The Jülich Supercomputing Centre Launches the New SimLab Quantum Materials

The SimLab Quantum Materials (SLQM) was officially established on January 1st 2017 by the Jülich Supercomputing Centre, following the sun-setting of the JARA-HPC SimLab "ab initio methods in Chemistry and Physics". Strategically positioned at the intersection between HPC and materials science, two of the pillars of the Strategic Priority "information" of the Forschungszentrum Jülich, SLQM naturally bridges the gap between material simulations based on quantum mechanical methods and high-performance computing.

From the onset of the first theoretical breakthrough in the early '60s, passing through the first computational codes based on Density Functional Theory (DFT) to arrive to modern simulations involving hundreds if not thousands of atoms, materials science (MS) has evolved in a mature field producing 20,000 publications per year. This success was achieved by the continuous and painstaking effort that code developers placed in increasing the functionalities of their codes and, above all, in adapting their simulation codes to newer and more powerful computing platforms. This effort is still present today but, as simulation software gets bigger and more complex, is becoming increasingly difficult to maintain scalability, performance, and portability all at the same time. The evolution of computing architectures on the road to exascale is making the task of executing large scale and complex material simulations even harder. Due to the limited concurrency of algorithms currently used in MS, there is a huge burden that weighs heavily on the capability of executing simulations on both state-of-the-art and emerging massively parallel platforms. Enabling materials science codes to overcome such burden crucially depends on the design, selection and optimization of modern high-performance scalable algorithms. At present, this is the most critical challenge in the advancement of scientific computing in materials science.

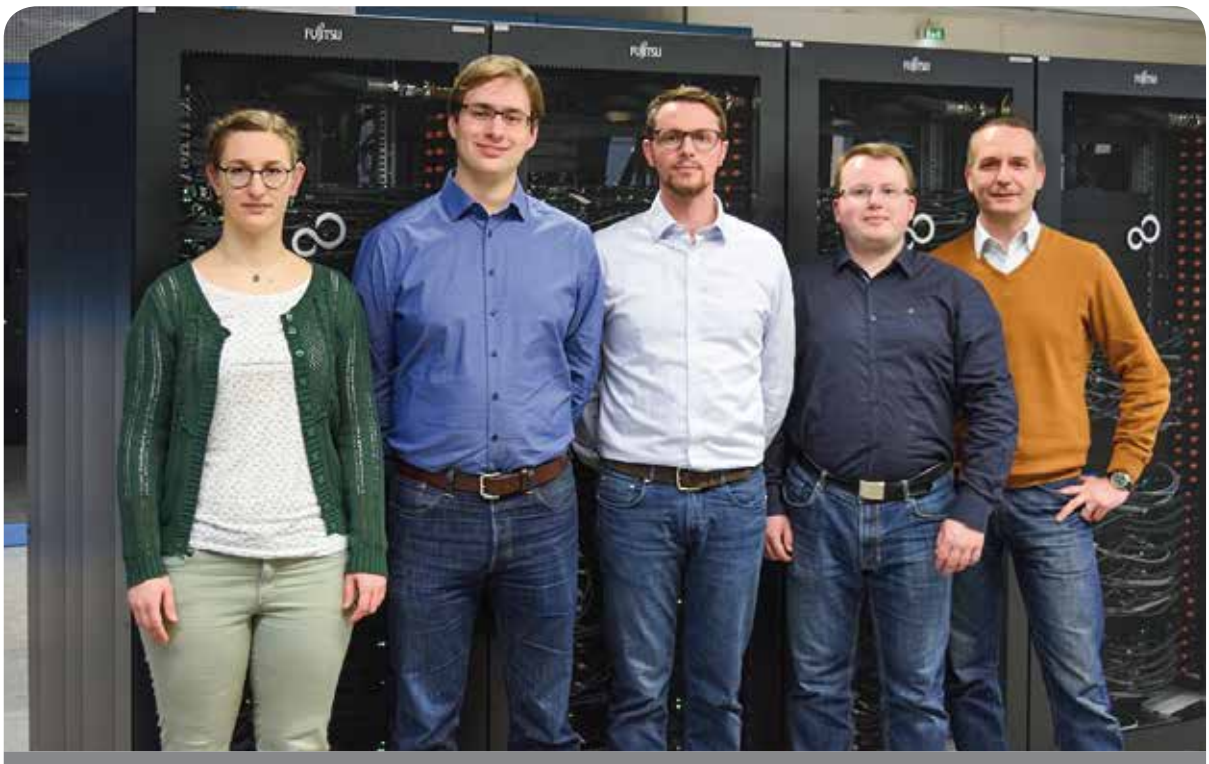
Research Activities

The new SimLab Quantum Materials [1] addresses the challenge exposed above with a research program centered on three specific activities. First, SLQM focuses on the development and maintenance of new modern numerical libraries tailored to specific linear algebra tasks emerging from materials science simulation software. For instance, a central task in DFT, as well as in more advanced methods dealing with excitation Hamiltonians, is the solution of an algebraic eigenvalue problem. Tackling the solution of large eigenproblems with traditional black-box libraries is not any more a feasible solution when the number of atoms (or the number of excited spectra) counts in the tens of thousands. To this end, SLQM develops and maintain new modern iterative eigensolvers [2] which are compute bound, portable and expose an increased level of parallelism.

A second area of activity deals with the design and implementation of high-performance algorithms targeting specific combination of operations extracted from simulation codes in the broad area of quantum materials. An example of recent work in this sense is the development of a performance portable algorithm, termed HSDLA, for the initialization of Hamiltonian and Overlap matrices in DFT methods based on the LAPW basis set [3]. Last but not the least, the Lab carries on research on the development of new mathematical models and computational paradigms aimed at improving performance, accuracy and scalability of simulations within a well-defined methodological framework. In this context an exemplary case is provided by the development of an adaptive preconditioner that would dramatically improve the convergence of Self-Consistent Field loops which appear almost ubiquitously in solving the Schrödinger equation.

Collaboration and Outreach

Inheriting the ongoing collaborations of the SimLab "ab initio", SLQM has an extensive network of contacts both at the national and international level. Such collaborations orbit around research activities on specific projects as well as more systematic cooperations on a number of cross-disciplinary topics. For instance, the Lab maintains a strong presence within the Aachen Institute for Computational Science



SimLab Quantum Materials team

and Engineering at the RWTH Aachen university and in particular with the High Performance and Automatic Computation group. At the international level, SLQM has active collaborations with groups working on algorithm and method development in the US and Japan.

The SimLab also has a keen commitment to outreach and education. Members of the Lab actively participate to international conferences and workshops. The Lab also organizes events and minisymposia that reach out to different materials science communities as well as to the more general Computational Science and Engineering crowd. SLQM is actively engaged to form a new generation of interdisciplinary scientists that will constitute the backbone of future communities engaged in computational materials science.

Opening Workshop

On the 4th of April 2017, the SimLab Quantum Materials held a one-day event at the Rotunda Hall of the Jülich Supercomputing Centre [4]. The workshop represented the official opening introducing SLQM to the scientific community. This event aimed at bringing together scientists from the Forschungszentrum Jülich (FZJ), RWTH Aachen University as well as international research institutes who were interested in participating in the research and support activities of the SimLab. By sharing their work and scientific expertise the participants were given the chance to contribute to the definition of a platform allowing for the mutual collaboration and prioritization of the Lab's activities. Each talk dealt with diverse and emerging topics in computational materials science including correlated electrons materials, topological magnetism, materials for energy, and high-performance computing, just to name a few. Each contribution was followed by constructive discussions, which often spilled over into the break between sessions. The modern and interdisciplinary nature of the topics attracted a very lively audience, comprised of about 50 scientists from all over Germany.

References

[1] http://www.fz-juelich.de/ias/jsc/slqm

[2] M. Berljafa, D. Wortmann, and E. Di Napoli: An Optimized and Scalable Eigensolver for Sequences of Eigenvalue Problems. Conc. Comp.: Pract. Exper. 27, pp. 905-922, 2015.

[3] E. Di Napoli, E. Peise, M. Hrywniak and P. Bientinesi: High-performance generation of the Hamiltonian and Overlap matrices in FLAPW methods. Comp. Phys. Comm. 211, pp. 61-72, 2017

[4] http://indico-jsc.fz-juelich.de/event/42/

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