

Big Days on JUWELS

In the past, JSC successfully provided users with the option to run large jobs exclusively within a reserved time frame on the leadership-class system JUQUEEN – an offer known as “Big Weeks”. After the resolution in 2019 of initial problems affecting massively parallel jobs on its successor JUWELS, JSC now plans to continue this legacy, starting with regularly reserved days on JUWELS with exclusive access for large jobs – so-called “Big Days”.

Once the workflows are established, users will be able to profit to a greater extent from our state-of-the-art environment for massively parallel computing, including the upcoming JUWELS Booster Module. In the near future, the Big Days will lead to “Big Weeks”, an event series where a week is reserved for capability-size (large) jobs. Big Days and Big Weeks will provide an excellent opportunity for the execution of unique large-scale simulations and also aim to challenge the user community to enable their production workloads for higher levels of parallelism.

Both Big Days and Big Weeks are part of a wider initiative, our exascale application preparation services, which – amongst other activities – will also host the HPC Tunathon 2020, an optimization and scaling workshop on JUWELS CPUs and GPUs.

The first Big Day will take place on 10 March 2020, followed by another Big Day on 24 March. For more information on Big Days and Big Weeks, please refer to <https://fz-juelich.de/ias/jsc/exascale-preparation> and <https://fz-juelich.de/ias/jsc/juwels-bigdays>.

In case of questions, please contact the supercomputing support team at sc@fz-juelich.de.

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HPC Tunathon for CPU and GPU Optimization and Scaling on JUWELS

A five-day workshop will be held on 25–29 May 2020 at JSC for qualified teams of application developers to optimize and scale their code on the CPU and GPU nodes of JUWELS in preparation for forthcoming exascale systems.

Each team will be paired with and mentored by experts from JSC, Intel, NVIDIA, or the Performance Optimization and Productivity (POP) Centre of Excellence, who will be available to assist with a variety of tools and advice for executions with large numbers of nodes (up to the full system). The focus is on hands-on practical training in a cooperative atmosphere.

All users of JSC computer systems can apply to participate in the HPC Tunathon. However, only a limited number of teams of two or more developers can be accommodated and will be selected based on demonstrated and potential scaling to use large clusters of CPU and GPU nodes such as JUWELS (and JURECA). For further information, including a Tunathon Guide and registration, please visit the webpage <https://fz-juelich.de/ias/jsc/2020/HPC-tuna>

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Guest Student Programme 2020

JSC will once again host a guest student programme in summer 2020, supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and IBM. Within the programme, students with a major in natural sciences, engineering, computer science, or mathematics will get the opportunity to familiarize themselves with different aspects of scientific computing. Together with local scientists, they will work on a variety of current topics in research and development. Depending on the participants' previous knowledge and interests, their assignment can be chosen from different areas, including mathematics, physics, chemistry, neuroscience, software development tools, visualization, distributed computing, operating systems, and communication. Special emphasis is placed on the use of supercomputers.

Participants are expected to have knowledge and experience in the computer-oriented branches of their subjects. They should already have completed their bachelor's degree but not yet finished a master's course. Additionally, a letter of recommendation from a university lecturer or professor is required for application.

The programme will last ten weeks, from 3 August to 9 October 2020. Students are encouraged to apply for the programme online. The closing date is 14 April 2020. Further information can be found at <https://fz-juelich.de/ias/jsc/gsp/>.

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TOAR-II Started

The Tropospheric Ozone Assessment Report (TOAR), an international initiative with more than 200 participants from over 30 countries, has recently launched its second phase. TOAR-I has produced eight peer-reviewed articles in the journal "Elementa – Science of the Anthropocene" which have been cited about 240 times within less than two years, and a number of follow-up publications in other journals have also generated relatively high citation counts.

A big part of TOAR's success is its database of more than 1 billion global surface measurements, which is hosted and maintained at JSC. This database is unique in terms of the online analysis capabilities that are offered via the JOIN web interface (<https://join.fz-juelich.de>). JSC will play an even stronger role in TOAR-II as Martin Schultz from JSC has been appointed as co-chair of the initiative together with Owen Cooper from the National Oceanic & Atmospheric Administration in Boulder, Colorado, USA.

Work is ongoing to redesign the metadata schema of TOAR data to better adhere to FAIR data principles, optimize the performance of the database, and develop more automated workflows for data imports and metadata updates. Thanks to EUDAT's B2SHARE service, it is already possible to generate DOI-referenced data publications with rich metadata of datasets that have been submitted for inclusion in the TOAR database or that accompany a journal publication that is closely linked to the assessment report. Further information on TOAR can be found at <https://igacproject.org/activities/TOAR>.

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Retrospective of the 10th NIC Symposium

The John von Neumann Institute for Computing (NIC) supports research projects from a broad scientific spectrum including topics from astrophysics, biology, chemistry, elementary particle physics, material and matter sciences, earth and environment, computer sciences and numerical mathematics, fluid mechanics, and plasma physics. On 27 and 28 February 2020, computational scientists presented their research results at the 10th NIC symposium in Jülich. Since the first NIC symposium almost 20 years ago in 2001, this series of biannual meetings has become a valued tradition, highlighting a diverse range of computational sciences at NIC. As in previous years, the symposium was well attended this year with over 200 participants.

The participants were welcomed by the Director of JSC and NIC, Prof. Thomas Lippert. In his talk, Prof. Lippert emphasized the enormous importance of exascale

computing, which will shape the HPC landscape in the coming years, and gave some insights into the development of exascale computing at JSC. Additionally, he provided information on the latest status of the JUWELS Booster Module, which is scheduled to be installed and made available to scientists during the course of this year.

Recent results of the NIC projects were presented in 15 insightful talks and on about 120 posters. The symposium produced fruitful discussions after the talks and during the poster session and provided plenty of space for the exchange of ideas and experience in an interdisciplinary scientific environment. Following long-standing tradition, accounts of recent activities within projects on the Jülich supercomputers were compiled in the NIC proceedings. All accompanying materials are available at <http://www.john-von-neumann-institut.de/nic/nic-symposium-2020>.

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Looking Back at ESM User Forum 2020

A 20% share of the JUWELS Cluster dedicated to Earth System Modelling (ESM) has been financed by the Helmholtz Association (HGF). Researchers from all HGF institutions in the research field Earth and Environment are eligible to apply for resources on the ESM partition, together with their cooperation partners outside the HGF. Resources are primarily provided to the Helmholtz ESM project – advanced Earth System Modelling Capacity – for scientific software implementation and production runs as well as preparation of ensuing frontier simulations.

From 4 to 5 February 2020, the second ESM User Forum took place at Forschungszentrum Jülich. 31 scientists from the ESM community met at JSC to discuss issues and new developments related to the ESM partition of JUWELS and to prepare for the GPU-based JUWELS Booster, which will be installed later in 2020. This system will again feature a partition for ESM use. The first day of the ESM User Forum was dedicated to GPU usage and programming, and summarized first applications from the ESM project exploiting the existing GPU nodes on JUWELS. These nodes were also used for the hands-on session on GPU-accelerated libraries, where the group worked on the implementation of stencil operators using OpenACC, Cuda-Fortran, CUF, Python with NUMBA, and the domain-specific language GridTools.

On the second day, the focus was on pre- and post-processing of large datasets as well as I/O performance, an issue which was brought up by ESM project scientists during former workshops. During the hands-on session, the parallel performance of netCDF4 was explored and I/O optimization strategies were spotlighted. The ESM User Forum was followed on 6 February by the second project meeting of the Pilot Lab Exascale Earth System Modelling, a new Helmholtz incubator project led by JSC that aims to enable breakthroughs in ESM on future exascale computer architectures.

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