Access to US Supercomputers via UNICORE

The Grid middleware UNICORE will be deployed in the TeraGrid successor XSEDE, the largest US Grid infrastructure project to date. Offering free resources and services to more than 10,000 scientists, XSEDE has an overall budget of US $ 121 million and a grant period of five years. Among the 17 participating institutions that will receive funding from the US National Science Foundation (NSF), JSC is the only organization located outside the USA. UNICORE will play a prominent part in the project as it is to be deployed on all 16 supercomputers within the project. It will allow for easy and secure access to more than two petaflops of computing capability and more than 30 petabytes of online and archival data storage. JSC as a leading institution within the UNICORE Forum e.V. – a partnership of 26 organizations involved in developing and fostering the UNICORE Grid middleware – will manage and coordinate all XSEDE-related tasks and activities. Further information about XSEDE can be found at *http://www.xsede.org*
(Contact: Bastian Demuth, *b.demuth@fz-juelich.de*)

Tape Library Expansion to 80 PB

In January 2011, the regular monitoring of the two JSC tape libraries predicted that the filling degree will hit 100 % (15 petabytes) in 2012. At that time, it was thought that waiting for new tape technology to become available during summer 2011 would cause no problems: 5-terabyte tapes and corresponding tape drives were due to replace the old 1-terabyte components. For this reason, JSC contracted the upgrading of the tape libraries as soon as the new technology was obtainable and planned to install the new tape media in September 2011.

However, as some large projects produced more data than predicted in the first six months of this year, the projected growth of user data more than doubled. This led to a severe shortage of tapes as early as the end of July. Those users with the largest amount of data had to be informed that new space would not be available until October, as it would take some time to copy the old tapes to the new larger tapes.

The tape capacity bottleneck has now been eliminated. According to plan, the first step of the upgrade was completed in the second week of September. The current tape capacity is 25 petabytes. The contract foresees the delivery of new tape media with a total capacity of 80 petabytes within the next five years. If necessary, the contract can easily be expanded to 130 petabytes. More information is available at
http://www.fz-juelich.de/ias/jsc/tapes
(Contact: Lothar Wollschläger, ext. 6420)

Nu-FuSE Project Launched

Nu-FuSE (Nuclear Fusion Simulations at Exascale) is an international project funded through the G8 Research Councils Initiative on Multilateral Research Funding. It is coordinated by the University of Edinburgh,

and includes research teams in Cadarache, Garching, Jülich (JSC, IEK-4), Moscow, Princeton, and Tsukuba. The goal is to examine three specific scientific areas: fusion core plasma, the materials from which fusion reactors are built, and the physics of the plasma edge, scaling up the simulation codes in these areas to the "exascale" level. The ultimate aim is to couple these codes together as a step towards a fully integrated fusion tokamak model. To address this challenge, the project will initially concentrate on improving the performance and scaling of selected community codes, enabling larger orders of magnitude for simulations than is currently the case. In the process, the project will create an important new alliance between supercomputing and fusion science. Further information can be found at *http://www.nu-fuse.com/*
(Contact: Dr. Paul Gibbon, ext. 1499)

EUDAT – Data as an Infrastructure

The three-year EU-funded project EUDAT (European Data) will deliver a federated data infrastructure with the capacity and capability for meeting future researchers' needs in a sustainable way. The design will be driven through the data service requirements of the research communities in Europe and beyond. This infrastructure will become increasingly important over the next decade as we face the challenges of massive expansion in the volume of data being generated and preserved (the so-called "data tsunami") and in the complexity of that data and the systems required to provide access to it. JSC will be a cornerstone of the federated European data infrastructure and will develop core services for basic use as well as specialized services for communities. More information will be available at *http://www.eudat.eu* after the project starts in October 2011.
(Contact: Daniel Mallmann, ext. 2433)

CBSB11 in Retrospect

The fifth workshop in the series "From Computational Biophysics to Systems Biology" (CBSB) took place from 20 to 22 July 2011 at Forschungszentrum Jülich. This particular workshop was dedicated to the forthcoming 90th birthday of Harold Scheraga who pioneered the use of computers in chemistry and biology. It was jointly organized by JSC, the German Research School for Simulation Sciences, and Michigan Technological University. Fourteen invited talks covered the wide spectrum of workshop themes for the more than 100 participating scientists from all over the world. Particular highlights were five award talks by young scientists, selected by the organizers from the submitted posters, and five panel sessions where the invited speakers exchanged their varying views and opinions on understanding molecu-

lar biological systems among themselves and with the audience. The participants eagerly exploited this opportunity to get first-hand information on controversial approaches and on perspectives about the future of the various fields. In his closing remarks, Prof. Scheraga emphasized that he was thrilled with the quality of the discussions and talks, particularly those by the young scientists, and by the wide range of topics covered.

For the full programme and pictures from the workshop, visit *http://www.fz- juelich.de/cbsb11*. Online proceedings of the workshop will be available soon.
(Contact: Dr. Walter Nadler, ext. 2324)

MATSE: Exams Passed, New Course Started

At the end of August 2011, 33 MATSE trainees (mathematical technical software developers) passed their final examinations. During a ceremony on 6 September 2011, they proudly received their certificates and the congratulations from representatives of Forschungszentrum Jülich, the Chamber of Commerce Aachen (IHK), and Aachen University of Applied Science (FH Aachen). More than half of the trainees achieved an overall grade of at least "good"; a grade of "excellent" was achieved by Robert Elles (PGI-JCNS-TA), Sebastian Lührs (IEK-8), and Anna Westhoff (JSC).

On 5 September 2011, 34 new students started the bachelor's course in Scientific Programming at FH Aachen in combination with the training course as a MATSE at Forschungszentrum Jülich. Of these students, 22 will receive their practical training in various institutes at Forschungszentrum Jülich, while 12 students are with external partners (seven industrial companies and FH Aachen). Both the vocational training and academic studies are designed to take three years. The curriculum and further information can be found at *http://www.fz-juelich.de/matse*
(Contact: Prof. Paul Jansen, ext. 6430)

Events

Scientific Python
Instructors: Dr. Olav Zimmermann, Dr. Jan Meinke, JSC
Date: 10-12 October 2011, 09:00 - 16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Registration: *olav.zimmermann@fz-juelich.de*, ext. 1520

International Workshop on Simulation and Manipulation of Quantum Systems for Information Processing
Date: 17-19 October 2011
Venue: Jülich Supercomputing Centre, Rotunda
Info: *http://www.fz-juelich.de/smqs-ip2011*

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

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