



Jülich Supercomputing Centre

Real-Scale Fire Experiments in an Underground Station

In January 2017, the third real-scale fire experiments in the framework of the OR-PHEUS project were implemented. Again, the underground station Osloer Straße in Berlin was used for the fluid and heat flow experiments while it was closed overnight (01:00 to 03:30). This station consists of three underground levels with a platform length of about 100 metres. With a total heat release rate of about 150 kW, created by an array of propane torches, the initial phase of a fire was imitated. This initial phase is of special interest for determining safety measures. As the burners produce no smoke, artificial smoke was added to the hot air plumes to visualize the air movement and to reduce visibility. The mass and heat transport were captured with 660 temperature sensors, 20 carbon dioxide sensors, 10 sulfur hexafluoride sensors, 16 ultrasonic anemometers and 196 multi-criterion sensors for smoke, temperature and carbon monoxide. This data will be used to validate the simulation model and also to test small-scale models.

The artificial smoke allowed us to assess the visibility of information signs, which may be the only aid to orientation in a complex station. Optical measurements were made and also observations by individuals.

The Berlin fire brigade deployed about 50 firefighters and 15 fire engines to practise their new tactical approach under low visibility conditions in a complex underground station. Additionally, new technical equipment supporting orientation was evaluated under quasi-realistic conditions.

Further information about the partners and other activities is available on the project's website *http://www.orpheus-projekt.de/* (in German).

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JUQUEEN Extreme Scaling Workshop 2017

From 23 to 25 January 2017, JSC organized its eighth IBM Blue Gene Extreme Scaling Workshop. The entire 28-rack JUQUEEN Blue Gene/Q was reserved for over 50 hours to allow six selected code teams to investigate and improve the scalability of their applications. Ultimately, all six codes managed to run using the full complement of 458,752 cores, most with over 1.8 million threads.

MPAS-A (from KIT / NCAR) and the pe rigid body physics engine (University of Erlangen) were both able to display strong scalability to 28 racks and thereby become candidates for High-Q Club membership. After participating in the 2015 workshop, MPAS-A returned with a higher resolution dataset and substantially improved file I/O using SIONlib to successfully manage its largest ever global atmospheric simulation. While ParFlow (University of Bonn/IBG at Jülich) had recently demonstrated execution scaling to the full JUQUEEN without file writing enabled, during the workshop the focus was on investigating file I/O performance which remains a bottleneck. High-Q Club member KKRnano (IAS at Jülich) investigated the scalability of a new solver algorithm developed to handle a million

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jsc@fz-juelich.de www.fz-juelich.de/jsc atoms, while the latest version of **CPMD** was tested with a large 1500-atom system. Both of these quantum materials codes revealed performance limitations at larger scales. The final code was a prototype multi-compartmental neuronal network simulator, **NestMC** (JSC SimLab Neuroscience), which compared scalability of different threading implementations.

Detailed results for each code provided by the participating application teams were published in the JSC technical report FZJ-JSC-IB-2017-01, see *http://juser.fzjuelich.de/record/828084*.

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5th PRACE Implementation Phase Project

PRACE-5IP is the fifth in a series of PRACE implementation phase projects. It is funded as part of the H2020 framework programme and started on 1 January 2017. Like its predecessors, PRACE-5IP is coordinated by Forschungszentrum Jülich. It has a budget of nearly € 15.9 million, a duration of 28 months and 26 partners. Over 250 researchers from 49 organizations (including 3rd parties) in 25 countries will assist the PRACE Research Infrastructure and support the PRACE users. The PRACE-5IP kick-off meeting took place at the Greek Research and Technology Network S.A., Athens, from 1-2 February 2017 with over 130 participants. The project is designed to build on and seamlessly continue the successes of the Partnership for Advanced Computing in Europe (PRACE) and start new innovative and collaborative activities. These include: preparing strategies and best practices towards Exascale computing; coordinating and enhancing the operation of the multi-tier HPC systems and services; continuing advanced training and expanding the network of PRACE Training Centres; promoting take-up by industry and new communities and special offers for SMEs; collaborating with the ETP4HPC, CoEs and other European and international organizations on future architectures, training, application support and policies; and supporting users in exploiting massively parallel systems and novel architectures. The project will continue to organize well-known events such as PRACEdays, Summer of HPC or the International HPC Summer School in order to promote and support innovative scientific approaches in modelling, simulation and data analysis.

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PRACE 2017 Winter School in Israel

The PRACE 2017 Winter School "Fuelling Scientific Discovery with HPC Infrastructure" took place at Tel Aviv University, Tel Aviv, Israel, from 6 to 9 February 2017. The school was organized by the Inter-University Computation Center (IUCC) and attended by 58 participants from Israel, Spain, Italy, Turkey and Austria. Four lecturers from Israel and three from JSC provided expert knowledge on a range of topics. The school programme focused on providing a thorough introduction and overview of how to use PRACE resources and to raise awareness of the value of the resources available to local and regional users.

After an introduction to MPI and OpenMP, the participants learned why they should pay attention to parallel I/O and how to use it in their own program. This was followed by an introduction to parallel performance analysis and tuning. Next the focus moved to many-core architectures such as GPUs and Xeon Phi Knights Landing, including a session on how to approach GPUs from an algorithmic point of view. The school concluded with parallel sessions on LAMMPS and multiprocessing with Python. Each session consisted of a mix of lectures and hands-on exercises, for which the participants were granted access to computing resources in Tel Aviv and Jülich. A social event at the Milk & Honey Distillery, Israel's first whisky distillery, rounded off the event. (Contact: Dr. Jan Meinke, *j.meinke@fz-juelich.de*)

GPU Hackathon in Jülich

From 6 to 10 March, JSC hosted the first GPU Hackathon of 2017. In this series of events, programmers come together to enable scientific applications for GPUs, optimize the performance and parallelize them to many GPUs. The events are organized by Oak Ridge National Laboratory and hosted by different sites in Europe and the USA.

Ten scientific applications were accepted for this Hackathon. Every team was paired with two expert mentors who guided them through their individual acceleration process. The teams came from a broad range of disciplines including brain research, lattice QCD, materials science and fluid dynamics. While some teams already had a mature GPU application and used the event for more in-depth tuning, other teams came without any prior GPU knowledge and worked on taking their very first steps into the realm of GPUs. All the teams made optimum use of the available time, spending long hours at JSC. Every day, each team had to present their status and report on challenges during a scrum session. Fernanda Foertter (ORNL), who moderated the event, gave working items for each day to guide participants through the classical stages of GPU acceleration.

When the Hackathon concluded with final presentations by all the teams, everyone found that the time had been well spent and praised the intense working atmosphere. The closeness to the experts from science (CSCS, JSC, HZDR/MPI-CBG, RWTH) and industry (IBM, NVIDIA, PGI) was regarded as especially valuable. By Friday afternoon, over 1000 jobs had been submitted to JURECA and JURON. Four more Hackathons will take place in 2017, see *https://www.olcf.ornl.gov/training-event/2017gpu-hackathons/*

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