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ORPHEUS Project Successfully Finished

In January 2018, the ORPHEUS project concluded its activities at a one-day public workshop in Berlin. The aim of the JSC-coordinated project was the investigation of new experimental and numerical methods for fire safety in underground stations. The BMBF-funded consortium consisted of 13 partners from academia and industry as well as fire brigades. One of the major activities was the real-scale smoke dynamics experiments at the metro station Osloer Straße in Berlin. These experiments were mainly used for underground climate investigations and model validations. They were accompanied by test runs of new firefighting strategies for Berlin's fire brigade. To date, the project members have published more than 20 contributions at national and international conferences and in journals.

Within the project, four JSC PhD students contributed to the research activities. While two of them have already finished their doctoral theses, the other two are in the final stages of their studies. JSC's scientific contribution to the project was the development of new numerical methods for pedestrian and smoke dynamics in complex infrastructures. This covers the coupling and multi-variate analysis of smoke spread and evacuation simulations, as well as dynamic mesh refinement and GPU-based real time concepts for smoke spread simulations.

Further project and contact information, a publications list, and the agenda of the closing workshop can be found on the project webpage *http://www.orpheus-projekt.de*. (Contact: Dr. Lukas Arnold, *l.arnold@fz-juelich.de*

Guest Student Programme 2018

During summer 2018, JSC will again be offering 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 bachelor's degree 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 various current topics in research and development. Depending on previous knowledge and on the participant's interest, the assignment can be chosen from different areas. These fields include mathematics, physics, chemistry, neuroscience, software development 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. Students should already have completed their bachelor's degree but have not yet finished their master's. Additionally, a letter of recommendation from a university lecturer or professor is required for application.

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The programme will last ten weeks from 6 August to 12 October 2018. Students are encouraged to apply for the programme online. The closing date for applications is 25 March 2018. Further information can be found on the web at *http://www.fz-juelich.de/ias/jsc/gsp/*.
(Contact: Dr. Ivo Kabadshow, *jsc-gsp@fz-juelich.de*)

Third Big Blue Gene Week

In late January, JSC held its third Big Blue Gene Week on JUQUEEN and enabled users to run highly parallel applications for more than seven consecutive days. The interest in the event was particularly high and even made it necessary to limit the submission half way into the event. At the same time, it was extended by about 1.5 days to complete as many requests as possible. Scientific areas of interest included finite-element computations (FEM), computational fluid dynamics (CFD), neuroscience and quantum materials. Once more, users took the chance to perform highly complex and demanding calculations and leveraged the accessible compute power to tackle their scientific challenges. With JUQUEEN due to be decomissioned in late spring this year, this event was the last of its kind on this machine. JSC will continue to offer similar events on successor architectures. In particular, JSC plans to schedule a Big Week on its newly implemented JURECA Booster module.
(Contact: Dr. Daniel Rohe, *d.rohe@fz-juelich.de*)

CECAM Events 2018 at Forschungszentrum Jülich

Within the context of CECAM activities, Forschungszentrum Jülich organizes and runs a number of events each year focused on scientific computing with respect to electronic structure, materials science, soft matter and biophysics. This year, there are three central events planned at Jülich.

From 6 August to 12 October, the International Guest Student Programme on Scientific Computing will take place. JSC offers about 12 students the opportunity to work with scientifc groups on specific topics in the fields of scientific computing, data analysis or visualization (see 2nd article in this issue).

From 24-28 September, a tutorial on Monte Carlo methods for biophysical simulation will be organized by the Simulation Laboratory Biology at JSC. After an introduction to the basic concepts of Monte Carlo, more advanced topics like generalized ensembles will be introduced and put into the context of protein simulations. The tutorial is designed as a hands-on course, where attendees will be introduced to the simulation code ProFASi, a C++ written code, which is used for e.g. protein folding simulations.

This year, a new type of workshop – an Extended Software Development Workshop – will be organized in collaboration with the Centre of Excellence E-CAM. The topic for this workshop will be "Load Balancing for Particle Simulation Codes". Based on some implementations, which were developed or implemented at JSC, the aim is to collate different methods within a library, which can then be used in various simulation codes. The workshop will address state-of-the-art load balancing, technical necessities for existing simulation codes, and the requirements as well as design of interfaces between the library and existing codes. The workshop will be split into three phases. In May, there will be a first meeting to exchange ideas and create an initial first structure for implementation issues. The next two phases will consist of implementation stages, where participants will be invited to discuss and implement the software together and test it on available parallel architectures. The date of the last two phases has not yet been fixed. The workshop is mainly intended for members of E-CAM. Other interested parties should contact Godehard Sutmann (*g.sutmann@fz-juelich.de*).

All activities of the Jülich CECAM node can be found at *http://www.fz-juelich.de/ias/jsc/cecam*.
(Contact: Prof. Godehard Sutmann,
g.sutmann@fz-juelich.de)

Events

Parallel I/O and Portable Data Formats
Instructors: Sebastian Lührs, Dr. Michael Stephan, Benedikt Steinbusch, Dr. Kay Thust, JSC
Date: 12-14 March 2018, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 2
Info: *http://www.fz-juelich.de/ias/jsc/events/parallel-io*

Introduction to parallel programming with MPI and OpenMP
Instructors: Benedikt Steinbusch, Thomas Breuer, JSC
Date: 19-22 March 2018, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Info: *http://www.fz-juelich.de/ias/jsc/events/mpi-intro*

From zero to hero: Understanding and fixing intra-node performance bottlenecks
Instructors: Andreas Beckmann, Dr. Ivo Kabadshow, JSC
Date: 11-12 April 2018, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Info: *http://www.fz-juelich.de/ias/jsc/events/intranode*

GPU Programming with CUDA
Instructors: Dr. Jan Meinke, Jochen Kreutz, Dr. Andreas Herten, JSC; Jiri Kraus, NVIDIA
Date: 23-25 April 2018, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Info: *http://www.fz-juelich.de/ias/jsc/events/cuda*

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