

CECAM Tutorials at JSC



Since 2010 Forschungszentrum Jülich is an integral part of the node structure of the Centre Européen de Calcul Atomique et Moléculaire, which consists of the central organization in Lausanne and by now of 18 nodes in Europe and Israel. Since then Jülich organizes workshops, tutorials and visiting programs on a regular basis. In 2013, four events were organized, consisting of two tutorials, one workshop and a visiting programme for students. The tutorials took place at Jülich Supercomputing Centre in September.

The first tutorial, Fast Methods for Long Range Interactions in Complex Particle Systems (www.fz-juelich.de/fcs-2013), September 9 to 13 focused on providing an overview of algorithms and methods for treating long range interactions in computer simulations of particle systems. During this school, the scalable library ScaFaCoS (www.scafacos.de), which was developed in a nationwide network project funded by the Federal Ministry of Education and Research, was used to illustrate examples. Participants were encouraged to bring their own simulation codes to include the ScaFaCoS functionality. About 17 participants from 9 countries attended this event to learn about modern methods to treat long-range Coulomb interactions and reduce the numerical complexity from $O(N^2)$ to $O(N \log(N))$ or $O(N)$. Important objectives of the lectures were the introduction of modern concepts to implement these methods on parallel computers and to learn about parallel algorithms. Lecturers from the Universities of Bielefeld, Chemnitz, Stuttgart, Wuppertal and Forschungszentrum Jülich presented state-of-the-art methods, algorithms and implementations for parallel computers of various ap-

proaches to tackle the long range interactions in many-particle systems.

The second international tutorial, Multi-scale modelling methods for applications in materials science (www.fz-juelich.de/mmm-2013), was jointly organized by KIT Karlsruhe and Forschungszentrum Jülich. About 30 participants from 14 countries attended this event. 12 Lecturers from 8 countries gave lectures on research including a range of mutually coupled methodologies to overcome limitations induced by various length- and time-scales in the physical problem. The tutorial was closely related to the FP7 funded project MMM@HPC. It focused on the introduction of different methods, ranging from ab initio to coarse graining techniques. It also provided insight into modern workflow design and simulation tools. Various aspects from multiscale modeling, ranging from general overview over the field to more specific topics like coarse graining techniques or electronic properties of materials were introduced. Special focus was also given to introductions to community codes, used as parts in multiscale problems, like BigDFT, DFTB+, DL_POLY or Elmer. Furthermore, the middleware UNICORE was introduced as a basic part for designing workflows in complex simulation protocols. During the afternoon sessions, the participants could get first-hand experience with tools and application codes during practical programming lessons.

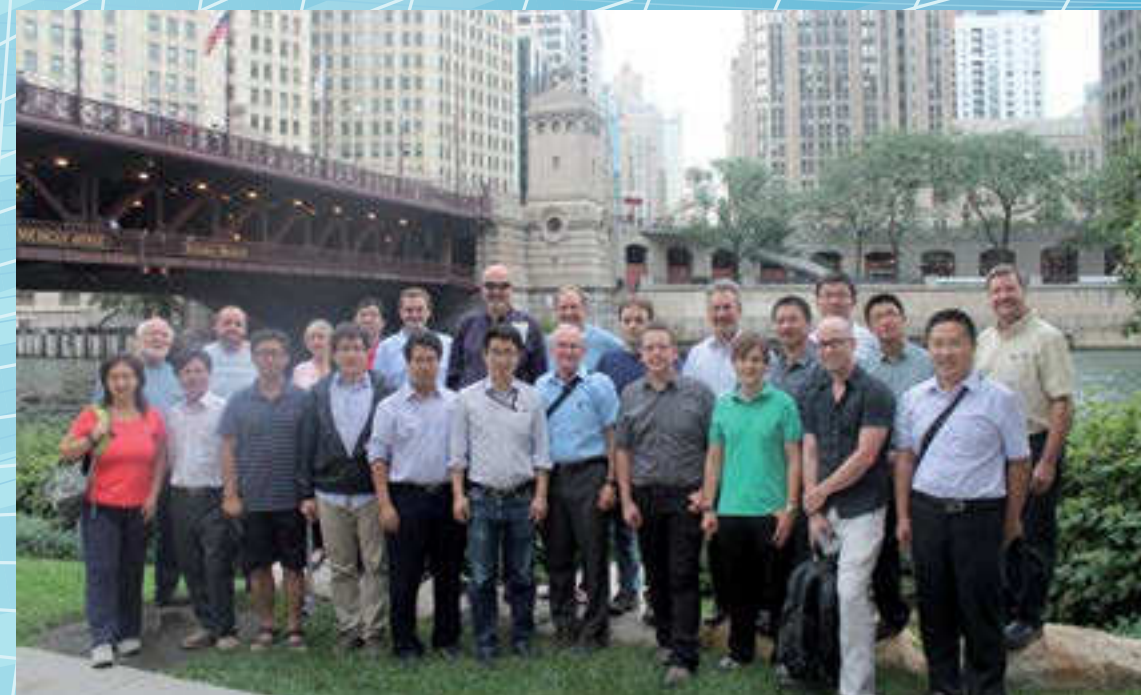
The other two CECAM events, i.e. the International Guest Student Programme and the workshop on Frontiers of computational biomolecular spectroscopy and mass spectrometry organized at Forschungszentrum Jülich are still ongoing and will be reported at a later stage.

CHANGES Workshop

The second workshop of the CHANGES series took place from September 10 to 12, 2013 in Chicago. CHANGES stands for CHinese-AmericaN-German E-Science and cyberinfrastructure.

This second CHANGES workshop addressed Data-Driven Science: "Data Management, Analytics and Visualization".

Again about 40 well-known experts



Partners are the Computer Network Information Center (CNIC) of the Chinese Academy of Sciences (CAS), the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC) and the Jülich Supercomputing Centre at Forschungszentrum Jülich. CHANGES provides a high-level platform to discuss latest trends in supercomputing, sophisticated information techniques and interdisciplinary applications. It will not only consider the issues of the partner institutions, but will also take national topics into account. The workshop series was founded in October 2011 and the first workshop took place in September 2012 in Jülich, where the topic High-Performance Computing "Performance Tools, Performance Modelling, and Algorithms" was covered.

came together by invitation and discussed latest data-related challenges in their research fields. In addition to several computer and domain scientists from JSC, Prof. Katrin Amunts from the Institute of Neuroscience and Medicine (INM-1) and Düsseldorf University, Prof. Henning Gast and Prof. Torsten Kuhlen from RWTH Aachen University were members of the German delegation. They talked about Big Data problems in their specific field of research. Besides the presentations, the workshop provided a forum for bi- and trilateral cooperations on student exchanges and mutual research projects. Special emphasis was placed on the question, how to select promising common research projects and how to secure funding for them.

• Godehard Sutmann

Jülich
Supercomputing
Centre (JSC)

• Norbert Attig

Jülich
Supercomputing
Centre (JSC)