5th International ABINIT developer workshop

11-14 April 2011, Han-sur-lesse (Belgium)

Summary

Initiated in 2002, the series of ABINIT developer workshops, organized each other year, 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 started on Monday 11 April 2pm, and finished on Thursday 14 April 4pm. This year, the number of participants was 57, nearly half of which were young (non-permanent) scientists. There were two invited speakers from different communities (N. Holzwarth and JJ Rehr), who presented the AtomPAW generator and OCEAN and AI2NBSE postprocessors for core and valence spectra.

There were 32 scientific presentations, 5 discussion sessions, and 1 poster session (17 posters). The scientific presentations were grouped in the following topical sessions :
- software development ;
- many-body perturbation theory I ;
- PAW and pseudos ;
- spectroscopy ;
- strong correlations ;
- phonons ;
- many-body perturbation theory II ;
- magnetic and electric fields ;
- structure and dynamics ;
- Bigdft and Wannier90 extensions ;
- exchange-correlation.
The discussion sessions, each of about one hour, covered software engineering aspects of ABINIT and the organization of future developments (the build system, the test farm, the Web site, modularization, libraires, pseudopotentials, beautification and documentation). These were very fruitful, with several people engaging to organize things in the forthcoming months and years.

The advisory committee of ABINIT also met, elected new members, and planned the next developer workshop, several schools, issued recommendations about the readibility of the software.

With all these diverse contributions, science-oriented as well as software engineering - oriented, the meeting was considered by the attendees as a very fruitful event resulting in several achievements.

The presentations can be dowloaded from http://ftp.abinit.org/ws11 .

Scientific content

A rather specific characteristics of the ABINIT workshop series, compared to traditional scientific workshops, is to allow integrated discussions of scientific developments with software engineering concepts and tools. The ABINIT software community pays attention not keeping such expertise inside the community only, but to disseminate it through :

(1) schools, like the CECAM Tutorial "Basic techniques and tools for development and maintenance of atomic-scale software" (Zaragoza, Spain, June 21-25, 2010), where about half of the tutors originate from the ABINIT community ;

(2) publications, like the recent "Organizing software growth and distributed development : the case of Abinit" published in Computers in Science and Engineering, Jan-Feb 2011, pp. 62-69, by Y. Pouillon, J.-M. Beuken, T. Deutsch, M. Torrent and X. Gonze,

Also, experts outside the core ABINIT community are invited to participate (usually between two and four invited speakers), to favour the exchange of ideas.

The 5th ABINIT developer workshop continued implementing this philosophy.

X. Gonze opened the workshop, and also provided an update on the current status of the ABINIT project (some statistics, like the number of members on the forum, the mailing lists, size of the package, etc.). The first session focused on recent software developments, by Y. Pouillon and the current status of the test farm, by J.-M. Beuken, followed by a discussion session on these aspects, and also on the Web site. A noticeable evolution of the build system consists in the development of plug-ins and fall back mechanisms, to allow a much more flexible link with external tools and libraries (e.g. NetCDF, LibXC, Wannier90, ...). The test farm includes now nearly twenty "slaves", testing a large variety of compilers, operating systems, configurations, presence or absence of plugins, also checking not only for numerical accuracy and portability, but also the fulfillment of coding rules, documentation etc . This test farm is used only for testing ABINIT, but also for testing other software applications within the EUropean Theoretical Spectroscopy Facility.

This session continued on the theme of modularization and libraries, with a presentation of the recent advances in the LibXC library by M. Oliveira, and the development of a library for molecular dynamics and geometry optimization, by G. Franco.

The next day, the first session was more scientifically oriented (speakers mixed implementation considerations with formalism or numerical considerations, though), focusing on Many-Body Perturbation Theory. The presentations by M. Giantomassi, A. Berger, F. Bruneval and M. Stankovski covered aspects from the Bethe-Salpeter equation to the RPA total energy, passing through GW calculations with new model vertex corrections. In particular, GW results for supercells up to 200 atoms were presented.

The second Tuesday session evolved around the concept of pseudopotentials. N. Holzwarth, the main developer of the AtomPAW generator, presented the status and future development of this important tool. Present as a plugin to ABINIT, AtomPAW will likely play a more important role in the future of ABINIT, especially in the

framework of the generation of a whole periodic table of PAW atomic data, discussed after her presentation.

In the afternoon, J. Rehr, the second "external" invited speaker presented two post-processors of ABINIT, dubbed OCEAN and AI2NBSE. In particular, they allow to obtain core spectra including multiplets. The session continued with two contributions related to core-level spectroscopy by F. Bottin and S. Mazevet.

The last session of the Tuesday afternoon focused on strong correlation. B. Amadon described the recent progress in the implementation of the LDA+DMFT within ABINIT. The full self-consistency is now possible. The implementation of the computation of U and J values for LDA+U was then described by D. Adams.

At the end of this day, a discussion session focused on the improvement ("beautification") of the code and its documentation, especially, the datastructures to be used in the future in ABINIT. Although object-oriented programming style is already present in numerous places in ABINIT, it is felt that this should be improved, and also done in a more systematic way.

Wednesday 13 April started with a session related to phonons, for which the linear-response approach implemented in ABINIT is a rather strong point. M. Torrent described the PAW implementation, in final debugging phase. P. Boulanger focused on the computation of the temperature-dependence of electronic structure, driven by phonons, while M. Verstraete describes his implementation of the self-consistent ab-initio lattice dynamics technique proposed by Souvlakis, Johansson and co-workers.

A second many-body perturbation theory session (the first was on tuesday) focused more on applications than the first one : the computation of defect formation energes (D. Waroquiers), GW band structure calculations for nanowires (H. Peelaers), electronic structure of materials for white LED (M. MIkami and B. Bertrand). This scientific session was followed by a brief presentation of a simple GUI for ABINIT, by F. Abreu. The audience was particularly pleased by this presentation, where the portability aspects, and also the access to remote machines, have been incorporated from the very start.

The afternoon of the Wednesday was dedicated to a social activity : the visit of the renowned Han-sur-Lesse caves. Then, the poster session started. The idea of the poster session in the ABINIT workshop consists in allowing the presentation of works not related to the software engineering or new implementation/formalism in ABINIT. Indeed, like many others, most of the ABINIT developers do not restrict their work on theory/implementation. Moreover, it is interesting to have during the poster session an idea of the range of applications of ABINIT : transparent conducting oxides, thermoelectric power, water on plutonium oxyde, a database of Rama spectra, interfaces of MgO, hydration and proton migration in Gd-doped BaCeO3, superlattices ...

To start the last day, the treatment of magnetic and electric fields was emphasized. J. Zwanziger presented the recently finalized implementation of the finite electric field approch, based on Berry phase, as well as a new technique to treat homogeneous magnetic field. E. Bousquet draw the attention of the audience to problems with the

treatment of non-collinear spin-polarization in DFT, while S. Blackburn described his implementation of the computation of the de Haas van Alphen frequencies.

The next session focused on structure and dynamics, for which the recent implementation of images in ABINIT allowed to consider path integrals in Born-Oppenheimer space (G. Geneste), or population of images (A. Romero), for powerful global search strategies. The parallelisation on several levels, combining parallel treatment of images, with the one of electronic wavevectors and spin, and bands and planewave coefficients, should allow for efficient parallel runs on more than ten thousand processors. The remaining issues, involving modifications of some ABINIT coding rules, were discussed after G. Geneste presentation.

Extensions of ABINIT (libraries) were then presented : Bigdft (L. Genovese), and the computation of transport properties using the externall developed Wannier90 as well as WanT software applications by T. Rangel.

In the afternoon, the focus shifted on exchange-correlation functionals, with the work of C. Espejo on van der Waals interactions, and the positron lifetime computation, by M. Torrent.

The final discussion session examined the roadmap of development for the next two years.

Assessment of the results and impact of the event on the future directions of the field.

The results of such a developer workshop are of several types :
- the information of the community of recent developments in ABINIT, thanks to the organized oral presentations and posters, in view of further collaborative research and development ;
- the information of the community of software engineering concepts recently implemented in ABINIT, usually facilitating their own future development, also thanks to oral presentations ;
- thanks to external invited speakers, creation of links between ABINIT developers and some scientists outside of the community ;
- broad discussions of the link and interplay between scientific and software engineering progresses ;
- more specific discussions of topics for which a consensus should be reached by the developer community ;
- also, even more specific discussions between some subset of developers that are currently collaborating, usually in the breaks and during the evenings.

As in the previous workshops of the series, the workshop has been quite succesfull in term of such interaction. This is witnessed by the numerous questions and answers that followed each presentation, leading to very intense discussions, and causing some difficulty to keep right on the planned schedule. The participants actually stayed quite late in the evening (sometimes up to 1am), and made the best of the time that they could spend together.

As concerns more concrete decisions :
(1) it was decided to improve some of the tutorials that guide the beginner in the use of ABINIT :
- the analysis tools (vizualisation) tutorial, on the basis of Vesta and VSim ;
- the tutorial explaining the use of spin ;
- the tutorial explaining parallel use of ABINIT ;
the GW tutorial :
- moreover a new tutorial to present tools of ABINIT should be written (cif to ABINIT, AbinitBandStructureMaker, AbinitStructureViewer.py with JMol .
(2) It was decided to Study the possibility to include Objects in ABINIT to simplify the high level
subroutines,
(3) it was decided to clean up a set of subroutines, as well as to simplify the FFT subroutines
(4) it was decided to improve failing/error messages, errors, macros,
(5) remove/comment OpenMPI code
(6) rename keywords
(7) improve the web page (logo, presentation, include a ABINIT feature sections, improve the Wikipedia description of ABINIT).

Program

Most of the presentations will be 25 minutes + 5 minutes discussion.
Some are 20 minutes + 5 minutes discussion.

Monday 11 April afternoon
Chair : Michel Côté.

Welcome!
14:00 [10'] Xavier Gonze : Current status of the ABINIT project

Software Development
14:15 [25'] Yann Pouillon : The build system of Abinit 6: on the road again
14:45 [20'] Jean-Michel Beuken : ABINIT test farm
15:10 [50'] Discussion session, organized by Matthieu Verstraete :
Build system / test farm / testing / the Web site (the latter if time permits).

16:00 Coffee break

16:30 [20'] Micael Oliveira : Advances in LibXC
16:55 [20'] Guillermo Franco : Ab-initio molecular dynamics and geometry optimization, new developments.
17:20 [40'] Discussion session, introduced and organized by Damien Caliste :
Modularization / libraries

Tuesday 12 April morning

Many-Body Perturbation Theory I
Chair : G.-M. Rignanese.

9:00 [25'] Matteo Giantomassi : Implementation of the Bethe-Salpeter formalism in Abinit.
9:30 [25'] Arjan Berger : The effective-energy technique: GW calculations without summing over empty states
10:00 [25'] Fabien Bruneval : The RPA total energy in Abinit
10:30 [25'] Martin Stankovski : Non-local model vertex corrections for GW calculations

11:00 Coffee break

PAW and pseudos
Chair : B. Amadon.

11:30 [25'] Nathalie Holzwarth : The ATOMPAW generator
12:00 [50'] Presentation / Discussion session, introduced and organized by Alain Jacques and Xavier Gonze :
Generation of pseudopotentials and PAW atomic data for the whole periodic table

Tuesday 12 April afternoon

Spectroscopy
Chair : N. Holzwarth.

14:00 [25'] John Rehr : OCEAN and AI2NBSE - Postprocessors of ABINIT for Core and Valence Spectra
14:30 [25'] Francois Bottin : Core-level X-ray photoelectron spectra
15:00 [25'] Stéphane Mazevet : Calculations of the transport properties within the PAW formalism
15:30 Coffee break

Strong Correlations
Chair : M. Torrent.

16:00 [25'] Bernard Amadon : LDA+DMFT: a fully self-consistent PAW implementation
16:30 [25'] Donat Adams : Hubbard U from first principles: Cococcioni's scheme within the PAW
17:00 [60'] Discussion session organized by J. Zwanziger
Future beautification / documentation

Wednesday 13 April morning

Phonons
Chair : Ph. Ghosez.

9:00 [25'] Marc Torrent : Miscellaneous features in DFPT+PAW available now and soon in ABINIT
9:30 [25'] Paul Boulanger : Theoretical approaches to the temperature and zero-point motion effects on the electronic band structure of semiconductors
10:00 [25'] Matthieu Verstraete : The SCAILD method for self-consistent phonons in ABINIT
10:30 Coffee break

Many-body Perturbation Theory II
Chair : F. Bruneval.

11:00 [20'] David Waroquiers : Computing defect formation energies in GW
11:25 [20'] Hartwin Peelaers : GW calculations of electronic band structure for nanowires
11:50 [20'] Masayoshi Mikami and Bruno Bertrand : Materials for white-LED
12:15 [20'] Rolando Saniz : Self-consistent GW study of the quasiparticle spectrum and optical properties of SnO2

Additionally :
12:40 [15'] Brief presentation of a GUI for ABINIT, by Flavio Abreu.

Wednesday 13 April afternoon

14:15 Departure : visit of the Han-sur-Lesse grotto.

17:00 Poster session
      Space available for each poster : maximum 2m x 1m <u>vertical</u> (not landscape).

18:30 Dinner

19:30 Poster session / Meeting of the ABINIT advisory committee.

Thursday 14 April morning

Magnetic and Electric Fields
Chair : M. Verstraete.

9:00 [25'] Joe Zwanziger : Finite homogeneous electric field and magnetic field in insulators
9:30 [20'] Eric Bousquet : Issues with simulations of non-collinear magnets in DFT
9:55 [20'] Simon Blackburn : Calculations of de Haas van Alphen frequencies using maximally localized Wannier functions

10:20 Coffee break

Structure and dynamics
Chair : B. Partoens

10:50 [25'] Aldo Romero : Random methods to predict novel crystalline structures
11:20 [25'] Gregory Geneste : Path Integral molecular dynamics

Bigdft and Wannier90 extensions
Chair : J. Rehr.

11:55 [25'] Luigi Genovese : The BigDFT project: results, advancements and potentialities
12:25 [20'] Tonatiuh Rangel : Transport properties Wannier90/WanT + ABINIT

12:50 Lunch

Thursday 14 April afternoon
Chair : A. Romero.

Exchange-correlation
14:00 [25'] Camillo Espejo : Two different approaches to include van der Waals interactions within ABINIT
14:30 [25'] Marc Torrent : Computation of positron lifetime with ABINIT: Two-Component Density-Functional Theory
15:00 [60'] Discussion session, prepared by M. Côté
Roadmap of development: the next 2+ years

16:00 Final Coffee and farewell ...