series, will begin with quantum computing. New quantum technologies promise applications with unprecedented speed, precision, and efficiency. The quantum computer is probably the best-known example. Forschungszentrum Jülich is a European hotspot for quantum research, combining basic research, theory, and development.

JSC will offer all of its quantum computing courses, workshops, and summer schools under this new umbrella. Since the JSA will also provide insights into other topics of future computing technologies, JSC will also run selected high-performance computing courses, workshops, and its guest student programme within this framework. Further information on the JSA and its programme can be found at https://fz-juelich.de/en/jsa.

**Contact:** **Dr. Sabine Höfler-Thierfeldt**

## Guest Student Programme 2023

In summer 2023, JSC will again offer a guest student programme supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM). Within this programme, students studying natural sciences, engineering, computer science, or mathematics have an opportunity to familiarize themselves with different aspects of scientific computing. Together with local scientists, the programme participants work on different current topics in research and development. Depending on previous knowledge and on the participant's interest, the assignment is chosen from different areas. These fields include mathematics, physics, chemistry, neuroscience, software development tools, visualization, distributed computing, operating systems, and communication systems. Special emphasis is on the use of supercomputers.

The participants are expected to have knowledge of and experience in the computer-oriented branches of their subjects. The students should already have completed their first degree but have not yet finished their master's

degree. Additionally, a letter of recommendation from a university lecturer or professor is required for application.

The programme lasts ten weeks and takes place at JSC from 7 August to 13 October 2023. Students are encouraged to apply for the programme online. The closing date for applications is 30 April 2023. Further information can be found at: https://www.fz-juelich.de/ias/jsc/gsp.

**Contact: Ivo Kabadshow**

## JSC in New EU Centres of Excellence

Following a call by the EuroHPC JU in the EU's Horizon Europe Framework Programme for Centres of Excellence (CoEs), three new CoEs with JSC participation were recently selected for funding and held their kick-off meetings earlier this year. The aim of the CoEs is to advance the transition to exascale capabilities by developing and scaling up parallel codes, resulting in effective applications to address scientific, industrial or societal challenges and meeting the needs of the user communities. The CoEs target scientific and industrial applications and user communities running codes that aggregate pre-exascale workloads and may require exascale resources in the future, such as those provided by Europe's first exascale system, JUPITER, to be hosted at JSC. The new CoEs will run for four years (2023-2026). The German project partners receive 50% co-funding from the Federal Ministry of Education and Research (BMBF).

In a team of 12 project partners led by the Barcelona Supercomputing Centre, **ESiWACE3** focuses on preparing existing operational weather and climate prediction systems for the exascale era. The main objectives of ESiWACE3 are to transfer and establish knowledge and technologies for efficient and scalable Earth system modelling (ESM), to fill common technology knowledge gaps, to provide toolboxes based on co-developments, and to provide a sustainable community hub for training, communication, and dissemination of HPC for ESM in Europe. As a new partner in ESiWACE3, JSC will contribute to the establishment of a common ESM software stack across the participating EuroHPC sites. JSC will also contribute to the networking of training activities and the organization of hackathons focusing on the exploitation of JUPITER. Further information: https://www.esiwace.eu/

**Contact: Dr. Lars Hoffmann**

The **MaX CoE** is entering its third phase, focusing on the adaptation, optimization, and deployment on the upcoming exascale computers of world-leading applications that use quantum mechanics to study material sciences. The sixteen European partners under the lead of CNR (Italy) bring Europe's leading scientific software developers in this field together with HPC experts from the European supercomputing centres. FZJ is represented by PGI-1/IAS-1 in the field of application development, and by JSC in the area of computer technology exploration and co-design. The knowledge and experience gained in the project will be used to further develop the HPC and AI infrastructure at JSC. Further information: http://www.max-centre.eu/

**Contact: Prof. Estela Suarez**

**MultiXscale** builds on the success of E-CAM, a Horizon 2020 HPC CoE. It combines the competence of 14 partners from eight European countries and is coordinated by the National Institute of Chemistry in Slovenia. The overarching objective of the MultiXscale CoE is to increase productivity across the entire spectrum of scientists active in the domain of multiscale material simulation. It couples the scientific expertise of the CECAM network with the technical expertise of the European Environment for Scientific Software Installations (EESSI) to develop and deliver architecture-optimized application software stacks that support this community. MultiXscale will empower application developers with exascale-relevant continuous integration capabilities, including access to all architectures relevant to the European HPC ecosystem. It will provide a software stack that runs on laptops, personal workstations, in the cloud, and on the largest HPC systems and it will provide extensive training and support to the user and developer communities. The role of JSC is the extension and porting of a library for electrostatics solvers for particle simulations and the adoption of the load balancing library ALL to multiscale simulations and hybrid architectures. Further information: https://www.fz-juelich.de/en/ias/jsc/projects/multixscale

**Contact: Prof. Godehard Sutmann**

## Quantum Computing for Earth Observation Study (QC4EO)

On 15 March 2023, the project QC4EO study was launched with the participation of the ESA Technical Officer as the representative of the European Space Agency, which is funding this study. The project consortium is led by Forschungszentrum Jülich, a joint effort of Jülich Supercomputing Centre (JSC) and the Institute for Quantum Computing Analytics (PGI-12), and it includes Thales Alenia Space (France and Italy), the National Institute of Nuclear Physics (INFN), and IQM Quantum Computers.

The primary objective of this study is to investigate whether quantum computing (QC) can provide a quantum advantage to Earth observation (EO) applications within a medium to long timeframe, i.e. between the next 3–5 to 15 years. Specifically, the study aims to answer the following questions: How can QC enhance EO applications, and what software and hardware developments are required to achieve this quantum advantage? The study is scheduled to last 5 months and will involve multiple activities that will be carried out by its multidisciplinary consortium, comprising partners with different competencies, each a leader in their respective areas. In this way, a broad view will be obtained, ranging from state-of-the-art quantum technologies (with related bottlenecks) and

commercial needs to pure research and the development of innovative solutions with the potential to be breakthroughs in EO and beyond.

**Contact:** **Prof. Gabriele Cavallaro**

## JSC's Research Software Engineers at the deRSE Conference

On 20 February, the 2nd Conference for Research Software Engineering in Germany (deRSE) opened in Paderborn. The three-day event was the first in-person conference since the pandemic, but despite current uncertain times, members from the HiRSE_PS and OS4FZJ teams at JSC were enthusiastic to work hard as conference co-chairs, and made sure the conference went ahead with great success. Attendance was excellent with 150 research software engineers (RSEs) from across Germany and 15 JSC employees presenting and volunteering over the three-day conference. This conference brings together people who develop software for any field of research. These roles exist under many job titles from doctoral researchers and postdoctoral researchers to research associates.

If you missed out on this RSE Conference, save the date for the 'un-deRSE23' in September. In the Dornberger Schloss in Jena, the unconference format will allow attendees to truly create their own programme from a choice of short talks followed by round table discussions or breakout sessions, which can be workshops, demos, discussions, code reviews, or whatever you think should be part of this event. The call for submission is now open and you can get in touch with Claire Wyatt for further information.

If you would like to meet other like-minded research software engineers (with any job title) at Forschungszentrum Jülich, join the RSE chat channel #rse at https://chat.fz-juelich.de/channel/rse.

**Contact:** **Claire Wyatt**

## Highly-Cited Article in *Philosophical Transactions*

The paper "Can deep learning beat numerical weather prediction?", published by Martin Schultz and his team members in the Royal Society journal *Philosophical Transactions* in February 2021 was listed as the fifth most cited paper from this journal in that year and has also been highlighted as highly-cited paper in Web of Science. In this article (DOI: 10.1098/rsta.2020.0097), the authors claim that it should be possible to make accurate weather forecasts that are purely based on modern deep learning approaches. Less than two years later, three papers from major industry labs have demonstrated that this vision is becoming reality.

**Contact:** **Dr. Martin Schultz**

## Events

### GPU Programming Part 1: Foundations
Instructors: Dr. Jan Meinke et al., JSC
Date: 17–19 April 2023, 09:00–17:00
Venue: JSC, building 16.3, room 213a
https://go.fzj.de/2023-cuda

### EuroCC AI for Science Bootcamp
Instructor: Miguel Martinez, NVIDIA
Date: 17–18 April 2023, 13:30–17:00
Venue: online
https://go.fzj.de/2023-bootcamp-ai

### Celebration of the 25th anniversary of NIC
Date: 21 April 2023, 09:00–17:00
Venue: Dorint Hotel am Heumarkt, Köln
https://indico3-jsc.fz-juelich.de/event/95/

### Interactive High-Performance Computing with Jupyter
Instructors: Jens Henrik Göbbert, Christian Witzler, JSC
Date: 25–27 April 2023, 09:00–13:00
Venue: online
https://go.fzj.de/2023-interactive-hpc

### Programming in C++
Instructor: Dr. Sandipan Mohanty, JSC
Date: 8–12 May 2023, 09:00–16:30
Venue: JSC, building 16.3, room 213a
https://go.fzj.de/2023-cplusplus

### EuroCC Nways to GPU Programming Bootcamp
Instructor: Paul Graham, NVIDIA
Date: 15–16 May 2023
Venue: online
https://go.fzj.de/2023-bootcamp-gpu

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