FIRST WORKSHOP

JARA-HPC Simulation Laboratory
"ab initio Methods in Chemistry and Physics"

Date: 8th of November 2013

Preliminary Program

All talks have an allocated time of 20 + 10 minutes.

08:50 – Opening address by the organizers

09:00 – First session

- *FLEUR: the Jülich Full-Potential Linearized Augmented code*
  Dr. D. Wortmann (PGI-1/IAS-1)

- *GPU accelerators for PAW calculations: curse or blessing?*
  S. Maintz (RWTH-Chemistry)

- *Ab initio molecular dynamics simulations of phase-change materials*
  Prof. Dr. R. Mazzarello (RWTH-Physics)

- *JuRS: the Jülich Real Space code*
  Dr. P. Baumeister (JSC)

11:00 – Coffee break

11:30 – Second session

- *High-performance and automatic computing for simulation science*
  Prof. P. Bientinesi, PhD (RWTH-AICES)

- *The SoftWare Analysis and Tools (SWAT) Team @ JSC*
  Dr.-Ing. B. Mohr (JSC)

12:30 – Lunch break (Catering provided)

14:00 – Third session

- *Numbers and understanding in chemistry: hybrid methods (QM/MM and all other things)*
  Prof. A. L. Tchougréeff, PhD (RWTH-Chemistry)

- *Molecular Electronic Structure Methods*
  Dr. T. Müller (JSC)

- *KKRnano: the Jülich Korringa-Kohn-Rostocker code*
  E. Rabel (PGI-1/IAS-1)

15:30 – Coffee break

16:00 – Wrap-up session and concluding remarks

Workshop Objectives

This event aims at bringing together scientists from the main institutes within JARA participating in the Simulation Laboratory:

- The Institute for Advanced Simulation (PGI-1/IAS-1) – FZJ
- The Chair of Solid-State and Quantum Chemistry – RWTH
- The Jülich Supercomputing Centre – FZJ
- The Institute for Theoretical Solid State Physics – RWTH
- The High-performance and Scientific Computing group – RWTH.

Scientists from RWTH and FZJ institutes involved in *ab initio* computations are encouraged to take part in the workshop so as to favor exchange of scientific expertize conducive to future collaborations.

Simulation Laboratory Focus

The Simulation Laboratory *ab initio* Methods In Chemistry and Physics (SLAI) is funded by the Jülich Aachen Research Alliance--High-Performance Computing (JARA-HPC). The main activities of the laboratory are centered on:

- Supporting DFT-based simulations – The laboratory will act as an intermediary between the DFT community and experts in computing at

JSC, assist users in utilizing existing DFT codes, and participate in the organization of educational activities.

- Research on scalable DFT methods – Within the Laboratory research will focus on developing new DFT-inspired algorithmic variants, a novel framework for the handling and re-use of large data sets for code optimization, regression testing and statistics analysis. Moreover the Laboratory will take steps towards the expansion of the mathematical modeling of existing DFT methods leading to the development of new computational frameworks.

- Assisting with best programming practices – The Laboratory will provide assistance for porting and optimizing DFT codes on large parallel architectures, support for new parallel programming modeling as well as task-scheduling paradigms leading towards workflow scaling.