JSCNews

Jülich
Supercomputing
Centre

First JARA-HPC Symposium

The Jülich Aachen Research Alliance (JARA) will host its first JARA-HPC Symposium on 4-5 October 2016 in Aachen. Scientists from JARA-HPC combine a knowledge of massively parallel computing on supercomputers with the respective expertise from different research fields.

This symposium is jointly organized by members of simulation labs and cross-sectional groups from JARA-HPC at the Jülich Supercomputing Centre of Forschungszentrum Jülich and the IT Center of RWTH Aachen University. It aims at providing a platform for discussions on various aspects of the development of HPC applications. Participants will have the opportunity for an in-depth exchange with colleagues from different research fields who also make use of HPC systems in their scientific work. Focusing on the merits of interdisciplinarity, the symposium specifically addresses visualization methods and performance optimization in connection with application development in engineering and materials science as well as neuroscience.

Scientists are encouraged to submit extended abstracts on related topics by 27 June 2016. Authors of accepted abstracts will be invited to give a presentation at the JARA-HPC Symposium and will have the chance to extend their initial submission into a full paper of 8 to 10 pages LNCS style to be published in the LNCS Symposium proceedings after the symposium. Details on the submission format and further information about the symposium are published on the symposium website at *http://hpc-symposium.jara.org*. (Contact: Marc-André Hermanns, *m.a.hermanns@fz-juelich.de*)

BMBF Project ParaPhase Started

From 2 to 3 June 2016, the kick-off meeting of the BMBF-funded project "ParaPhase – Raum-zeit-parallele adaptive Simulation von Phasenfeldmodellen auf Höchstleistungsrechnern" took place at JSC, marking the official start of this three-year project. Led by Robert Speck's group at JSC, the consortium of six German partners targets the development of space-time parallel adaptive algorithms and high-order discretization methods to enable industry-relevant phase-field simulations with unprecedented resolution in space and time.

Phase-field models are an important class of mathematical techniques for the description of a multitude of physical and technical processes. Examples are the modelling of cracks and fracture propagation in solid media like ceramics or dry soil, the representation of liquid phase epitaxy for solar cells, semi-conductors or LEDs, as well as melting and solidification processes of alloys. The broad applicability and mathematical elegance of this approach comes at a cost, namely the significant computing effort required for the simulation of phase-field equations at large scales, demanding the use of modern HPC architectures.

The interdisciplinary consortium consists of two partners with long-standing experience in the particular field of applications (the groups headed by Heike Emmerich at Universität Bayreuth and Christian Miehe at Universität Stuttgart) as well as four partners with a strong background in methods, algorithms and HPC (the groups headed by Carsten Gräser at FU Berlin, Oliver Sander at TU Dresden, Robert Speck at JSC and Jiri Kraus from the NVIDIA Application Lab). While the algorithms developed in this project will be primarily used for studying fracture propagation and liquid phase epitaxy, these problem classes already represent a wide range of challenges in industrial applications. Based on the open-source software DUNE, the "Distributed and Unified Numerics Environment", the resulting algorithms will help to make large-scale HPC simulations accessible for researchers in these fields.

With two post docs and three PhD students fully funded by BMBF, this work will also contribute to educational efforts in the field of computational science and engineering, enabling young scientists to address the challenges of real-world applications with HPC-ready methods and algorithms.
(Contact: Dr. Robert Speck, *r.speck@fz-juelich.de*)

NIC Excellence Project May 2016

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its April meeting, the board decided to honour Dr. Alberto Martinez de la Ossa (DESY, Hamburg), who works in the field of plasma physics. The goal of his project is to study and design electron-injection techniques in plasma-wakefield accelerators for the production of high-energy and high-quality beams, suitable for applications in free-electron lasers (FELs). For more details, please see *http://www.john-von-neumann-institut.de/nic/exzellenz-2016* (in German).
(Contact: Dr. Alexander Schnurpfeil, *nic@fz-juelich.de*)

CECAM Tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems"

From 19-23 September 2016, JSC will again host the CECAM tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems" organized by SimLab Biology at JSC. Participants will be given an in-depth introduction to the theory and practice of simulating proteins and other biomolecules by atomistic Markov chain Monte Carlo (MC) methods. These methods are a computationally efficient alternative to molecular dynamics simulations, in particular for studying processes that act on longer time scales such as protein folding and peptide aggregation. While there are numerous training courses for molecular dynamics, students rarely get useful exposure to Monte Carlo techniques. To fill this gap, CECAM (Centre Européen de Calcul Atomique et Moléculaire) is now funding this five-day tutorial for the

second time. The open-source protein folding and aggregation package ProFASi developed at SimLab Biology will be used as a demonstration tool for the highly transferrable MC techniques. Participants will have access to JURECA for realistic tests of advanced parallel simulation techniques like replica exchange MC or Wang-Landau. Interested researchers can still apply and obtain detailed information on the tutorial content on the web page for the CECAM school: *http://www.cecam.org/workshop-1339.html*.
(Contact: Dr. Sandipan Mohanty, *s.mohanty@fz-juelich.de*)

Initial Phase of SAGE Project Successfully Completed

Capacity and performance requirements for future storage architectures can hardly be met by one single storage device technology. While hard drives continue to provide more capacity, they remain slow. Storage devices based on non-volatile memory are much faster, but also much more expensive. Hierarchical storage architectures with tiers optimized for capacity and others optimized for performance allow us to solve this dilemma. While the hardware technologies are available, integrated architectures including a suitable software layer are still lacking. The EC-funded project SAGE (Percipient StorAGe for Exascale data centric computing) addresses this gap.

At the beginning of June the project was subject to an interim review. The reviewers highlighted the good progress that had been made during the first 9 months of the three-year project. In this period, the focus was on establishing a co-design process and deriving requirements for the final architecture for different workloads. SAGE's application portfolio comprises a broad range of applications from a variety of research fields, which share the common aspect that they are coping or will have to cope with data volumes at extreme scales, as their problem domain scales upward.

The identified requirements are now used as input for the different R&D tasks within SAGE. In parallel, the application experts in the project will start to develop strategies for refactoring applications in order to efficiently exploit the features of SAGE. While there will be support for legacy codes, applications will have to be adapted in order to optimally exploit hierarchical storage architectures. Further information at *http://www.sagestorage.eu/*.
(Contact: Prof. Dirk Pleiter, *d.pleiter@fz-juelich.de*)

Events

International Workshop on Quantum Annealing and its Applications in Science and Industry
Date: 26-28 July 2016, 09:00-18:00
Venue: Jülich Supercomputing Centre, Rotunda
Info: *http://www.fz-juelich.de/ias/jsc/events/quaasi16*

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