News from the NIC Scientific Council

The Scientific Council of the John von Neumann Institute for Computing (NIC) held its annual meeting on 14 April at GSI in Darmstadt. Prof. Kurt Binder from the Johannes Gutenberg University Mainz was elected new chairman, while Prof. Gernot Münster, the current chairman, was elected new deputy chairman. Also several new members were elected at the meeting: Prof. Dr. David P. DiVincenzo (RWTH Aachen University and Forschungszentrum Jülich), Prof. Dr. Volker Lindenstruth (Goethe University Frankfurt am Main), Prof. Dr. Marcus Müller (Georg August University of Göttingen), and Prof. Dr. Wolfgang Wenzel (Karlsruhe Institute of Technology). All will begin their terms of office in January 2012.
(Contact: Dr. Walter Nadler, ext. 2324)

NIC Excellence Projects 2011

At its meeting on 15 April at GSI, the NIC Peer Review Board decided to honour two outstanding simulation projects by awarding them the title of NIC Excellence Project. The projects receiving the distinction this year come from the fields of elementary particle physics and polymer physics. "Computing B_K with 2+1 flavors at the physical mass point", submitted by Dr. Christian Hoelbling, University of Wuppertal, for a Wuppertal-Jülich collaboration group, investigates nuclear matter with the goal of understanding the asymmetry between matter and antimatter. "Long-range correlations at polymer-solid interfaces", submitted by Prof. Dr. Wolfgang Paul, Martin Luther University Halle, has the goal of understanding the puzzling intermediate phase of nanocomposite materials using molecular dynamics simulations. For more details see *http://www2.fz-juelich.de/nic/Projekte/exzellenz-2011.html* (Contact: Dr. Walter Nadler, ext. 2324)

High Demand for Supercomputer Resources

Following the latest call for projects in February, the NIC Peer Review Board once again had the difficult job of assigning supercomputing resources for the next computing time period. About 50 groups from all over Germany requested more than four times as much computing time than was available for NIC projects on JUGENE, Jülich's Petaflop supercomputer. The demand was even higher for JUROPA, Jülich's general purpose supercomputer; more than 70 groups applied for about seven times the available resources. At the beginning of May, all applicants received information about the allocation of computer time.
(Contact: Dr. Walter Nadler, ext. 2324)

On the Origin of Carbon-Based Life

A major breakthrough in research into the creation of elements in the universe was recently made by simulations on JUGENE. Prof. Dr. Ulf-G. Meißner from IAS and IKP at Forschungszentrum Jülich gives a short description of his team's findings:

"Life on earth is based on carbon-12. Carbon is produced in massive, hot stars by the fusion of three alpha particles (helium-4 nuclei). More than 50 years ago, the astronomer Fred Hoyle predicted an excited state of the carbon nucleus with its energy tuned in such a way that a sufficient amount of carbon is generated. This new state was later called the Hoyle state. It was experimentally verified in 1957, but no one had ever been able to reproduce the Hoyle state from scratch, starting from the known interactions of protons and neutrons. This has now changed.

Earlier at IKP and IAS, Evgeny Epelbaum (now at Ruhr University Bochum), Ulf Meißner and collaborators had developed an effective field theory of the nuclear forces that had been successfully tested in few-nucleon systems. In collaboration with Dean Lee from North Carolina State University, they now put six protons and six neutrons on a discretized representation of space-time and calculated the spectrum of carbon-12 using Monte Carlo methods. In order to access the spectrum of carbon-12, they developed a new determinantal projection Monte Carlo scheme. Such an algorithm is ideally suited for JUGENE. The total CPU time used for the Hoyle state calculations was about 4 million CPU hours. Each run used 2048 parallel processors on JUGENE.

The Hoyle state appeared together with other observed states of carbon-12, proving the theory to be correct from first principles. The total disk storage used for the Hoyle state calculations is about 4 terabytes. With these stored configurations, we will now be able to analyse in detail the structure of the Hoyle state, such as its spatial extension or electromagnetic transition strengths. The method paves the way for solving other problems relevant to astrophysics, such as a precise calculation of the cross section of the carbon-12 alpha-particle fusion, which is of prime importance for the generation of oxygen-16."

(Contact: Prof. Dr. Ulf-G. Meißner, *u.meissner@fz-juelich.de*, *meissner@hiskp.uni-bonn.de*)

New PRACE Calls for Proposals – Tier-0 and DECI

The Partnership for Advanced Computing in Europe (PRACE) allows researchers from across Europe to apply for time on high-performance computers from a series of hosting nations.

The 3rd PRACE Project Access call for proposals for Tier-0 systems, the highest supercomputer class, is now open. Researchers can apply for access to three Tier-0 systems:

- IBM Blue Gene/P "JUGENE" (GCS@Jülich, Germany);
- Bull cluster "CURIE" (GENCI@CEA, France) and
- Cray XE6 "HERMIT" (GCS@HLRS, Germany).

Synchronized with this call, the PRACE Pilot Call for national systems (Tier-1) has also opened. After the end of the DEISA project (Distributed European Infrastructure for Supercomputing Applications), the former DECI calls are to be continued under the PRACE banner. The abbreviation DECI stands now for "Distributed European Computing Initiative". As part of this call, researchers can apply for support and access to Tier-1 HPC systems in Bulgaria, Finland, France, Germany, Ireland, Italy, The Netherlands, Poland, Spain, Sweden, and the UK.

Both calls will close on 22 June 2011, 16:00 CEST. Successful projects will start on 1 November 2011. For further information and the appropriate application forms, please go to *http://www.prace-ri.eu/Calls-for-Proposals*.

(Contact: Dr. Florian Janetzko, ext. 1446)

JSC @ ISC11

The International Supercomputing Conference ISC11 will take place this year from 19 to 23 June, once again at the Congress Center Hamburg. JSC will present its wide-ranging supercomputing activities at booth #132 in close collaboration with its partners in the Gauss Centre for Supercomputing (GCS) and the Gauss Alliance.

In particular, JSC will showcase scientific results obtained with its supercomputers JUGENE and JUROPA in 2D and 3D presentations. LLview, the comprehensive interactive monitoring software for supercomputers developed in house, will be presented in live demonstrations.

During the conference, JSC director Prof. Thomas Lippert will participate in the sessions on "Transpeta Flop/s Initiatives" and on the "European Open File System Initiative (EOFS)". JSC staff member Dr. Bernd Mohr (JSC) will present a "Crash Course on High Performance Computing", Wolfgang Frings will present a paper on "A System Level View of Petascale I/O on Blue Gene/P", and Dietmar Erwin will give a presentation on "E-Infrastructure for Science in Europe". JSC staff will also be present at the PRACE (#125), the UNICORE (#122), and the Intel (#530) booths. Do pay us a visit if you plan to attend the conference!

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

Events

Workshop: From Computational Biophysics to Systems Biology 2011
Date: 20-22 July 2011
Venue: Forschungszentrum Jülich, Auditorium
Info: *http://www.fz-juelich.de/cbsb11/*

If you would like to receive regular information on our events, please send an e-mail to *jsc-events-join@fz-juelich.de*.

Further events, talks, and training courses:
http://www.fz-juelich.de/ias/jsc/events