

JSCNews

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Centre

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JUROPA – Successor System

In summer 2009, the first general-purpose part of JSC's dual architecture strategy – the supercomputer JUROPA together with the HPC-FF partition for the European Fusion Community – went into operation. It quickly became obvious that this system co-designed by JSC was very useful for our users, and in a final step, over 220 projects and more than 1000 users benefited from more than 95 % operational availability of the system. The demand for computing time on JUROPA in the bi-yearly calls was up to seven times higher than the maximum time available on the system.

After a five-year period, the end of this workhorse's lifetime cycle is now rapidly approaching. For this reason, the Supervisory Board of Forschungszentrum Jülich approved JSC's proposal to procure a successor system for JUROPA in its May meeting. This system will increase the total peak performance to about 2 petaflop/s without consuming more energy or requiring more cooling capacity. It is planned to have this system installed by the end of 2014. Until installation, the current system will still be available for user operation.

Currently, JSC is soliciting system proposals from different companies and hopes to finalize a contract as soon as possible. Additionally, we plan to make a small prototype system available in late summer with a similar architecture to the final system. Current users will be granted early access to ease the migration of their programs and to facilitate efficient use of a more modern

system architecture.

(Contact: Klaus Wolkersdorfer,
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Low Friction Using Immiscible Polymer Brush Systems

Within the NIC Research Group of JSC, Prof. Martin Müser and Dr. Sissi de Beer developed a method to reduce friction and wear between surfaces in relative sliding motion. The method is inspired by biological lubricants in which hydrophilic polymers keep an aqueous liquid from flowing out of the contact. The latter is the reason why – for example – human joints keep their lubricating properties at all times. Anchoring polymers to solid surfaces is an approach to mimic these biological lubricants: in good solvents, the polymers will swell and keep the solvent from flowing out of the contact.

A critical shortcoming of polymer brush lubrication is, however, that polymers on the opposing surfaces can interdigitate, which induces friction and wear. To prevent the latter, Müser reasoned that contacts between solvated hydrophilic and hydrophobic brushes would not interdigitate. Therefore, de Beer performed large-scale molecular dynamics simulations on JUGENE and JUQUEEN to show that employment of such asymmetric contacts between two different brushes, each of which prefers its own solvent, does indeed eliminate interdigitation of the polymers, which results in low friction and negligible wear. Experiments, which were performed in coopera-

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tion with Prof. Julius Vancso's group at the University of Twente, confirmed the results.

More information can be found in the article "Solvent-induced immiscibility of polymer brushes eliminates dissipation channels" in Nature Communications (DOI: 10.1038/ncomms4781).

(Contact: Prof. Martin Müser, m.mueser@fz-juelich.de)

New Deputy Chairman for NIC Scientific Council

The Scientific Council of the John von Neumann Institute for Computing (NIC) held its annual meeting on 10 April 2014 at the GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt. Prof. Marcus Müller (Georg August University of Göttingen) was elected new deputy chairman. He will support the re-elected current chairman, Prof. Kurt Binder (Johannes Gutenberg University Mainz), for the next three years, starting January 2015.

(Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

NIC Excellence Project 2014

At its April meeting, the NIC Peer Review Board decided to award an outstanding simulation project with the title of NIC Excellence Project. "The Strong Interaction at Neutron-Rich Extremes", submitted by Prof. Dr. Achim Schwenk (Technische Universität Darmstadt, Institut für Kernphysik), develops and employs new computational methods for the prediction of extreme neutron-rich matter in astrophysics and of exotic nuclei. The latter can be investigated, for example, at the Facility for Antiproton and Ion Research (FAIR).

(Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

Parallel-in-Time Workshop Held at JSC

At the threshold of the exascale era, there is an urgent demand for improved and new numerical algorithms. For time-dependent problems, the idea of concurrency in the time domain is attracting growing interest in many different communities. From 26 to 28 May, JSC and SPPEXA, the German Priority Programme "Software for Exascale Computing" (DFG SPP-1648), organized the 3rd Workshop on Parallel-in-Time Integration with a special focus on parallel multi-level methods in space and time. With 42 participants from academia, research and industry coming from 11 different countries, a broad spectrum of expertise was brought together to create a great ambiance for the successful exchange of ideas, new approaches and also pressing questions. The topics ranged from applied mathematics to climate and earth sciences as well as engineering sciences. With sufficient time for discussions and individual meetings, new collaborations were initiated and long-lasting contacts

renewed. This workshop was the third in a series of workshops for a fast-growing community, following the events at the universities of Lugano in 2011 and Manchester in 2013. In 2015, the 4th workshop will be held at TU Dresden as announced here at JSC, and further events are already envisaged for the following years.

(Contact: Dr. Robert Speck, r.speck@fz-juelich.de)

New Projects from JARA-HPC Seed Funds Granted

The High-Performance Computing section of the Jülich Aachen Research Alliance (JARA-HPC) has provided Seed Funds with the incentive to develop new ideas up to the point where they can attract subsequent third-party funding. The proposed projects should demonstrate a significant HPC reference and strengthen the collaboration between RWTH Aachen University and Forschungszentrum Jülich. In the recent Seed Fund Call, JSC researchers together with their colleagues from RWTH secured grants for three projects: "Interactive Volume Rendering of Massive Data on the Blue Gene Active Storage Architecture", "Development of a DEM process model for HPC of vibratory finishing", and "A method framework for high-performance data mining of Monte Carlo protein simulations". The projects will be funded for two years.

(Contact: Michaela Bleuel, Michaela.Bleuel@rwth-aachen.de)

JSC Expert Joins ISC Organization Team

Dr. Bernd Mohr, the performance tool team leader of JSC, has joined the organization team of the International Supercomputing Conference (ISC) as an Executive Consultant. In the past two years, he helped to organize the ISC scientific programme as a freelancer. Starting this year, he will divide his time between his existing tasks at JSC and new responsibilities for ISC. JSC wishes Bernd all the best for his new task!

Events

High-performance computing with Python

Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC

Date: 26-27 June 2014, 09:00-16:30

Venue: Ausbildungsraum 2, Jülich Supercomputing Centre

Registration: j.meinke@fz-juelich.de

Introduction to parallel programming with MPI and OpenMP

Instructors: Dr. Florian Janetzko, Dr. Alex Schnurpfeil, JSC

Date: 5-8 August 2014, 09:00-16:30

Venue: Ausbildungsraum 1, Jülich Supercomputing Centre

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