

## JSC @ SC21

The SC21 supercomputing conference will take place as a hybrid event (a mix of live and virtual participants) from 14 to 19 November 2021 in St. Louis, Missouri. JSC together with its partners ParTec and the Jülich Aachen Research Alliance (JARA) will present their diverse range of activities in November at JSC's virtual booth.

This year's highlight will be our virtual interactive event hosted on <https://www.virtualchair.net/events/sc21-fair>. Join us on 16 November starting at 19:00 MET and get the latest news on JSC@GCS's pathway to exascale with our pathfinder modular system JUWELS, obtain insights into the performance and application of the 75 PFLOP/s JUWELS Booster Module, Europe's first D-Wave system made available through the Jülich UNified Infrastructure for Quantum Computing (JUNIQ), and learn about intriguing research results from the Earth System Modelling community in four exciting talks. Furthermore, take the opportunity to virtually meet our experts and discuss these and other fascinating topics, such as our activities in the EBRAINS research infrastructure and the Fenix Infrastructure, or new developments and new features of our in-house developed HPC tools like LLview, SIONlib, JUBE, and Scalasca.

At the virtual booth, our co-design partner ParTec will present its expertise in the field of HPC and its significant contribution to the modular software stack. The DEEP projects will also present their latest developments. The activities and services of the JARA Center for Simulation and Data Science (CSD) will also be highlighted.

As part of the conference programme, JSC employees will organize the all-day online tutorial "Hands-On Practical Hybrid Parallel Application Performance Engineering", co-organize the "Research Software Engineers in HPC" workshop, give presentations in the "Efficient Distributed GPU Programming for Exascale" tutorial, present talks, and participate in special interest group sessions and panel discussions. For detailed information and access to our virtual event, please visit <https://go.fzj.de/jsc-at-sc21>.

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## Artificial Intelligence Enhances View into Space

In their search for distant galaxies, rapidly rotating neutron stars, and black holes, radio astronomers are collecting an ever increasing amount of data. Data will be generated from the next generation of radio telescopes at rates comparable to the entirety of today's Internet traffic. Scientists are therefore looking for entirely new ways to cope with this flood of data. In future, machine learning and artificial intelligence will help researchers to filter out the exciting signals of the universe from the enormous volume of data.

To this end, eight institutions in North Rhine-Westphalia have joined forces under the leadership of the Max Planck Institute for Radio Astronomy (MPIfR) to form the "NRW Cluster for Data-Intensive Radio Astronomy: Big Bang to Big Data" (B3D). JSC's Simulation and Data Laboratory Astrophysics and Astronomy led by Prof. Dr. Susanne Pflanzner is part of this consortium. The main purpose of the alliance is to share knowledge as part of a network and to coordinate the activities of radio astronomers, data scientists, and industry partners. The JSC team will mainly focus on bridging the gap between simulations and observational data, preparing algorithms, and developing hardware concepts for the expected flood of data. The state is providing the B3D project with up to € 3 million in funding. Further details can be found at <https://b3d.nrw/>.

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## News from Jupyter-JSC

Jupyter-JSC was first launched four years ago and continues to grow at JSC with new functions and tasks. Today, it is part of the Helmholtz Cloud (<https://cloud.helmholtz.de>) and enables the use of the HPC systems at JSC. It also allows for the use of the HDF Cloud in everyday work entirely in the web browser and with just a few clicks via <https://jupyter-jsc.fz-juelich.de>.

JupyterLab's modern user interface is a highly functional, highly flexible intuitive web application that offers direct access to the login and compute nodes of our HPC

systems. While the classic terminal remains in the interface, the main advantage of JupyterLab is its modern access to data analysis. The short paths in JupyterLab from simulation to data analysis to visualization in the remote desktop have impressed many users over the course of four years. Today, about 500 JupyterLab sessions are initiated by around 100 different users via Jupyter-JSC each week.

As the number of users has grown, so too have the demands on Jupyter-JSC. The backend of the service was therefore fundamentally revised this year and made fit for further challenges. Kubernetes, in combination with Rancher, was chosen to ensure that the growing number of containers are stable, scalable, and easy to administer, and thus to significantly increase resilience.

Of course, these changes are not immediately visible to the user. More obvious is the possibility to now use JupyterLab 3 in addition to JupyterLab 2 via Jupyter-JSC. The highlights of JupyterLab 3 include the integration of a debugger frontend (currently for Python) and the simplified method of extending your own JupyterLab with prebuilt extensions.

As always, we welcome your feedback and suggestions and invite our HPC users to use Jupyter-JSC.

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## New GCS Large-Scale Projects Started in November 2021

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, 45 x 10<sup>21</sup> 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 15 projects from various scientific fields. In total, five projects were granted 955 Mcore-h on Hawk, six projects were granted 375 x 10<sup>21</sup> FLOP/a on JUWELS, and four projects were granted 270 Mcore-h on SuperMUC-NG.

For further information on these projects, please visit <https://www.gauss-centre.eu/results/large-scale-projects/>.

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## News Concerning the MaTSE Trainees

At the end of August 2021, 27 mathematical and technical software developer (MaTSE) trainees, who started their vocational training in 2018, passed their final examinations. Despite the severe restrictions in place as a result of the coronavirus pandemic, such as basic operations mode, home office, and digital learning, the latest set of trainees achieved good results. Lucas Reichert (IEK-4) achieved the top grade "very good", fourteen others were awarded the second best grade "good". These newly graduated trainees increase the number of MaTSE trainees successfully trained at JSC (since 1964) to 1232.

Twenty-six of the graduates decided to stay at Forschungszentrum Jülich. After graduating with a bachelor's degree in "Applied Mathematics and Computer Science", some of them will continue with the corresponding master's program at the Aachen University of Applied Sciences, Campus Jülich (FH Aachen).

On 1 September 2021, 26 new students began their bachelor's degree course in "Applied Mathematics and Computer Science" at FH Aachen (Jülich) in combination with MaTSE training at Forschungszentrum Jülich. They will complete their training at various Jülich institutes. The planned duration of the vocational training and the studies combined amounts to three years.

Those interested can already apply for the MaTSE training course starting in September 2022. The curriculum and further information can be found at <https://fz-juelich.de/matse>.

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## Events

### Introduction to Supercomputing at JSC – Theory & Practice

Instructors: JSC employees, representatives of Atos, Intel, and ParTec

Date: 22–25 November 2021

Venue: online

<https://fz-juelich.de/ias/jsc/2021/sc-2>

### Advanced Parallel Programming with MPI and OpenMP

Instructor: Dr. Rolf Rabenseifner, HLRS Stuttgart

Date: 29 November – 1 December 2021, 08:45–17:30

Venue: online

<https://fz-juelich.de/ias/jsc/2021/adv-mpi>

### 41<sup>st</sup> VI-HPS Tuning Workshop

Instructors: JSC employees, members of the VI-HPS collaboration

Date: 7–11 February 2022, 09:00–16:00

Venue: online

<https://go.fzj.de/2022-vi-hps>

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