

## JSCNews

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### Dr. Rüdiger Esser retires

After 20 years at the institute, Dr. Rüdiger Esser says goodbye to JSC. Starting as head of the former "Information Centre" division, he played a decisive role in organizing the support structure for supercomputer users. This role was continued when he later took over the "Programming Techniques" division and, finally, the "Computational Science" division. For a short time in 2003, he was acting director of the institute and has continued to be deputy director since Prof. Lippert's appointment.

At Esser's farewell party, Prof. Lippert and the previous director Prof. Hoßfeld expressed their gratitude to him for his good teamwork for the institute and emphasized his fairness, reliability and talent for organization. The staff thanked him for the pleasant working atmosphere he created at the institute by a medley of humorous speeches and poems. JSC wishes Rüdiger Esser all the best for his retirement!

In the future, the position of the deputy director of JSC will be taken over by Wolfgang Gürich and the "Computational Science" division will be headed by Dr. Paul Gibbon.

### Winter School on Multiscale Simulation Methods

Jülich will continue its successful series of Winter Schools in computational science. From 2 - 6 March 2009, the Winter School on "Multiscale Simulation Methods in Molecular Sciences" will be held in the rotunda at Jülich Supercomputing Centre.

More than 20 renowned scientists will present lectures on so-called "eclecticism in simulation". Eclecticism is a conceptual approach that does not keep rigidly to a single paradigm, but instead draws upon multiple theories or ideas to gain complementary insights into a subject. In particular, three sets of topics will be covered focusing on how to deal with hard matter, soft matter, and biomatter when it is necessary to handle different length and time scales:

- coarse graining of molecular systems and solids, quantum/classical hybrid methods, embedding and multiple time step techniques, creating reactive potentials, multiscale magnetism, hydrodynamic interactions
- mathematical and algorithmic aspects of multiscale approaches and their implementation on large, multiprocessor platforms including techniques such as multigrid and wavelet transformations
- fundamental simulation methods such as molecular dynamics, Monte Carlo simulation, and electronic structure calculations in the flavour of both wavefunction-based and density functional based methods

This Winter School is designed for PhD students and young postdocs from physics, chemistry, materials science or related disciplines with a solid background in basic quantum mechanics. Applications for participation must be received by the end of December 2008. On the basis of the applications, about 50 participants will be selected by the scientific organizers.

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Details of the School and the application procedure can be found at <http://www.fz-juelich.de/wsms>  
(Contact: Prof. Dr. Johannes Grotendorst, ext. 6585)

## Hermes Project

The Hermes Project, funded by the Federal Ministry of Education and Research (BMBF) and coordinated by JSC, started on 1 November 2008. In this project, JSC is cooperating with companies (PTV AG, Imech, Vitracom and TraffGo HT) and universities (Cologne, Wuppertal and Bonn). The aim is the development of an evacuation assistant to support security services in case of emergency and thus to improve safety at mass events. The main task of JSC is to build a model for pedestrian dynamics especially designed for real-time forecasting of the emergency egress of large crowds on parallel computers. The simulation core will be coupled with an extensive smoke detection system and a camera system for automated people counting in order to incorporate the actual status. In 2011, a test system of the evacuation assistant will be verified in the LTU Arena in Düsseldorf in cooperation with the Düsseldorf Fire Department and the North Rhine-Westphalia Police (LZPD). BMBF is funding the Hermes Project in line with the "Research Programme for Civil Security" as a part of the German High-Tech Strategy. The kick-off meeting for the project will take place at BMBF in Bonn on 25 November 2008.

(Contact: Dr. Armin Seyfried, ext. 3437)

## UNICORE 6 Migration Workshop

On 29 October 2008, the UNICORE 6 Migration Workshop took place in Langen (near Frankfurt), jointly organized by T-Systems SfR, the German Weather Service DWD, FhG-SCAI and JSC. The workshop addressed end users and system administrators from DWD in particular and the broad D-Grid community in general. Five presenters from T-Systems SfR, FhG-SCAI and JSC covered the following topics: architecture, client solutions, application integration, migration from UNICORE 5 to UNICORE 6 as well as data management and UNICORE 6. About 25 participants from DWD and the D-Grid community attended the workshop and initiated fruitful discussions. The presentations were recorded by the SuGI training project within the D-Grid initiative in order to preserve the training material for future use. The presentations in PDF form and also more information can be found at: <http://www.t-systems-sfr.com/u6/>  
(Contact: Dr. Achim Streit, ext. 6576).

## Young Stargazers Present Their Results

On 7 November 2008, the online workgroup project as part of the Year of Mathematics ended with a closing event in JSC's rotunda. This event attracted one third of the more than 130 active participants from 22 schools. During the

project period from 18 August to 30 September 2008, senior pupils downloaded small data sets of a computation describing the interaction and motion of 100,000 stars, computed next simulation steps, and uploaded their own partial results. Thus, the pupils simulated the formation of a spiral galaxy as well as the operation mode of the JUGENE supercomputer. The highlight of the closing workshop was a presentation of the 3D visualization of the collected results in the virtual reality showroom at JSC. The 2007 Nobel Laureate Professor Peter Grünberg congratulated the participants and awarded several internships at Forschungszentrum Jülich to the most active workgroups. Further information including a video is available at: <http://jdm.fz-juelich.de>  
(Contact: Oliver Bucker, ext. 3176)

## New MATSE and Bachelor Course Started

On 1 September 2008, 38 students started the bachelor course in Scientific Programming at Aachen University of Applied Sciences (FH Aachen) in combination with an apprenticeship as a mathematical technical software developer (MATSE) at Forschungszentrum Jülich. About half of the MATSE qualification is devoted to practical training. 24 students will receive practical training in various institutes at Forschungszentrum Jülich, 14 students are with external partners (seven industrial companies, the Max Planck Institute of Iron Research 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/jsc/matse>  
(Contact: Prof. Paul Jansen, ext. 6430)

## End of Year Colloquium 2008

- 09:00 Prof. Dr. Dr. Thomas Lippert: Begrüßung
- 09:15 Binh Trieu: Mögliches und Unmögliches in der Quanteninformation
- 09:45 Marc-André Hermanns: ParMA – Schinken und andere Köstlichkeiten
- 10:45 Annika Schiller: Schnelle Wavelets auf JUICE
- 11:15 Tom Schröder: Warum vertrocknende Pflanzen numerisch schwierig zu behandeln sind!
- 11:45 Dr. Jan Meinke: Proteine & Petaflops
- 14:00 Thomas Oistrez: Fit for Grids – Firewall-Hole-Punching als Dateitransfer für UNICORE
- 14:30 Morris Riedel: Der Multi-Grid-Mensch
- 15:00 Dr. Thomas Eickermann: PRACE – Petaflops für Europa
- 15:30 Prof. Dr. Dr. Thomas Lippert: Von Engeln auf Nadelspitzen zu Petaflops und Femtometern

The talks will be given in German.

Date: Thursday, 18 December 2008, 9:00 - 16:00 h

Venue: Hörsaal, JSC

Programme: <http://www.fz-juelich.de/jsc/events/eyc-2008>

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