ABINIT hands-on 2019
A newcomer-oriented school to ab initio nanoscience simulations. From laptop to supercomputer

Proposal for partial funding by CECAM IdF French node

Proposed dates and place

A 5-day tutorial (4 nights) at Teratec campus (TGCC), Bruyères-le-Châtel.
January 21, 2019 to January 25, 2019.
30 participants, with access to the TGCC HPC resources.

Organizing committee

- Bernard Amadon (contact organizer), Sandra Boullier, Boris Dorado, Gregory Geneste, François Jollet, Marc Torrent (CEA Bruyères-le-Châtel)

Proposal – Scientific summary

With more than 1500 registered users, ABINIT [1-3] is nowadays a well-established open-source software package for the first-principles calculations of the properties of condensed matter (more than 2000 cites of ABINIT papers on ISI-WEB). One of the strengths of the package is the possibility of computation and analysis of **various physical quantities response to perturbation** (using the linear and non-linear responses formalism), **excited states** (using the many-body perturbation theory), **strong electronic correlations** (using the Dynamical Mean Field theory). Study of **transition paths** (NEB, string methods) and **energy landscapes** are also available

Some of these functionalities have been implemented fairly **recently** [1]. Extensive on-line tutorials and an active forum already provide a helpful basic support to users [4]. However, regular and recurrent questions on the forum highlight the limitation of such interactive formation tools and the need of additional concrete training formations in direct contact with ABINIT developers.

Moreover, with the experience of years, it appears that, although the basic usage of the code is available to everyone, an advanced and effective use **requires practice and advice from experienced users**. To use efficiently ABINIT, it is very important to deeply understand the connection between the input parameters and the physics. It is also essential to know how to adapt the calculation cases to the computing architecture. The use of supercomputers, in particular, requires some expertise.
The goal of this tutorial is to enable participants to learn the relevant techniques to tune ABINIT in order to use it most efficiently. The final challenge is to perform simulations on more complex or larger systems, and/or for longer simulation times.

The proposed tutorial is addressed mainly to the community of young French and European students and postdocs interested in the field of nanoscience simulation.

The school with be user oriented: **for each theoretical courses, a hands-on session will follow.** Note that each participant will benefit of *hundreds of processors* on a supercomputer of the TGCC.

(Preliminary) program

Topic	*Duration (time slot)*
Introduction to ABINIT	0,5
Installation of ABINIT	0,5
DFT : - Theory, solids, magnetism, … - Practice : plane-waves, mixing, iterative diagonalization,. - Pseudopotentials, PAW	1.5
Magnetism	0.5
Parallelism, theory and practice	1
Structural optimization, Molecular Dynamics, Minimum Energy Paths,.	1
Efficient use of ABINIT (tuning)	1
Analyze, postprocessing	1
Optional sessions : DFPT, DMFT, Study of transition paths (NEB, String method)	2
Hands-on session	7
TOTAL	16

2 time slots in the morning, 2 time slots in the afternoon

Tentative list of speakers

Xavier Gonze (UCL, Louvain-la-Neuve), Belgium
Marc Torrent, François Jollet, Bernard Amadon, Jordan Bieder, Boris Dorado, Grégory Geneste (CEA Bruyères-le-Chatel)
Eric Bousquet (Liège)

> Note that the CEA-Bruyères-le-Chatel "Condensed Matter" group is one of the main developer group of the ABINIT software, especially as regards *High Performance Computing* features, DFPT, strongly correlated theories (DMFT), and transition paths methods.

Financial support

The workshop will be supported by the CEA ("Condensed Matter" group).
We plan to cover the cost of lunches/breaks, social dinner and facilities/buses. Fees will be asked to participants to cover housing/dinners.
We would like to limit to fees and keep the workshop accessible to students.

We ask for additional support from CECAM IdF node : 2000 euros will cover the expenses for break and the buses (from hotel to Teratec/TGCC).

References

[1] *Recent developments in the ABINIT software package*. Gonze at al. Computer Phys. Comm. 205, 106 (2016).

[2] *First-principle computation of material properties: the ABINIT software project*. Gonze et al. Comput. Materials Science 25, 478-492 (2002).

[3] *ABINIT: First-principles approach to material and nanosystem properties. Gonze et al.* Comput. Phys. Commun. 180, 2582 (2009).

[4] *http://www.abinit.org ; https://wiki.abinit.org ; http://forum.abinit.org*