Développement de codes de chimie théorique dans un environnement HPC

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Maximilien Levesque
Pôle de physico-chimie théorique, École Normale Supérieure
maximilien.levesque@ens.fr

Bernard Lévy
Laboratoire de Chimie Physique, Université Paris Sud
bernard.levy@u-psud.fr

Jean-Philip Piquemal
Laboratoire de Chimie Théorique, Université Pierre et Marie Curie
jpp@lct.jussieu.fr

1. Proposal

1.1 Introduction and motivation

Theoretical chemistry codes, including Molecular dynamics, Monte-Carlo or Qunatum Chemistry have been mostly written (in the best cases) in the 90s and 2000s. They thus fit to the computational paradigm of this time. They've been developed, distributed and maintained by large academic labs or dispersed communities, mainly anglo-saxon. They have indeed become important tools for chemists in both academic and industry laboratories.

However, these codes do not fit to the new paradigm of high performance computing, i.e., they are not designed for massively parallel architectures.

It is timely for the French community to take advantage of this change of paradigm, and to try to assess what are the strengths of the community, where are the needs for new methodological or algorithmic developments, which codes can be indentified within the community that could benefit from the expertise of HPC engineers at, e.g., Maison de la Simulation, a joint effort of CEA, CNRS, INRIA, Upsud and UVSQ in Saclay, or Institut du Calcul et de la Simulation at Sorbonne Universités, UPMC. Finally, the main objective of the workshop would be to identify a few grand projects which could gather the community around a few codes that are looking to the future.

1.2 State of the art

The 2013 report on French calculation centers [1] shows that the total processing power of these centers has increased by 188 % from 2012 to 2013. The order of magnitude has been the same for the last few years. This evolution is not explained by an increase of the processing power of a single cpu, but by the explosion of the number of cpu per (super)computer. Top 500 worldwide supercomputers have now exceeded the million of cpus. Very high parallelism is reached on the national machines at IDRIS, CINES, or TGCC.

Theoretical chemistry codes have not followed this change of paradigm. Gaussian, for instance, that is the most widely used quantum chemistry code, is limited to shared memory parallelism that implies at most few tens of cpu working together [2]. Today, very few theoretical chemistry codes do better than a few hundred cpus, even if there are some exceptions for Molecular Dynamics codes such as NAMD, GROMACS, LAMMPS or Amber, [3], and improved scaling for ab-initio MD codes working with plane waves. It should be noted that the production of the theoretical chemistry codes that are discussed above has been undertaken by academic players only. This is no more the case. It is now challenged by several other private companies like QChem, Schrodinger QuantumWise, [4] etc….

It is a well-known statement that the French community, although having always been at the heart of the initial developments (the Verlet group at Orsay for MD, or la rue du

Maroc in Quantum chemistry), has failed to produce and diffuse its own codes. This is only partly true nowadays, and a few initiatives have emerged, like QMCCHEM for quantum Monte Carlo (MC) or BIGDFT for materials. On the other hand, many French groups are deeply involved in international initiatives such as ABINIT, CP2K, TINKER, DeMON. Others have begun to develop their own libraries, like DOMINO for MC.

Aware of the changes in machine architectures and programming paradigms, French institutions have very recently supported new infrastructures dedicated to producing HPC codes, like La Maison de la Simulation [5], and L'Institut du Calcul et de la Simulation [6]. These laboratories are designed as places where computer scientists, chemists and physicists can meet and produce top-level HPC codes for state-of-the-art scientific problems. They can thus greatly help the code development initiatives noted above.

[1] http://calcul.math.cnrs.fr/IMG/pdf/2013_rapport_meso.pdf
[2] http://www.gaussian.com
[3] a) http://www.ks.uiuc.edu/Research/namd/ ; b) http://www.gromacs.org/;
c) http://ambermd.org/; d) http://lammps.sandia.gov
[4] a) http://www.q-chem.com/; b) http://www.schrodinger.com/;
c) http://quantumwise.com
[5] http://www.maisondelasimulation.fr
[6] http://www.ics.upmc.fr

1.3 Objectives

The aim of this discussion meeting is thus to gather major actors and code developers of the theoretical chemistry community, and as well as HPC specialists from L'Institut du Calcul and La Maison de la Simulation, in the perspective of promoting (a few) high performance code initiatives in theoretical chemistry. The code developers in the various fields will present their codes and will have to focus on the methodology, algorithms, code architecture rather than the science produced with it. The HPC specialists will set the state of the art in terms of code architecture and HPC programming.

1.4 Participant List

Andreas Savin	UPMC	savin@lct.jussieu.fr
Antony Scemama	Université Paul Sabatier	anthony.scemama@irsamc.ups-tlse.fr
Ari P. Seitsonen	ENS	apsi@iki.fi
Aurélien de la Lande	UPSud	aurelien.de-la-lande@u-psud.fr
Bastien Mussard	UPMC, ICS	bastien.mussard@upmc.fr
Bernard Lévy	UPSud	bernard.levy@u-psud.fr

Daniel Borgis	ENS, MdS	daniel.borgis@ens.fr
Eric Cances	ENPC	cances@cermics.enpc.fr
Fabien Leydier	IDRIS	
Fabio Sterpone	IBPC	fabio.sterpone@ibpc.fr
Francesco Sottille	Polytechnique	francesco.sottille@polytechnique.fr
François Jollet	CEA	francois.jollet@©cea.fr
François-Xavier Coudert	ENSCP	fx.coudert@chimie-paristech.fr
Guillaume Jeanmairet	ENS	guillaume.jeanmairet@ens.fr
Isabelle Demachy	UPSud	isabelle.demachy@u-psud.fr
Jean-Philip Piquemal	UPMC	jpp@lct.jussieu.fr
Julien Derouillat	MdS	Julien.derouillat@cea.fr
Julien Toulouse	UPMC	toulouse@lct.jussieu.fr
Louis Lagardère	UPMC, ICS	louis.lagardere@upmc.fr
Luc Belloni	CEA	luc.belloni@cea.fr
Lucia Reining	Polytechnique	lucia.reining@polytechnique.fr
Marco Saitta	UPMC	marco.saitta@upmc.fr
Maximilien Levesque	ENS	maximilien.levesque@ens.fr
Michel Caffarel	Université Paul Sabatier	caffarel@irsamc.ups-tlse.fr
Pascal Frey	UPMC	frey@ann.jussieu.fr
Philippe Dereumeaux	IBPC	philippe.dereumeaux@ibpc.fr
Pierre Kestener	MdS	pierre.kestener@cea.fr
Rodolphe Vuilleumier	ENS	rodolphe.vuilleumier@ens.fr
Thierry Deutsch	CEA	thierry.deutsch@cea.fr
Xavier Gonze	UCLouvain	xavier.gonze@uclouvain.be
Yvon Maday	UPMC	maday@ann.jussieu.fr

2. Financial Support

We ask CFCAM a support of 3000 €, for this Meeting, in order to cover logistic expenses, like coffee breaks (~ 500€), lunches for the participants coming from abroad (~ 500€), and travel expenses for selected young participants.