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Launch of the Simulation Laboratory Quantum Materials

On 4 April 2017, the opening workshop for the new Simulation Laboratory Quantum Materials (SLQM) took place at JSC. The workshop featured a number of scientific talks given by leading experts from Forschungszentrum Jülich, RWTH Aachen University, and the University of Liège. Each talk dealt with diverse and emerging topics in the field of computational materials science, including correlated electron materials, topological magnetism, energy materials, and high-performance computing, to name but a few. The modern and interdisciplinary nature of the topics attracted a very lively audience of about 50 scientists from all over Germany. Each talk was followed by constructive discussions, which often spilled over into the break between sessions.

Thanks to its specific focus on high-performance computing within the context of quantum-based simulations beyond equilibrium, the SLQM workshop sparked interest in scientific communities recently introduced to computational science as well as established groups delving into new and challenging areas. Such interest is critical to the mission of the new SimLab, which intends to act as a high-level support structure for dedicated projects and to host research projects dealing with fundamental aspects of code development, algorithmic optimization, and performance portability. Current SLQM research activities are already focused on a large variety of topics, including the development of specialized eigensolvers, efficient preconditioners for density functional theory (DFT), massively parallel simulations of heterogeneous photovoltaic materials, and investigating material properties using machine learning methods. Further information can be found at *http://www.fz-juelich.de/ias/jsc/slqm*.
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CECAM Events 2017 in Jülich

Since 2010, Forschungszentrum Jülich has been an integral part of the node structure of CECAM, which now comprises the central organization in Lausanne and 18 nodes in Europe and Israel. This year, four events are scheduled to take place at the Jülich CECAM node, consisting of three tutorials and the well-established guest student programme.

The first event is a hands-on tutorial about the DFT code FLEUR, developed at Jülich by the group headed by Prof. Stefan Blügel (IAS-1/PGI-1). The tutorial is scheduled for 8–12 May 2017 and will take place at JSC.

The Guest Student Programme on Scientific Computing, which has been organized at JSC since 2000, is an integral part of CECAM activities and has continuously developed to become an international programme attracting students from all over Europe. From 7 August to 13 October, about 12 students will work in research groups at JSC in the fields of scientific computing, receiving an introduction to parallel computing with access to JSC's high-performance computing facilities.

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Another hands-on tutorial entitled "Explicit Chemical Bonding Analysis of Materials from High Performance First Principles Simulations" will run from 25 to 29 September 2017 at JSC and is organized by RWTH Aachen University. It provides an introduction to the *Lobster* code, which was developed in the group headed by Prof. Richard Dronskowski at RWTH. Realistic case studies will be considered by the participants, which will subsequently be executed and analysed on the parallel cluster JURECA.

A third hands-on tutorial, co-organized by the Jülich and Daresbury CECAM nodes, will take place from 4 to 6 October 2017. It focuses on computational fluid dynamics (CFD) introducing the community code *Saturne* and concentrating on large-scale applications. In addition to providing theoretical background information and an introduction to CFD, this workshop will run several case studies on the JUQUEEN supercomputer, which participants will have limited access to.

Tutorials are still open for applications and those interested are encouraged to visit the web pages for further information, *http://www.fz-juelich.de/ias/jsc/cecam*.
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Experiments with Pedestrians Conducted at the University of Melbourne

In March 2017, Prof. Majid Sarvi conducted a series of laboratory experiments together with colleagues from the Transport Engineering Group at the University of Melbourne to investigate the dynamics in pedestrian streams and to study the wayfinding inside complex spatial structures. Two JSC staff members from the Civil Security and Traffic division were invited to these studies. Within the framework of the cooperative project, which was entitled "A real-time modelling of crowd dynamics for disaster prevention", they supported the study in the planning phase and during the realization of the experiments through the collection of trajectories. Eight experimental setups were built and examined, including bottlenecks and rooms with multiple exits. In addition, different motivation levels were tested to analyse the influence of competition on the performance.
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Data Publication with B2SHARE

B2SHARE is a service developed within the EUDAT and EUDAT2020 projects. It is one of the services of the EUDAT CDI (Collaborative Data Infrastructure), which was established to sustain the operation of EUDAT services beyond the end of the projects. B2SHARE offers a solution for the publication of small-scale research data – approximately 1 GB – from diverse contexts. The service instance (*https://b2share.fz-juelich.de*) is operated by JSC and available to all researchers and scientists of Forschungszentrum Jülich as well as users of the Jülich supercomputers.

B2SHARE can manage research data in a single file as well as data distributed across multiple files. The research data and additional metadata are stored in a record. During the creation of a record, the user is asked to fill in the (community-specific) metadata. A persistent identifier (PID) is assigned to each record as a reference that allows users to find the data. The PIDs of B2SHARE can be used in publications to refer to the research data and are resolvable through the Handle System, which is the infrastructure for DOIs that are assigned to paper publications (*http://dx.doi.org*).

Before using B2SHARE, you need to create an EUDAT user account on the central EUDAT user identification service B2ACCESS, which is operated by JSC. You can easily create your account and login using, for example, your email address and password from Forschungszentrum Jülich GmbH. More information about using B2SHARE is available at *https://eudat.eu/services/userdoc/b2share-usage*.
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HPSC TerrSys Fall School 2017

The Centre for High-Performance Scientific Computing in Terrestrial Systems (Geoverbund ABC/J), together with the JSC SimLab Terrestrial Systems and supported by the Energy oriented Centre of Excellence for computing applications (EoCoE), is organizing the second international Fall School on Terrestrial Modelling and High-Performance Scientific Computing (HPSC) from 25 to 29 September 2017. The objective of this applied course is to provide the theoretical and technical context for terrestrial modelling in HPC environments utilizing stand-alone and coupled hydrologic, land surface, and atmospheric models. Using the Terrestrial Systems Modelling Platform (TerrSysMP), the course will take a comprehensive look at terrestrial modelling and HPSC in connection with real-world observations and data assimilation. Topics covered by condensed lectures and hands-on sessions will include model system setup, parallel performance and profiling, coupled models, big data strategies, and data assimilation. The course will be held at the University of Bonn with practical afternoon sessions on the JURECA HPC system. The school is intended for master's students and doctoral researchers, or postdocs with a keen interest in terrestrial modelling. The registration deadline is 15 May 2017. Further information and registration procedures at *http://www.hpsc-terrsys.de/fallschool*
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