Opening Workshop of the Simulation Laboratory "Ab Initio"

Ab initio methods play a major role in the fields of chemistry, solid-state physics, nano-science and materials science. The impact of such methods has been steadily growing, currently generating computations which result in several thousands of scientific papers per year [1]. In order to keep up with this impressive output, it is crucial to preserve the performance and accuracy of ab initio simulations as the complexity of the physical systems under scrutiny is increased. Maintaining high performance and great accuracy poses significant challenges such as, for instance, simulating materials with interfaces, parallelizing and porting codes on new architectures, and converging the self-consistent field in Density Functional Theory (DFT) computations. In order to address these challenges, expertise in the fields of numerical mathematics, algorithmic development and hardware evolution is required.

There are three major factors hindering a straightforward achievement of performance and accuracy: 1) model diversity, 2) a need for scientific interdisciplinarity and 3) implementation heterogeneity. Model diversity emerges from the necessity of solving for a large spectrum of diverse scientific problems (e.g. band gaps, structural relaxation, magnetic properties, phonon transport, chemical bonds, crystallization, etc.) by simulating different aspects of a physical system. As a consequence ab initio methods have been realized in a rich variety of mathematical models, some examples of which are Density Functional Theory assorted discretizations, hybrid Quantum Mechanics/Molecular Mechanics methods and the Functional Renormalization Group approach, just to name a few. Driving the progress in all these methods requires an increasing cooperation within a multidisciplinary community which almost no working group worldwide can afford. Specifically there is a necessity to establish extensive collaborations between Physicists, Chemists, Computer Scientists and Applied Mathematicians.

Figure 1: Participants to the opening workshop of the ab initio Simulation Laboratory.

State-of-the-art codes are usually the result of a multi-person effort maintained over many years. The outcome is a large number of heterogeneous implementations, each one focusing on distinct physical aspects such as, for example, finite-size versus periodic systems or molecular versus solids compounds. Moreover, codes are written in a variety of styles and programming languages culminating in huge legacy codes which are difficult to maintain and port on new parallel architectures.

The Jülich Aachen Research Alliance–High-Performance Computing (JARA-HPC) [2] has established the Simulation Laboratory "ab initio methods in Chemistry and Physics" (SLai) [3] with the purpose of addressing all three main classes of issues. SLai is part of the strategic effort to improve the scientific collaboration between RWTH Aachen and the Forschungszentrum Jülich. Multidisciplinarity is deeply encoded in the DNA of the SimLab which connects the large community of ab initio application users with the code developers and the supercomputing support team. The mission of the Lab is to provide expertise in the field of ab initio simulations for physics, chemistry, nano-science and materials science with a special focus on High Performance Computing at the Jülich supercomputer facilities. It also acts as a high-level support structure in dedicated projects and hosts research projects dealing with fundamental aspects of code development, algorithmic optimization and performance improvement. Examples of current SLai activities are

- development of fast eigensolvers tailored to DFT methods;
- implementation of efficient tensor contraction kernels for Coupled Cluster methods;
- generation of improved data structures for FLAPW-based methods;
- development of a universal pre-conditioner for the efficient convergence of the charge density in DFT.

On November 8, 2013 SLai held its kick-off event at the Jülich Supercomputing Centre Rotunda Hall [4]. The workshop was designed to introduce the SimLab to the local condensed-matter physics and quantum chemistry communities, bringing together 50 scientists from institutes within JARA. By sharing their work and scientific expertise, the participants established a platform defining opportunities for mutual collaboration and prioritization of the SimLab's activities. Short informal talks were given by speakers from each of the main participating partner institutes and cross-sectional groups, followed by extensive constructive discussions between the speakers and the audience.

References

[1] Burke, K. Perspective on Density Functional Theory, J. Chem. Phys. 136, pp. 150901, AIP Publishing LLC 2012

[2] http://www.jara.org/en/research/jara-hpc/

[3] http://www.jara.org/hpc/slai

[4] http://www.jara.org/hpc/slai/kick-off

contact: Edoardo A. Di Napoli
e.di.napoli@fz-juelich.de

- Edoardo Di Napoli

JARA-HPC

Jülich Supercomputing Centre (JSC)

Activities