"Industry Relations" Team Paves the Way to HPC Expertise

Since January 2016, JSC has provided a new central contact point for enterprises that wish to use HPC cluster systems for their R&D activities, manufacturing, or their products. The work of the "Industry Relations" team is inspired by various existing cooperations between JSC and industrial companies and by a generally increasing interest in and need for parallel computing in various fields of engineering and technology.

JSC therefore offers its expertise in HPC to potential customers from industry in the form of "simulation consulting", which ranges from software analysis and optimization techniques targeting small systems up to elaborate means of running highly parallel code on compute clusters with thousands of cores. Cooperations can be established on different levels, varying from short-term core consulting services up to large-scale project partnerships with intensive code treatment and performance enhancement. Last but not least, the Industry Relations team enables industry partners and SMEs to access Jülich know-how and experts in the rapidly emerging field of big data analytics.

This essential new interface provided by JSC emerged naturally from existing services and capabilities and aims to facilitate the transfer of specific knowledge in the field of parallel computing to a wider industrial community and to further areas of applied research and development. It offers a tremendous opportunity for cooperations that can leverage the vast potential HPC is able to deliver to IT-based R&D. Further details can be found at *http://www.fz-juelich.de/ias/jsc/industry-relations.*
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Guest Student Programme 2016

During summer 2016, JSC will again offer a guest student programme. It is supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and IBM. Within this programme, students with a major in natural sciences, engineering, computer science or mathematics will have the opportunity to familiarize themselves with different aspects of scientific computing. Together with local scientists, the participants will work on different topics of current interest in research and development. Depending on previous knowledge and on the participant's interests, the assignment can be chosen from different areas. These fields include mathematics, physics, chemistry, neuroscience, HPC tools, visualization, distributed computing, operating systems and communication. Special emphasis is given to the use of supercomputers.

The participants are expected to have knowledge of and experience in the computer-oriented branches of their subjects. The students should have completed their first degree but not yet finished their master's course. Additionally a letter of recommendation from a university lecturer or professor is required.

The programme will last ten weeks from 1 August to 7 October 2016. Students are encouraged to apply for the programme online. The closing date is 31 March 2016. Further information can be found at
http://www.fz-juelich.de/ias/jsc/gsp/.
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SiME - New Project in Civil Security

In order to help disabled people gain easier access, many buildings, e.g. sheltered workshops, as well as other venues are now accessible barrier-free. But how can such places be evacuated effectively if disabled people are involved? How can stakeholders be trained, evacuation plans be adjusted, and facilities be designed to make these sites safer? To answer these questions the joint project "Safety for people with physical, mental or age-related disabilities" (SiME) has been funded in the context of the "Research Programme for Civil Security" by the German Federal Ministry of Education and Research (BMBF) for three years since the beginning of February 2016. The project is coordinated by the Federal Institute for Materials Research and Testing (BAM). Other partners are Otto-von-Guericke University Magdeburg, Hochschule Niederrhein, Werkstatt Lebenshilfe, PTV Transport Consult GmbH, and Forschungszentrum Jülich.

The simulation of the process of evacuating a building enables bottlenecks to be identified and the evacuation time calculated. For this purpose, parameters of the realistic movement of persons involved are needed, but such data are as yet only available for people with unrestricted mobility. In SiME, the team from JSC will execute parameter studies for mixed traffic, i.e. for people with and without disabilities, and also analyse the process of movement of disabled people, e.g. transfer from a wheelchair to an evacuation chair, during an evacuation process. With the collected data, more reliable models should be obtained to also simulate the evacuation of sheltered workshops or homes for people with disabilities.
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Centre of Excellence MaX Operational

Materials research is an area that is expected to strongly benefit from the growing performance capabilities of future supercomputers towards exascale. Significant efforts are, however, necessary to enable applications for materials simulations, design and discovery for extremely parallel architectures. This is the mission of the European Centre of Excellence (CoE) MaX "Materials design at the exascale", which is coordinated by the Modena Laboratory of CNR Nanoscience (Italy). The CoE brings together five leading institutions for materials research and five leading European computing centres as well as other part-

ners. From Forschungszentrum Jülich, those involved are the Peter Grünberg Institute for Quantum Theory of Materials (PGI-1/IAS-1) and JSC. In December, the coordinator hosted a kick-off meeting of the CoE.

Within the CoE, leading European experts for computational materials science work together with experts for high-performance architectures and technologies. They collaborate on advancing a set of open-source materials simulation codes not only to add new functionalities but also to enable these applications for future exascale architectures. By developing domain-specific libraries and promoting sustainable programming models, the community as a whole will benefit from these efforts.

The CoE will also address new approaches to data-driven materials research. Future HPC systems will enable high-throughput calculations that generate large amounts of data. Translating data into knowledge requires a data ecosystem that allows data to be shared by different research groups who then will be able to apply different data analytics methods. For further information, visit *http://www.max-center.eu/*
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Intensive HPC Training for European Doctoral Students

Together with 16 other partners, JSC organizes a European joint doctoral programme that is highly interdisciplinary and brings together experts from various disciplines in computational science to train doctoral students to exploit high-performance computing for their research. The doctoral programme HPC-LEAP started in September 2015 and is coordinated by the Cyprus Institute.

In January, a very intensive training event on HPC architectures and large-scale numerical computation took place at JSC. Over a period of three weeks, experts from JSC, other Jülich institutes and external institutions held lectures on computer architectures, parallel algorithms, performance analysis, modelling and optimization, MPI and OpenMP programming, GPU programming, visualization, parallel I/O and mathematical libraries. The programme was supplemented by lectures on novel HPC architectures, brain simulation, scalable materials research and various exercises. The students were challenged by the projects, where small teams worked on the parallelization and optimization of different numerical tasks. Finally, the teams presented their results at a concluding colloquium and demonstrated how much they had learned during these weeks. All the students left JSC enthusiastic about the opportunities of using supercomputers for their research. We would like to thank all the lecturers and project tutors for making this intensive training course such a success. Further information at *http://hpc-leap.eu/*.
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