FINAL REPORT

8TH INTERNATIONAL ABINIT DEVELOPER WORKSHOP

Organizers

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Summary

ABINIT is an open-source software (*http://www.abinit.org*) for the atomistic modelling of the properties of periodic solids and nanostructures. It is clearly identified in the scientific community of first–principles calculations as a major tool for scientists. Initiated in 1997, ABINIT rapidly became an international project involving groups from all over the world. Nowadays, ABINIT counts more than 1700 registered users and a yearly 40 contributors from a wide variety of research groups, mainly in Europe.

The package has beyond 700 000 lines of source code.

Basic capabilities of ABINIT include DFT computation of total energy (plane-wave based pseudopotential and Projector Augmented-Waves formalisms), its first-, second- and third- derivatives (e.g. phonon band structure calculations, Raman efficiencies, piezoelectricity ...), molecular dynamics, excited states determination (GW, Bethe-Salpeter and TD-DFT formalisms).

In addition, in the recent years, several more specific theories have been implemented in ABINIT, making it – for some of them – a unique tool: fully self-consistent DFT+DMFT to include electronic correlations, two-component DFT to have access to electron-positron interactions, Path-Integral Molecular Dynamics to add quantum effect of the light nuclei, AHC theory (Allen-Heine-Cardona) to determine the temperature dependence of the electronic gap, perturbative (DFPT) treatment of the strain, Berry phase treatment of a finite electric field, etc. All these recent developments have been detailed in a specific article published in 2016 [1].

Efficient adaptation to High Performance Computing (speed up beyond 10000 CPU cores) is available for most of the important functionalities of ABINIT. A major effort is being currently carried out to adapt the code on future supercomputer architectures that announce a technological breakthrough.

The ABINIT software project, because to its open-source characteristics, is linked/interfaced to many other software projects in the field of atomistic modeling, either by sharing of routines or libraries (LibXC, ELPA, TRIQS, BigDFT, Wannier90), or thanks to common file formats: FHIPP, OCTOPUS, YAMBO, SIESTA, ATOMPAW, OCEAN, ASE. Some developers of these software are usually invited to the ABINIT developer workshop.

Initiated in 2002, the series of ABINIT developer workshops are organized every two years (Louvain-la-Neuve 2002, Paris 2004, Liège 2007, Autrans 2009, Han-sur-Lesse 2011, Dinard 2013, Liège 2015) and plays an important role in the life of the ABINIT community. It is the occasion for the most active ABINIT developers —as well as a few expert users — and selected invitees, to gather and exchange information,

and present recent developments. The future of ABINIT is also discussed, and recommendations are issued.

The workshop in Fréjus followed the spirit of preceding workshops and was particularly fruitful. This year, the number of participants reached 39 people. Workshop program, abstract and oral presentations (pdf) are permanently available on the website of the conference (https://abidev2017.abinit.org/program) linked from ABINIT website.

The workshop started with a half-day session on Tuesday. After a first presentation with an update by X. Gonze of the current status of the abinit package, the software ecosystem was presented. Several speakers showed the latest developments related to addition of new libraries, the integrated effort for better pseudopotentials, and the automation of certain tasks focused towards data mining and large-scale computing of material properties.

The second day of the workshop, Wednesday, addressed the newest developments related to fundamental physics. The morning session was about the electronic properties. A special attention was paid for treating strongly correlated materials in various approximations (DMFT, Hubber U, GW). The afternoon session was about lattice dynamical properties and the effort of going beyond the quasi-harmonic approximation with the incorporation of higher-order energy derivatives, and advanced molecular dynamics techniques leading to the treatment of the anharmonicities.

Morning of the third day was dedicated to algorithms and implementation techniques. With the passage of most supercomputing centers to many integrated core architecture with vector calculation units and hyperthreading (in an effort to save energy), Abinit, like many other ab initio software packages took a hit in terms of performance and accuracy. This has been recently solved with the implementation of new algorithms. This was an important effort from the abinit developers' community that led to regaining the lost efficiency. Other presentations dealt with numerical stability and automation of the test series on various platforms.

Thursday afternoon we came back to response function, one of the pillars of the abinit package. The presentations were about the determination of the elastic and the Raman tensors, van der Waals effects, coupling of the phonons with magnetic and electronic properties. This part brought new flavors to this traditional line of development of ABINIT.

During the last half-day, Friday morning, the participants were split in several working groups, whose tasks were related to improvements of the code and of the user experience. We discussed and came with suggestions about the overall efficiency and speed of the code and making the interface, and about making the website and the documentation more user-friendly. The conclusions stemming from these working groups were shared with all the participants at the end of the workshop, and were centralized by the steering committee.

Assessment of the results and impact on the future

The International ABINIT Developer Workshop is the opportunity for everybody active in the development of ABINIT to get an overview of the main advances realized over the last 2 years. The workshop gives the possibility to keep a global view on the project, to learn how to use the most recent advanced capabilities of the software and to define the future of the code with respect to both the scientific lines and the IT development.

At the end of the 2017 session, all the attendees considered the meeting as a very good working session resulting in several achievements; among them it is worth noting particularly that:

- the ABINIT ecosystem adapted well to new computing environments,
- the code gained in efficiency, parallelism and saw several advanced implementation techniques realized
- there is an ongoing effort for simplicity towards the users
- there is a sustained effort towards implementing advanced and complex physical problems

The workshop was an opportunity to raise different questions and take collective decisions.

A total of 16 participants out of the 39 were PhD students and post-docs. Most of them had the opportunity to give a presentation

Finally, the Advisory Committee of ABINIT had the opportunity to have a meeting. A new chairman has been elected: Aldo Romero from West Virginia University (Virginia, USA). New members have been proposed; the program for future events based on ABINIT (tutorials, schools …) has been set.

Program and speakers

The meeting will start on tuesday, May 9, 2017 at 2pm and ends on friday, May 12, 2017 after lunch. Arrival is possible on monday, May 8.

Below is a list of topics to be covered in each session. Schedules will be communicated later
This program is likely to (slightly) change...

A 20' slot consists of a 16' presentation and 4' of questions.
A 10' slot consists of a 8' presentation and 2' of questions.

Tuesday, 9 May

Welcome

Status of ABINIT project - X. Gonze - SLIDES

Abinit ecosystem, Big data

- The Delta project: current status and future directions - K. Lejaeghere (20') - SLIDES
- The MULTIBINIT software project - P. Ghosez (20') - SLIDES
- MULTIBINIT: how to scale up simulations from 2nd principles models - A. Martin (20') - SLIDES
- Python ecosystem for scientific computing with ABINIT: challenges and opportunities - M. Giantomassi, G.-M. Rignanese (30') - SLIDES
- News from the PAW dataset table - F. Jollet (10') - SLIDES
- The PseudoDojo: training and grading a 85 element optimized NCPP table - M. van Setten (20') - SLIDES
- High-throughput DFPT - G. Petretto (20') - SLIDES

Discussion/round table: ABINIT survey

Wednesday, 10 May

Electrons: advanced theories

- LOBSTER and ABINIT: perfect partners for chemical bonding studies - R. Dronskowski (20') - SLIDES
- Develoment of DFT+DMFT + cRPA in ABINIT - B. Amadon (20') - SLIDES
- Hybrid functionals in ABINIT: state of the art and perspectives - F. Jollet (20') - SLIDES
- Metaheuristic searchers Applied to Strongly Correlated Materials - A. Romero (20')
- Ab initio calculation of U within cRPA for early Lanthanides - J.-B. Morée (10') - SLIDES
- High-Throughput GW: automation methodologies and large scale validation - M. van Setten (20') - SLIDES
- Band gaps of extended systems through efficient vertex corrections in GW - W. Chen (20') - SLIDES

Discussion/round table: ABINIT ecosystem

Dynamics

- Supercritical silicate melts - R. Caracas (10') - SLIDES
- Temperature dependent phonons, but faster! - O. Hellman (20') - SLIDES
- Anharmonic effects in solids: an implementation in ABINIT - F. Bottin, J. Bouchet (20') - SLIDES
- Nuclear quantum effects in ab initio MD simulations - H. Dammak (20') - SLIDES
- Implementation of the Blue-Moon Ensemble in ABINIT - G. Geneste (20') - SLIDES
- AGATE - Abinit Graphical Analysis Technical Engine - J. Bieder (10')

"Exploration" in Fréjus

Conference dinner (restaurant "Ray'Son" in Fréjus)

Thursday, 11 May

Software/hardware environment

- Adapting ABINIT to new computing architectures - M. Torrent (20') - SLIDES
- ABINIT on manycore-based supercomputers - J. Bieder (20') - SLIDES
- Verificarlo applied to ABINIT: detecting numerical instability - Y. Chatelain (20') - SLIDES
- The ABINIT test farm and its evolution - J.-M. Beuken (20') - SLIDES

Discussion/round table: development tools: gitlab, testfarm, ...

Discussion/round table: ABINIT forum

Response functions

- Phonons and elastic constants including van der Waals - B. van Troeye (20') - SLIDES
- Counterintuitive dyn. charge, vdW Interaction in Transition Metal Dichalcogenides - N. Pike (10') - SLIDES
- van der Waals DF - c. Espejo (10') - SLIDES
- Phonon unfolding: real and reciprocal space methods - X. He (20') - SLIDES
- Non-collinear magnetism in Abinit for DFPT - F. Ricci (20') - SLIDES
- DFPT with magnetic field and noncollinear XC functionals - S. Prokhorenko (20') - SLIDES
- The ElectronPhononCoupling module - G Antonius (20') - SLIDES
- New Abinit driver for the calculation of electron-phonon interactions - M. Giantomassi (20') - SLIDES
- Ab-initio computation of Raman spectra within DFPT+PAW - L. Baguet (20') - SLIDES
- 1st-principle HT approach for linear and non-linear optical properties - F. Naccarato (10') - SLIDES
- Resonant Raman in ABINIT - X. Gonze (10') - SLIDES
- Precise effective masses from DFPT - X. Gonze (10') - SLIDES

Friday, 12 May

Several small meetings: improving ABINIT

- How to improve user experience with the code?
- How to improve electronic experience (website, forum, wiki...)?
- How to improve development efficiency?

Discussion/round table in working groups

Sharing of working groups

List of participants

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