

Retrospect on 25th Anniversary of the John von Neumann Institute for Computing (NIC)

The John von Neumann Institute for Computing celebrated its 25th anniversary in April in Cologne. The event showcased current research and explored disruptive computing technologies through keynotes and exciting discussions. In addition, tribute was also paid to Prof. Kurt Binder who unfortunately passed away last autumn. He was former chair of the NIC Scientific Council and one of the driving forces in the high-performance computing (HPC) community in Germany and particularly in the NIC.

The programme for the event reflected the organization's mission and achievements over the last quarter century. In particular, two keynote talks by Prof. Hidetoshi Nishimori and Prof. Steve Furber gave a deeper insight into current disruptive technologies. Nishimori's work helped to lay the theoretical foundations for the field of quantum annealing, and his insights continue to be important in advancing the state-of-the-art in quantum computing. Furber is one of the key designers of the ARM processor, which is extensively used to develop neuromorphic computing today. The ARM processor is a type of microprocessor architecture that is widely used in mobile devices, embedded systems, and other low-power applications.

In a panel discussion, Prof. Thomas Lippert and Prof. Thomas Schulthess together with Furber and Nishimori focused on the topic "beyond digital computing". This subject of high topicality and relevance also encouraged the audience to address their questions to the panel.

The NIC research groups are an integral part of the NIC and some of the groups' former and current leaders gave talks that proved to be another highlight. Further information is available at: <https://go.fzj.de/nic-25>.

Contact: [Dr. Alexander Trautmann](#)

Norbert Attig Retires

Having worked for over 34 years at the institute, Dr. Norbert Attig started the leisure phase of his partial retirement at the end of May 2023. In 1988, he joined the Central Institute for Applied Mathematics – the predecessor of JSC – as a young postdoc working as administrator of the then existing CRAY systems. A few years later, he took over new tasks to strengthen the support of supercomputer users. Within this framework, he organized several winter schools and conferences, and pushed the idea of participating in the ISC and SC exhibitions with a booth. Starting with the SC'98 exhibition, Norbert organized JSC's participation in these conferences for at least ten years.

In 2007, Norbert became head of the application support division at JSC – a position he held until October 2022. He also was very active as a science manager: he served as the topic speaker for the supercomputer facility in the Helmholtz programmes over three periods, represented the JSC in almost all compute time granting meetings, and became JSC's deputy head together with Thomas Eickermann in 2012. He made major contributions to the setup of the Gauss Centre for Supercomputing (GCS), its governance, and the GCS scientific steering committee, and he was involved in numerous nationally and EU-funded projects.

JSC bid farewell to Norbert Attig at JSC's summer event in September last year. In April, his achievements were also honoured at the celebration of the 25th anniversary of the John von Neumann Institute for Computing by the NIC community and collaborators from Poland and Cyprus with whom he maintained good connections over years.

JSC wishes Norbert Attig all the best for the coming years and finally for his retirement!

The position of deputy director of JSC has been taken over by Dr. Thomas Eickermann. The application support division is now headed jointly by Dr. Wolfgang Frings and Dr. Bernd Mohr.

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JUNIQ's Summer School on Quantum Information Processing

The Jülich Supercomputing Centre will host the summer school on "Quantum Information Processing – Applications on Gate-based and Annealing Systems" from 28 August to 1 September 2023. The school focuses on hands-on experience in developing and implementing algorithms on both gate-based devices and quantum annealers. The attendees will make use of the cloud-programming platform of the Jülich UNified Infrastructure for Quantum computing (JUNIQ) to access quantum devices located at the Jülich Supercomputing Centre. The hands-on sessions will be accompanied by several lectures covering basic concepts of gate-based and annealing systems, the design and implementation of use-cases, and big-picture lectures, all given by experts in the field. The summer school will be complemented by a poster session where attendees will present their research activities to each other. Further information and the registration form can be found at: https://go.fzj.de/juniqs_summer_school.

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News from the NIC Scientific Council

The Scientific Council of the John von Neumann Institute for Computing (NIC) held its annual meeting on 20 April 2023. The meeting was conducted by the chair of the council, Prof. Marcus Müller (University of Göttingen). After six years of enormous dedication, his term ends on 31 December 2023. Deputy chairwoman Prof. Christine Peter (University of Konstanz) has unanimously been elected as chairwoman and will take up office at the beginning of next year. Prof. Müller will still remain on the council as deputy chairman. Furthermore, Prof. Szabolcs Borsanyi (University of Wuppertal), Prof. Timo Dickscheid (FZJ), and Dr. Patrick Jöckel (DLR) were elected as new members and will begin their terms in January 2024.

Prof. Stefan Bornholdt (University of Bremen), Prof. Elena Innocenti (University of Bochum), Prof. Rolf Kuiper (University of Duisburg-Essen), Prof. Alexander Schug (University of Duisburg-Essen), and Prof. Ina Tegen (Leibniz Institute for Tropospheric Research) were elected as new members of the NIC Peer Review Board. Their terms of office will begin at the upcoming meeting of this body in October.

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NIC Excellence Project Awarded to Prof. Holger Gohlke

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its April meeting, the board decided to award the title to Prof. Holger Gohlke (University of Düsseldorf) for his project on ethylene-induced development processes in plants.

The small molecule ethylene is a gaseous plant hormone known to induce various developmental processes in plants, including fruit ripening, after binding to the plant receptor ETR1 (ethylene response 1). His project "Structural dynamics of apo, agonist-, and antagonist-bound full-length ETR1" studies how ethylene binding is transduced from the transmembrane domain of ETR1 to its C-terminal cytoplasmatic domains and how ethylene binding changes the structure and dynamics of full-length ETR1 using molecular simulations on the JUWELS Booster module. The studies are expected to provide pathways of information flow that lead to conformational or stability changes in the receptor. In collaboration with plant biochemists, an experimentally validated view of the structural dynamics of full-length ETR1 will be provided at the atomistic level.

For more details, see <https://go.fzj.de/nic-ep-2023-1>.

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New GCS Large-Scale Projects Started in May 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.

After computing time quantities were previously specified in core hours, the modularity of JUWELS requires the introduction of a new computing time unit. JSC is currently working with the peak floating point operations per year (FLOP/a) of the computing devices (CPU or GPU) available to approved projects. The computing time on Hawk and SuperMUC-NG continues to be given in core hours. Projects in this case fall into the category of large-scale only if they require at least 100 Mcore-h on Hawk, or 45×10^{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 19 projects from various scientific fields. In total, four projects were granted 1587 Mcore-h on Hawk, nine projects were granted 520×10^{21} FLOP/a on JUWELS, and six projects were granted 485 Mcore-h on SuperMUC-NG.

For more details of these projects, visit <https://www.gauss-centre.eu/results/large-scale-projects/>.

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Events

Introduction to parallel programming with MPI and OpenMP

Instructors: Ilya Zhukov, Dr. Jolanta Zjupa, Junxian Chew

Date: 14–18 August 2023, 09:00–16:30

Venue: JSC; Ausbildungsraum 1

<https://go.fzj.de/2023-mpi>