FINAL REPORT

6TH INTERNATIONAL ABINIT DEVELOPER WORKSHOP

LOCAL ORGANIZING COMMITTEE

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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 molecules. Initiated at the University of Louvain-la-Neuve, Belgium) in 1997, ABINIT rapidly became an international project involving groups from all over the world (Belgium, France, Germany, Spain, USA, Canada, Mexico, Colombia, Japan …).

Nowadays, ABINIT counts more than 1200 registered users and an average of 40 active developers. The package includes more than 600 lines of source code.

Initiated in 2002, the series of ABINIT developer workshops are organized every two years 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 *Dinard* followed the spirit of preceding workshops and was particularly fruitful. This year, the number of participants reached 48 people. Workshop program, abstract and oral presentations (*pdf*) are permanently available on a website (*http://sites.google.com/site/abinit2013workshop*) linked from ABINIT website.

The first 3 days of the meeting were devoted to talks and discussions. The topics covered were the ABINIT structure and modularisation, testing, parallelism, van der Waals interactions and Exchange-Correlation functionals, basis (PAW, Wavelets), spectroscopy, electron-phonon, dynamics, high-throughput, structure search, Many-Body physics and electronic correlations. Several discussions sessions were held about computing architectures, performances, modularisation and libraries, testing, documentation, high throughput.

The last day was devoted to small workgroups focused on specific points of the ABINIT development.

Scientific content of and discussions

The workshop was based on talks — developers of ABINIT, developers from external libraries and expert users —, group discussions, and ended finally with workgroups on the last day.

A first series of talks was focused on the software itself and libraries in view of efficiency, performance, and ease of use for developers and users: build system (Y. Pouillon), test farm (J.M. Beuken), automatic test scripts (M. Giantomassi), pre- and post-processing Graphical User Interfaces (Y. Gillet, A. Martin), memory profiling (D. Waroquiers), high levels functionalities through binding (D. Caliste).

The recent advances in parallelism in ABINIT were underlined by the talks on speed and parallelism on hybrid computers with a milestone on *shared-memory* and *GPU* architectures (M. Torrent, M. Giantomassi). Finally the link with libraries or the use of ABINIT as a library were presented in the talks on AI2PS (J. Rher), ASE (A.H. Larsen), Abipy (G. Antonius), libxc/lipspio (M. Oliveira).

A large amount of talks were devoted to pseudopotentials and new basis in view of High Throughput or performance: new libraries for pseudopotentials (libpspio projects) (M. Oliveira), pseudopotentials generation (N. Holzwarth), reading of PAW data in the XML format (F. Jollet), Wavelets (L. Genovese), Wavelets-based PAW formalism (T. Rangel), and High-Throughput (G.M. Rignanese).

Then the development of new functionalities took an important part of the meeting and focused on frontiers of DFT such as magnetism, Many-Body physics, strong correlations, and nuclear quantum effects: van der Waals interactions (C Espejo), orbital magnetic susceptibility (J. Zwanziger), refinements of Bethe-Salpether equation methodology (Y. Gillet), improvements in phonons spectra interpolation (M. Verstraete), genetic algorithm for finding new structures (A. Romero), Continuous-Time QMC in DFT+DMFT (J. Bieder), calculation of screened interaction for correlated systems (B. Amadon), fast GW calculations (J. Laflamme Janssen, B. Rousseau), hybrid functionals (F. Bruneval, C. Martins), Path-Integral Molecular Dynamics (G. Geneste)

Some selected applications of ABINIT were finally presented: GGA functionals benchmark for Density-Functional Perturbation Theory (L. He), Time-Resolved structure of Bismuth (B. Arnaud), Electron-Phonon calculations (S. Poncé), thermoelectricity (B. Xu), new materials from first principles (J.A. Flores Livas, M. Amsler), comparison of the Tran-Blaha functional with GW (D. Waroquiers).

Two invited contributions have allowed the participants to have an insight on related communities. The first one (N. Holzwarth) was devoted to the generation and testing of PAW datasets, the second one (A. H. Larsen) focused on the "Atomistic Simulation Environment (ASE)" project — a plate-form to perform electronic structure calculations recently connected to ABINIT —.

Large time slots were devoted to discussions on specific topics (see program); the participants also had time for discussions during the coffee breaks, the poster session and the outing in Saint-Malo.

The last day of the workshop was devoted to small workgroups on the development of the ABINIT software. Around 20 people attended to these workgroups. The subjects that have been discussed concerned the ABINIT website, the communication around ABINIT, the pseudo-potentials and PAW-datasets tables, the Object-Oriented programming, the improvement of the input file, the external libraries, the documentation, the management of the development, the test suite and bug reports,... Each workgroup produced a report and a roadmap up to the next developer meeting (2 years).

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 2013 session, the meeting was considered by all the attendees as a very good working session resulting in several achievements; among them it is worth noting particularly that:

- the coordination of ABINIT development of the software improves,
- ABINIT is evolving towards more flexibilities,
- ABINIT is evolving towards simplicity for users.

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

A large number of PhD students and post-doc attended the meeting and most of them had the opportunity to give a presentation; to encourage this, all the non-permanent speakers did not pay the registration fees. The massive participation of students suggests that the ABNIIT developer community is active and constantly renewed.

The last-day working groups produced a 30 pages document — available for people involved in ABINIT development —which brings together all the roadmaps for the future evolution of the code: important decisions have been taken for the development and the promotion of the code.

Finally, the Advisory Committee of ABINIT had the opportunity to have a meeting. A new chairman has been elected: Josef Zwanziger from *Dalhousie University* (Halifax, Canada). New members have been proposed; the program for future events based on ABINIT (tutorials, schools …) has been set.

Program

Presentations are either maximum 15' or maximum 25', followed by an additional 5' discussion.

MONDAY, April 15, 2013 — PM

Session 1 **ABINIT** (50')

14:40-15:00 Overview of the ABINIT project
Xavier Gonze (15'+5')

15:00-15:30 Paving the way towards ABINIT 8 in the post-Moore's law era
Yann Pouillon, Matteo Giantomassi, Jean-Michel Beuken, Thierry Deutsch, Damien Caliste and Xavier Gonze (25'+5')

Session 2 **Parallelism and GPU** (70')

16:00-16:30 ABINIT on High Performance Computers
Marc Torrent, Florent Dahm, Laurent NGuyen, Francois Jollet and Muriel Delaveau (25'+5')

16:30-16:50 Recent developments in parallelism for ABINIT
Matteo Giantomassi (15'+5')

16:50-17:10 Using ABINIT on Graphics Processing Units (GPU)
Marc Torrent and Florent Dahm (15'+5')

Discussion 1 (40')

17:10-17:50 **Architectures and Speed**

19:00 Dinner

20:30 Poster session

TUESDAY, April 16, 2013 — AM

Session 3 **Exchange-correlation / Magnetism** (80')

08:30-08:50 Accuracy of Generalized Gradient Approximation functionals for density functional perturbation theory calculations
Lianhua He, Fang Liu, Geoffroy Hautier, Gian-Marco Rignanese and Aihui Zhou (15'+5')

08:50-09:10 Libxc and Libpspio: towards better code sharing and reuse in DFT codes
Micael Oliveira (15'+5')

09:10-09:30 Implementation of vdW-DF functional in ABINIT
Camilo Espejo, Yann Pouillon, Aldo Romero and Xavier Gonze (15'+5')

09:30-09:50 Orbital magnetic susceptibility
Josef W. Zwanziger (15'+5')

Session 4 **PAW, BigDFT** (120')

10:20-10:50 Comments on generating and testing PAW datasets
Natalie A.W. Holzwarth (25'+5')

10:50-11:20 Interfacing ABINIT with PAW atomic data tables: Toward an XML reference format?
François Jollet and Marc Torrent (25'+5')

11:20-11:40 Wavelets opportunities for DFT and Post-DFT calculations
Luigi Genovese, Paul Boulanger, Laura Ratcliff, Damien Caliste and Thierry Deutsch (15'+5')

11:40-12:00 Wavelets within the Projector Augmented-Wave (PAW) method in ABINIT
Tonatiuh Rangel, Damien Caliste, Luigi Genovese and Marc Torrent (15'+5')

12:00-12:20 High level functionalities through bindings (or not), the BigDFT example
Damien Caliste, Luigi Genovese and Thierry Deutsch (15'+5')

12:30 Lunch

TUESDAY, April 16, 2013 — PM

Session 5 **Spectroscopy and phonons** (70')

14:20-14:40 Time-resolved X-ray diffraction in laser-excited bismuth from first-principles
Brice Arnaud, Alain Gellé and Yvelin Giret (15'+5')

14:40-15:00 Bethe-Salpeter methodology and resonant Raman spectroscopy
Yannick Gillet, Matteo Giantomassi and Xavier Gonze (15'+5')

15:00-15:30 AI2PS: An analysis tool for vibrational properties based on ABINIT
John J. Rehr, Shauna M. Story, Joshua J. Kas and Matthieu J. Verstraete (25'+5')

Session 6 **Electron-Phonon** (60')

16:00-16:20 Validation of calculations based on electron-phonon matrix elements in ABINIT and PWSCF/Yambo
Samuel Poncé, Martin Stankovski, Gabriel Antonius, Michel Côté and Xavier Gonze (15'+5')

16:20-16:40 Odd and ends. Novelties in phonon interpolation and treatment with ABINIT and anaddb
Matthieu Verstraete, Bin Xu and Georg Madsen (15'+5')

16:40-17:00 Calculation of thermoelectric properties using ABINIT
Bin Xu, Matthieu Verstraete (15'+5')

Discussion 2 (40')

17:00-17:40 **Modularisation / Libraries**

19:30 Dinner

Advisory board meeting

WEDNESDAY, April 17, 2013 — AM

Session 7 **Testing procedures / GUI** (60')

08:30-08:50 New test procedures
Matteo Giantomassi (15'+5')

08:50-09:10 ABINIT Test Farm
Jean-Michel Beuken and Yann Pouillon (15'+5')

09:10-09:30 Status of the ABINIT GUI
Yannick Gillet and Flavio Abreu Araujo (15'+5')

Discussion 3 (20')

09:30-09:50 **Testing / Web site / Documentation**

Session 8 **Dynamics, High-Throughput tools** (120')

10:20-10:50 Path-Integral Molecular Dynamics under fixed volume or fixed pressure and its parallelization
Gregory Geneste, Marc Torrent and Francois Bottin (25'+5')

10:50-11:10 ABINIT Post Process Application (APPA): Graphical tool for Molecular Dynamics simulation analysis
Alexandre Martin, François Bottin, Johann Bouchet and Marc Torrent (15'+5')

11:10-11:40 The Atomistic Simulation Environment
Ask Hjorth Larsen and the ASE development team (25'+5')

11:40-12:00 Abipy Tutorial: Managing ABINIT calculations in Python
Gabriel Antonius (15'+5')

12:00-12:20 Towards high-throughput *ab initio* calculations using ABINIT
Gabriel Antonius, Michel Côté, Matteo Giantomassi, Xavier Gonze, Geoffroy Hautier, Gian-Marco Rignanese, Martin Stankovski and David Waroquiers (15'+5')

12:30 Lunch

WEDNESDAY, April 17, 2013 – PM

Session 9 **Structure search** (60')

14:00-14:20 News from the genetic world: GA implementation in ABINIT
Aldo H. Romero and Xavier Gonze (15'+5')

14:20-14:40 Designing new materials from first principles:
Computational and experimental results
Jose A. Flores Livas, Sangeeta Sharma, John K. Dewhurst and Eberhard K. U. Gross (15'+5')

14:40-15:00 Novel structural motifs in alanates
Maximilian Amsler, Jose A. Flores Livas, Huan Tran, Miguel Marques, Silvana Botti and Stefan Goedecker (15'+5')

Discussion 4 (30')

15:00-15:30 **High-throughput and structure search**

Outing in Saint-Malo

16:30 Transportation (bus)

17:00 **Saint-Malo visit (free)**

19:30 Dinner at the Creperie "Le corps de garde"

22:00 Transportation (bus)

THURSDAY, April 18, 2013 — AM

Session 10 **Many-body theories and Hybrids I** (80')

08:30-08:50 DFT+DMFT and calculation of U in cRPA in ABINIT
Bernard Amadon, Thomas Applencourt and Fabien Bruneval (15'+5')

08:50-09:10 CTQMC solver for DMFT
Jordan Bieder and Bernard Amadon (15'+5')

09:10-09:30 Faster G_0W_0 implementation for more accurate material design
Jonathan Laflamme Janssen, Bruno Rousseau and Michel Côté (15'+5')

09:30-09:50 Efficient computation of GW energy level corrections for molecules described in a plane wave basis
Bruno Rousseau, Jonathan Laflamme Janssen and Michel Côté (15'+5')

Session 11 **Many-body theories and Hybrids II** (80')

10:20-10:50 Hybrid functionals in ABINIT à la GW
Fabien Bruneval (25'+5')

10:50-11:10 Hartree-Fock and hybrid functionals in ABINIT:
Implementation and first applications
Cyril Martins, Bernard Amadon, and Marc Torrent (15'+5')

11:10-11:30 Band widths and gaps from the Tran-Blaha functional:
Comparison with Many-Body Perturbation Theory
David Waroquiers, Aurélien Lherbier, Anna Miglio, Martin Stankovski, Samuel Poncé, Micael Oliveira, Matteo Giantomassi, Gian-Marco Rignanese and Xavier Gonze (8'+2')

Memory profiling in ABINIT
David Waroquiers and Xavier Gonze (8'+2')

Discussion 5 (50')

11:30-12:20 **The future ABINIT**

12:30 Lunch

Departure

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