

JSCNews

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New NIC Research Group in Jülich

The three partners in the John von Neumann Institute for Computing (NIC), Forschungszentrum Jülich, DESY, and GSI Darmstadt, support supercomputer-oriented research and development through special research groups in selected fields of physics and the natural sciences.

In April, the new NIC research group "Computational Materials Physics" started work at JSC. It is headed by Prof. Dr. Martin Müser from Saarland University, who has many years of experience in computer simulations. He graduated in 1995 in Mainz with Prof. Kurt Binder and has worked at several international universities and research centres, including IBM's Watson Research Center in Yorktown Heights, New York. His focus is on the computer simulation of materials out of equilibrium and under extreme pressure, as well as on simulations in tribology, i.e. the science and engineering of interacting surfaces in relative motion.

(Contact: Prof. Dr. Martin Müser, ext. 9095)

Workshop CBSB 2011

Since 2006, a series of successful workshops with the title "From Computational Biophysics to Systems Biology" (CBSB) has been held, three times in Jülich and once in the USA. Its goal is to bring together scientists from various scientific fields to

bridge the gap between biological simulations at the molecular level and approaches to describe biological systems at the cellular level and beyond.

This fifth workshop will take place from 20 to 22 July 2011 at Forschungszentrum Jülich. It is jointly organized by JSC, the German Research School for Simulation Sciences (GRS), and Michigan Technological University (MTU). The workshop is dedicated to Harold Scheraga who will celebrate his 90th birthday later this year. Dr. Scheraga pioneered the use of computers in chemistry and biology, and his work has inspired many of the research areas that are the topic of these workshops. In the spirit of Harold Scheraga's work, this workshop will enable researchers from physics, chemistry, biology, and computer science to acquaint each other with current trends in computational biophysics and systems biology, to explore avenues of cooperation, and together to establish a detailed understanding of cells at a molecular level. Invited talks will highlight recent algorithmic developments in the life sciences and successful applications of high-performance computing. Several panel sessions will stimulate the exchange of views between the various scientific fields and the different approaches to understanding the biological systems in question.

For the full programme, see <http://www.fz-juelich.de/cbsb11>, where links to the programmes and proceedings of the earlier workshops can also be found.

(Contact: Dr. Walter Nadler, ext. 2324)

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Three New SimLabs at JSC

In the first half of 2011, three new Simulation Laboratories were established at JSC: Climate Science, Highly Scalable Fluid and Solid Engineering, and Ab Initio Methods in Chemistry and Physics, adding to the established JSC portfolio of Biology, Molecular Systems and Plasma Physics.

The new SimLab Climate Science has strong ties to its counterpart Climate and Environment housed at the KIT Steinbuch Center for Computing, Karlsruhe, and is committed to improving popular atmospheric chemistry and climate prediction models. The engineering and ab initio labs have been set up by the HPC branch of the Jülich Aachen Research Alliance (JARA-HPC), and will focus on high-profile supercomputing applications developed by groups at Jülich and RWTH Aachen University.

Each of these Simulation Labs offers advanced user support for supercomputing projects and carries out research on new algorithms and methods relevant to its respective community. Last autumn, JSC issued its first call for high-level support from the Simulation Labs, covering a wide range of tasks, including code performance analysis, scaling and restructuring to exploit the JUROPA and JUGENE systems. In this current pilot phase, work packages range from 1-2 person-months of JSC staff resources and are supplemented by an equivalent amount of manpower from the project partners. A workshop is planned for autumn this year to present the results of this activity prior to the next support call.

(Contact: Dr. Paul Gibbon, ext. 1499)

HPC Enables Knowledge Mining

A new research project, called UIMA-HPC, has been initiated to enable data mining applications to make efficient use of high performance computing resources. In the first phase, the focus will be on the bio-pharmacological area for which e.g. the PubMed database holds more than 20 million entries. Researchers in this field need to find answers to questions such as the following: For a given base structure, are there any structure variants already mentioned in literature, and if so, are there any indications of their effects? Are structure variants protected by third-party rights or are they freely available? These questions cannot be answered by sheer keyword searches. The information has to be made available to researchers in a compact and structured way in a timely manner.

The project has been set up to develop fast and efficient procedures to extract knowledge from unstructured data from all kinds of sources, such as texts, graphics, tables, diagrams, captions, and blogs. The project partners FHG SCAI, JSC, Taros Chemicals, and scapos will develop a system which embeds the de facto standard protocol for information

extraction UIMA (Unstructured Information Management Architecture) into an HPC framework based on UNICORE, thus enabling a new class of applications. UIMA-HPC is funded in part by BMBF and started on 1 April with a duration of three years.

(Contact: Mathilde Romberg, ext. 3703)

New Group for Application-Oriented Technology Development

To strengthen its competence in the (co-)development of new HPC architectures JSC has established a new group for application-oriented technology development. On 1 April 2011, Dirk Pleiter joined JSC and was simultaneously appointed professor for theoretical physics at the University of Regensburg. He has been involved in the development and deployment of several generations of machines optimized for lattice QCD simulations. The latest generation of such machines, QPACE (QCD Parallel Computing on the Cell Broadband Engine), was based on IBM PowerXCell 8i processors, which were interconnected by a custom network implemented on FPGAs. By means of a highly efficient implementation of the HPL benchmark by IBM and JSC, the architecture was proven to be particularly power-efficient and put QPACE in the number one spot on the Green500 list in 2009. Ever-more powerful new HPC technologies are emerging, providing ample opportunities for future architectures optimized for particular classes of applications.

(Contact: Prof. Dr. Dirk Pleiter, ext. 9327)

Events

Einführung in ParaView zur Visualisierung von wissenschaftlichen Daten

Instructors: Marlene Busch, Dr. Herwig Zilken, JSC

Date: Tuesday, 10 May 2011, 09:00 - 16:30

Venue: JSC, Ausbildungsraum 2 (building 16.3, room 004)

Registration: ma.busch@fz-juelich.de, ext. 4100

Introduction to the programming and usage of the supercomputing resources at Jülich

Instructors: Representatives of IBM, Intel and ParTec, JSC staff members

Date: 16 May 2011, 13:00 - 17:30, and

17 May 2011, 08:30 - 16:00

Venue: JSC, Hörsaal (building 16.3, room 006)

Registration: dispatch.jsc@fz-juelich.de, ext. 5642

Agenda: <http://www.fz-juelich.de/ias/jsc/events/sc-agenda>

Debugging with DDT

Instructors: Representatives of Allinea Inc.

Date: Wednesday, 18 May 2011, 09:00 - 15:00

Venue: JSC, Hörsaal (building 16.3, room 006)

Registration: b.mohr@fz-juelich.de, ext. 3218

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