

## Earth System Modelling Symposium

JSC is organizing the Earth System Modelling (ESM) Symposium from 27 to 29 May 2019. The symposium brings together users of the Helmholtz ESM partition on JUWELS as well as computational scientists and system administrators from JSC. The event will take stock of Earth system modelling achievements that can be realized through the ESM partition, form the basis of problem-solving tutorials (with a focus on GPU usage), and provide a forum for discussing the future use of this resource and its integration in two planned Helmholtz-wide initiatives: Pilot Lab Exascale Earth System Modelling (PL-EESM) and Joint Lab EESM.

In 2016/17, the Helmholtz Association applied for and received supplementary funding for an additional compute partition (ESM partition) on the next-generation Tier-0/1 system JUWELS at Forschungszentrum Jülich, which is specifically dedicated to Earth system science simulations and big data workflows. This extension arrives in two instalments: the first part has been in operation since July 2018, while the second part will be set up in 2020.

The core concept of the Helmholtz ESM partition is to provide dedicated next-generation Tier-0/1 capability to Earth system science. This can be used for next-generation scientific software implementation, testing, performance analysis, and tuning, on the one hand, and for production runs and preparation of subsequent frontier simulations, on the other hand. Since the ESM partition is not realized as dedicated hardware, but instead as an equivalent share of compute time on the entire JUWELS system, it offers enormous flexibility to Earth system scientists within the Helmholtz Association. They can utilize the dedicated partition under their own governance, while at the same time making full use of the Tier-0/1 system at JSC, for example to perform frontier simulations. This concept offers strong synergies in terms of code optimization and project distribution within a fully equipped HPC system.

Further information on the symposium can be found at <https://indico-jsc.fz-juelich.de/event/94/>.

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## Data Projects Started at JSC

The migration to the new usage model at JSC in December 2018 initiated the separation of computing time and data projects. Data projects comprise a number of data resources that are located on specific file systems at JSC, each offering their very own characteristics regarding bandwidth, capacity, and retention time. They allow for project data to be managed beyond the scope of a computing time project. Among other things, this approach facilitates the prolongation of data resources across a series of computing time projects.

Initially, each ongoing computing time project has been granted a data project with its existing data resources and a duration aligned with that of the computing time project. In future, principal investigators of projects must apply for data projects in addition to their computing time projects in order to retain their existing data resources.

Four file systems are available within the scope of a data project: ARCHIVE, DATA, FASTDATA, and USER-SOFTWARE. The ARCHIVE filesystem offers high capacity for long-term storage at the expense of higher latencies when recalling data. The newly introduced DATA file system has been designed for large capacity at a reasonable level of performance. Its main usages are the sharing of data among projects, medium-term data storage, and making data available to JSC's OpenStack-based cloud environment, allowing for community-specific services based on community data. It is worth noting that the DATA file system is not available on the HPC systems' compute nodes, meaning that data staging must be employed to utilize the data within compute jobs. FASTDATA is intended for several higher volume projects that cannot employ data staging prior to executing jobs on JSC's HPC systems, for example because they use most of their entire data set for each job. USERSOFTWARE is a file system intended to share software installations among several projects. Other file systems, such as PROJECT and SCRATCH, are exclusively available to computing time projects and are not part of the data project grant.

The first round of applications for data projects resulted in approximately 50 projects requesting a total of about

15 PB storage space on ARCHIVE, 10 PB on DATA, and 10 PB on FASTDATA. These projects have now been set up and users are gathering first experiences with the new offering at JSC. Starting on 1 May 2019, users will be able to apply for data projects in a rolling call.

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## JSC at the 9th JLESC Workshop

From 15 to 17 April 2019, JSC colleagues participated in the JLESC Workshop at the University of Tennessee (UTK), Knoxville, USA. The event marked the ninth annual meeting of the Joint Laboratory on Extreme Scale Computing (JLESC) and was the first one hosted by UTK. The Joint Laboratory brings together researchers from the seven JLESC partners – Institut National de Recherche en Informatique et en Automatique (France), the National Center for Supercomputing Applications (USA), Argonne National Laboratory (USA), Barcelona Supercomputing Center (Spain), RIKEN Center for Computational Science (Japan), UTK, and JSC. The purpose of JLESC is to address science and engineering's most critical needs in the field of high-performance computing, and to enhance the ability of its member organizations and investigators to take advantage of the ongoing evolution of extreme-scale computing technologies.

With more than 100 scientists and students from the JLESC partners, the meeting in Knoxville covered a broad range of topics that are crucial to current and future supercomputing. Together with the other participants, 14 scientists and doctoral researchers from JSC and German partner universities learnt about the latest cutting-edge research from the fields of resilience, I/O and programming models as well as numerical methods, applications, big data, and performance tools. In addition to their talks, the participants had time for fruitful discussions about their ongoing and future research ideas during project meetings, round table sessions, and a social event.

Organized by JSC, the next JLESC workshop will take place at the Gustav Stresemann Institute in Bonn from 15 to 17 April 2020, building on this successful series of internationally recognized and highly valued meetings. For more information on JLESC and the workshops, please visit <https://jlesc.github.io/>.

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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 11 April 2019 at JSC. It was conducted by the chair of the council, Prof. Marcus Müller (University of Göttingen). At the meeting, Dr. Stephan Schenk (BASF), Prof. Berk Hess (KTH Royal Institute of Technology, Stockholm, Sweden), and Prof. Jochen Heitger (University of Münster) were elected as new members of the council and will take up their new positions in January 2020. The terms of office for Dr. Christian Beck (Siemens AG), Prof. Marc-Oliver Gewaltig (EPFL, Lausanne), and Prof. Hartmut Wittig (Johannes Gutenberg University Mainz) will end on 31

December 2019. Prof. Müller expressed his thanks to the researchers for the work that they have contributed thus far in the NIC Scientific Council.

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## NIC Excellence Project – May 2019

The NIC Peer Review Board regularly awards "NIC Excellence Project" status to outstanding simulation projects. At its April meeting, the board took the decision to honour Prof. Lars Pastewka (University of Freiburg) for his projects "Friction of (hydro-)carbons at surfaces: Adsorbed surfactant layers and amorphous carbon" and "Micro-mechanics of metals: non-affine deformations and phonons". The projects, which have been granted computing time on JUWELS, use large molecular dynamics calculations to understand frictional processes in exemplary material systems. Friction is responsible for 20% of global energy consumption and wear determines the lifetime of a mechanical component. There is still a lack of quantitative understanding regarding these phenomena, however, since the underlying processes require models that span many length scales and often depend on the material under consideration at the molecular scale. The results will reveal how energy is dissipated and how a material's microstructure and surface topography respond to mechanical load. This will enable a rational optimization of material systems for reliable and energy-efficient mechanical components.

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## New GCS Large-Scale Projects in May

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – currently Hazel Hen (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are classified as large scale if they require at least 35 million compute core hours (Mcore-h). During its April meeting at JSC, the GCS Peer Review Board decided to award large-scale project status to 13 projects from various scientific fields. Three projects were granted 524 Mcore-h on Hazel Hen, 3 projects were granted 105 Mcore-h on JUWELS, and seven projects were granted 542 Mcore-h on SuperMUC-NG. In total, the GCS has awarded about 1.2 billion compute core hours to large-scale projects. For more details on these projects, please visit <https://www.gauss-centre.eu/large-scale>.

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## Events

### 33<sup>rd</sup> VI-HPS Tuning Workshop

Instructors: JSC employees, VI-HPS members

Date: 24–28 June 2019, 09:00–16:30

Venue: Jülich Supercomputing Centre, Rotunda

<https://fz-juelich.de/ias/jsc/2019/vi-hps-tuning>