High Resonance on JSC's Support Offer for COVID-19 Research

JSC together with its partners in the Gauss Centre for Supercomputing and in PRACE announced their offer for unbureaucratic and rapid support for COVID-19 research in March. Starting with initially three projects, another nine national and international projects dealing with the spread of the virus and with research on a medical or molecular level are receiving computing resources on JSC's HPC facilities and are being supported by JSC experts in code and algorithm development.

From Forschungszentrum Jülich three further groups have started their search for effective molecular inhibitors of the virus using computational biophysics approaches. The group led by Valentin Gordeliy (IBI-7 and Institute de Biologie Structurale, Grenoble) as well as the two NIC research groups "Computational Biophysical Chemistry", led by Holger Gohlke (JSC), and "Computational Structural Biology", led by Alexander Schug (JSC) are being supported with computing resources on the JURECA and JUWELS supercomputers. Furthermore, the group led by Jenia Jitsev (JSC) is working together with an international team of experts to develop an effective and efficient deep learning model for COVID-19 pattern detection in X-ray images with resources on the new JUSUF system at JSC.

Erich Wanker and Christopher Secker from the Max-Delbrück Centre for Molecular Medicine, Berlin have started a screening study on the JURECA cluster module to investigate the docking of small molecules to SARS-CoV-2 proteins. Besides the provision of computing resources, JSC experts are currently optimizing the codes for the JURECA booster module in order to increase the throughput and efficiency of this and further campaigns.

The group led by Gordon Pipa (Osnabrück University) is working with COVID-19 data from the Robert Koch Institute to model and describe the speed and type of local spread of the virus. The simulations are being performed on JURECA and JSC is assisting with code development, optimization, and data visualization.

Finally, three international projects have been granted access to JSC's HPC infrastructure. Adolfo Poma (Polish Academy of Science) is exploring conformational changes using force-field simulations, Alexander Viguerie (University of Pavia, Italy) is performing simulations of spatio-temporal COVID-19 spread using a coupled diffusion-SEIR model, and the group led by Rafael J. Villanueva (Universitat Politècnica de València, Spain) is working on a network model for studying the transmission dynamics of SARS-CoV-2.

For an overview on the supported projects, please visit https://fz-juelich.de/ias/jsc/covid-19-projects.

JSC and its partners are continuing their offer to support COVID-19 research and any experts who are interested should contact Thomas Lippert.

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JUSUF – New Multi-purpose Computing Platform for Neuroscientists

In May 2020, the new JUSUF (Jülich Support for Fenix) system started operation in JSC's data centre. JUSUF is a novel multi-purpose computing platform providing HPC as well as cloud resources in two separate sub-systems whose sizes are reconfigurable according to demand.

JUSUF is part of the Fenix e-infrastructure (https://fenix-ri.eu), which combines infrastructure components at the major European supercomputing centres of BSC in Spain, CEA in France, JSC in Germany, CSCS in Switzerland, and CINECA in Italy. The Fenix infrastructure is built up as part of the EU-funded ICEI project, through which the procurement and operation of JUSUF is also co-funded.

Resources on JUSUF are made available to European neuroscientists via a dedicated share of the system for the Human Brain Project (HBP) and the broader European research community via the PRACE-ICEI calls for proposals.

JUSUF, which is delivered to Jülich by Atos, consists of 205 nodes, each equipped with two of the latest-generation of AMD EPYC "Rome" 64-core processors, 256 GB of main memory, and a local 1 TB NVMe device.

61 nodes are equipped with an additional NVidia V100-16G GPU. The nodes are interconnected with a 100 Gb/s HDR InfiniBand interconnect in a full fat tree topology. The cluster sub-system of JUSUF, whose system software configuration is compatible with JURECA and JUWELS, accesses the central file systems from the JUST storage cluster. JUSUF is also connected to a share of the new high-performance JUST NVM storage layer, which will be operational soon. The cloud sub-system is based on Red Hat's OpenStack Platform and enables virtual machine hosting in the form of an Infrastructure-as-a-Service offering.

More information about the system can be found at https://fz-juelich.de/ias/jsc/jusuf.

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Jupyter-jsc: Supercomputing in Your Browser

Interactive supercomputing is currently gaining in importance and with it the browser-based development, workflow, and analysis web application JupyterLab. For one and a half years now, users of the HPC clusters at JSC have been able to access JURECA and JUWELS directly from their web browser via https://jupyter-jsc.fz-juelich.de with JupyterLab. Last year, support for the HPC cluster JURON and the OpenStack cluster HDF-Cloud was added. With the current update of the Jupyter-jsc service, direct access via the browser to the new HPC clusters DEEP and JUSUF is also possible.

Jupyter-jsc has continuously matured into a first-class citizen in the JSC ecosystem. Under the hood, Jupyter-jsc builds on the software building blocks of JupyterHub, UNICORE, and Unity-IdM and uses the possibilities of the HDF-Cloud to provide 24/7 availability and high scalability, e.g. for workshops. In this way, every user of our systems can easily and intuitively start JupyterLab directly in their web browser.

The latest update of the Jupyter-jsc service brings support for more HPC clusters as well as many other new features, such as more configuration options at start-up, support for dashboards, a uniform design, and of course bug fixes and improved performance.

But most of all, Jupyter-jsc can do one thing: it can quickly and reliably start a modern and feature-rich JupyterLab directly on the computing resources of the JSC and make it accessible ad-hoc for the user. We would like to thank the users for their many constructive suggestions. This will allow the JupyterLab installation to continuously adapt its functional range to the wishes of the research groups. We therefore continue to ask for feedback and are convinced that interactive supercomputing with Jupyter-jsc via https://jupyter-jsc.fz-juelich.de is of great benefit to our users.

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NIC Excellence Project May 2020

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its April meeting, the board decided to honour Prof. Ulf-G. Meißner (University of Bonn and Forschungszentrum Jülich) for his project "Nuclear Lattice Simulations". Atomic nuclei make up the majority of the matter around us. These strongly interacting systems are made up of protons and neutrons. The aim of Meißner's project is to gain a deeper understanding of the many remarkable phenomena in nuclear physics. This includes element formation in stars, the limits of the stability of atomic nuclei, the occurrence of substructures (alpha clustering), the thermodynamics of hot and dense core matter and the calculation of the corresponding equation of state. For more details, see http://www.john-von-neumann-institut.de/nic/meissner (in German).

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New GCS Large-Scale Projects in May 2020

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). Until now, projects were classified as "large-scale" if they required at least a combined 35 million core-hours (Mcore-h) per year on the GCS member centres' systems. These specifications for large-scale projects have been changed. From now on, projects fall into the category "large-scale" only if they require at least 100 Mcore-h on Hawk, 15 Mcore-h on JUWELS, or 45 Mcore-h on SuperMUC-NG. These values correspond to 2 % of the systems' annual production in terms of estimated availability.

The GCS Peer Review Board decided to award the status of a large-scale project to 20 projects from various scientific fields. Five projects were granted 1,590 Mcore-h on Hawk, five projects were granted 105 Mcore-h on JUWELS, and ten projects were granted 640 Mcore-h on SuperMUC-NG. In total, the GCS awarded about 2.3 billion compute core hours to large-scale projects. For more details of these projects, visit https://www.gauss-centre.eu/results/large-scale-projects/.

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Susanne Pfalzner Awarded the Albertus Magnus Prize for Teaching

Prof. Susanne Pfalzner from JSC was awarded the Albertus Magnus Prize for Teaching by the University of Cologne, Department of Physics, for her special commitment to teaching during the summer semester of 2019 in the course of her lecture series entitled "Philosophical Foundation of Research in Physics". The prizewinner was selected by the students of the department. The prize includes € 1,000 to be used for teaching. JSC congratulates Susanne on this recognition.