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Excellence Prize 2014 Awarded to Armel Ulrich Kemloh Wagoum

Each year, Forschungszentrum Jülich awards the Jülich Excellence Prize for outstanding PhD theses. In 2014, Armel Ulrich Kemloh Wagoum from JSC was one of two winners. He accepted the prize during the official event "JuDocs 2014 - Karriere made in Jülich" on 14 June 2014, when Forschungszentrum Jülich bid farewell to 45 PhD students.

Armel Ulrich Kemloh Wagoum worked on his PhD thesis at JSC in cooperation with the University of Wuppertal between 2009 and 2012. The main topic of his thesis entitled "Route Choice Modelling and Runtime Optimisation for Simulation of Building Evacuation" was crowd management using computer simulation on HPC systems. He developed route choice techniques for pedestrians based on perception of the local environment and achieved a faster-than-real-time evacuation simulation of a stadium using a hybrid parallelization. The thesis was part of the BMBF-funded project Hermes, one aim of which was the conception and development of a real-time evacuation assistant for mass events. Dr. Kemloh Wagoum is currently working at JSC in the department of Civil Security and Traffic, where he is involved in the development of the Jülich Pedestrian Simulator (JuPedSim), for which his thesis laid the foundation. JuPedSim is a free, open-source tool for performing evacuation simulations with state-of-the-art pedestrian models. The first version of JuPedSim is being showcased on board the "MS Wissenschaft" – an exhibition ship which is currently traveling through Germany – and shows an interactive computer simulation of the evacuation of the ship.
We congratulate Armel Ulrich Kemloh Wagoum on receiving the prize!

CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-molecular Systems

Only a few bio-molecular processes happen on the microsecond time scale. Most take milliseconds or longer. This makes them inaccessible to atomistic molecular dynamics simulations. Atomistic Markov Chain Monte Carlo (MCMC), on the other hand, is a statistical method that is less sensitive to time scales and can be employed to study the thermodynamics of such processes. The Simulation Laboratory Biology is developing the open-source software package ProFASi to enable scientists to perform statistical investigations of bio-molecular systems using MCMC techniques.

From 15 to 19 September 2014, the SimLab Biology will hold a CECAM tutorial on atomistic Monte Carlo simulations of bio-molecular systems. Invited speakers and members of the SimLab will give lectures and practical sessions on the topic. These will be accompanied by hands-on sessions using ProFASi. Participants will learn how to perform and analyse MCMC simulations of bio-molecular systems. They will understand the principles behind this technique

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and recognize when MCMC would be helpful in their research and when not. Further information is available at *http://www.cecam.org/workshop-1067.html*.
(Contact: Dr. Sandipan Mohanty, *s.mohanty@fz-juelich.de*)

Calls for Computing Time Applications

The Gauss Centre for Supercomputing (GCS) will issue a new call for large-scale projects at the end of July. Proposals from publicly funded German academic and research institutions are eligible. Projects are classified as "large-scale" if they require 35 million core hours or more on a member centre's high-end system. Available systems are the IBM Blue Gene/Q system JUQUEEN in Jülich, the CRAY installation in Stuttgart, and the IBM iDataPlex SuperMUC in Garching. Further details can be found at
http://www.gauss-centre.eu/large-scale-application.

Applications can also be made for regular simulation projects on JUQUEEN and on the general-purpose supercomputer JUROPA at JSC. For more information, see
http://www.fz-juelich.de/ias/jsc/computingtime.

Finally, applications for computing time on the JARA-HPC Partition can be made via
http://www.jara.org/de/research/jara-hpc/partition/.

Online application will open on 29 July 2014. All applications should be submitted by Friday, 29 August 2014, 17:00 at the latest.
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

JSC Participates in the DFG Programme "Tailored Disorder"

The German Research Foundation (DFG) is establishing 16 new Priority Programmes (SPP), in which researchers will investigate fundamental scientific questions in particularly topical or emerging areas of research over the next few years. One of the programmes is the SPP "Tailored Disorder" with eight partners from German universities and research institutes, among them Prof. Kristel Michielsen from JSC. The research will focus on the development of novel optical technologies.

The last several years have witnessed considerable progress in the field of nanooptics. Up until now, a maximum degree of regularity was thought to be a prerequisite for perfect functionality – although nature itself yields a host of templates for how tailored disorder can be implemented on the smallest of structural scales. As such, the exact same starting material may produce the vibrant colours of the wings of a butterfly, while in beetles of the family Cyphochilus it yields a brilliant white, regularly scattered surface with an underlying three-dimensional nanoarchitecture. Only over the last couple of years have irregular structures been probed systematically for their potential relevance to optical applications. The programme partners will further tackle the potential inherent in this new class of materials.

The programme is coordinated by Prof. Silke Christiansen from the Helmholtz-Zentrum in Berlin (HZB) and will receive DFG funding to the amount of approx. € 12 million between 2015 and, foreseeably, 2021.
(Contact: Prof. Kristel Michielsen,
k.michielsen@fz-juelich.de)

Workshop Force Fields 2014

From 3 to 5 November, the NIC Research Group "Computational Materials Physics" will organize the workshop "Force Fields 2014 - From Atoms to Materials" at JSC. Force fields are, and will remain in the future, an indispensable tool for studying many-particle systems ranging from simple metals or ceramics to chemically heterogeneous systems including composite materials or biological molecules. The main advantage of force fields is their modest computational cost compared to first-principle-based approaches. However, in order to be both accurate and transferable, effective potentials need to be constructed properly to reflect the intricate quantum mechanics responsible for interatomic bonding and repulsion. Despite great progress during the last few decades, an abundance of materials cannot yet be simulated meaningfully in terms of classical force fields, in particular when defects, bond breaking, or chemical reactions matter.

The goal of the workshop is to focus on the construction of classical force fields while considering a broad variety of models such as bond-order, polarizable, charge-transfer, and embedded-atom potentials. It aims at informal discussions, a free exchange of ideas, and at the creation of new collaborations. Further information is available at *http://www.fz-juelich.de/ias/jsc/ForceFields2014*.
(Contact: Prof. Martin Müser, *m.mueser@fz-juelich.de*)

Events

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
Registration: *f.janetzko@fz-juelich.de*

CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-molecular Systems
Date: 15-19 September 2014
Venue: Rotunda, Jülich Supercomputing Centre
Registration: *http://www.cecam.org/workshop-1067.html*

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