UNIVERSITÉ de Liège

FINAL REPORT

Abinit Developer's Workshop 2007

29 – 31 January 2007

LIÈGE - BELGIUM

ORGANIZING COMMITTEE :

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Summary

ABINIT is an open-source software (http://www.abinit.org) for the atomistic modeling of the properties of periodic solids. Initiated by Prof. X. Gonze (UCL, Belgium) in 1997, ABINIT rapidly became an international project involving groups from all over the world (Belgium, France, Germany, USA, Canada, Japan, India…).

Nowadays, ABINIT counts more than 900 registered users and an average of 40 active developers. The package includes more than 300 000 lines of source code. The advisory board involves people from 5 countries.

Initiated in 2002, the international ABINIT developer workshops (IADW) constitue a very important series of events organized every two years (in alternance with Schools for users) and bring together the community of people actively working at the development of the software (members of the advisory committee and active developers),

Such periodic IADWs are mandatory to ensure the dynamics of the project and its long-term coherency. These meetings are the opportunity to :
- discuss the global structure of the package and its possible evolution,
- present the formalism and technical details of the most recent implementations,
- discuss and synchronize short-term future developments,
- discuss long-term strategy and developments
- highlight recent advanced use of ABINIT
- identify new needs and weaknesses.

The IADW-2007 workshop in Liège followed the spirit of preceding workshops and was particularly fruitful. It was gathering together 60 people. Workshop program, abstracts and support of oral presentations (in PDF) are permanently available on the ABINIT web site (http://www.abinit.org/workshops). Beyond a dense schedule including many talks on various topics (from software engineering to sharp applications in materials science) the program also included breaks and 2 discussion sessions to favor interactions and exchanges between the participants. This year the workshop also started with a poster session during the first evening. The posters remained available at coffee breaks during the whole workshop, offering a helpful support for the discussions.

Scientific content and discussions

The meeting included 29 talks and was divided into 9 sessions covering different main aspects of the ABINIT software.

- Two sessions (S1, S3) dealt with software engineering and concerned the ABINIT build system, software analysis tools and file formats

- Two sessions (S2, S5) were devoted to improvement of the global efficiency of ABINIT and were related to parallelism, preconditioning and recent achievements concerning the use of wavelets

- Two sessions (S4, S9) concerned two recent major modules of ABINIT : the PAW implementation and the GW part.

- Two sessions (S7, S8) were related to recent implementations allowing to access new physical properties: electron-phonon interactions, phonons under electric fields, Wannier functions, Raman and infrared spectra.

- One session (S6) was devoted to the presentation of advanced uses of ABINIT to tackle complex problems.

In addition to the formal talks, a poster session was organized that was gathering together 17 contributions treating of practical applications or technical issues of ABINIT.

Finally, besides the various informal interactions, two main discussions sessions took place at the workshop, during which various topics were discussed including : the setup of working groups for the ABINIT build system and the generation of a full table of PAW pseudopotentials, information of the place of ABINIT in European projects like Nanoquanta and BigDFT…

Results and impact on the future

The IADW is typically the opportunity for everybody active in the development of ABINIT to get an overview of the main advances realized over the last 2 years. ABINIT is indeed a broad software project with many independent modules (PAW, linear and non-linear responses, GW …) so that someone working on a specific aspect is not necessarily aware of all the other developments. The workshop is therefore the opportunity for everybody to fill in the gaps, to keep a global view on the project and to discover how to use the most recent advanced capabilities of the software.

Going beyond usual e-mail discussions, the IADW offers also the opportunity to the developers to meet physically which is particularly useful to boost the interactions. As an example amongst others, it was realized during the IADW that, combining the expertise at ULG on Berry phases and at CEA on PAW, it would be relatively straightforward to implement polarization calculations in PAW what was so realized in collaboration beginning of April.

The IADW was also the opportunity to raise different questions and take collective decisions. First of all, the built system of ABINIT is becoming rather advanced, the price to pay being that it is becoming less transparent. From the discussions it appeared that only few persons are at this stage still able to modify the built system. A working group has then been proposed to remedy to this problem and share the information amongst a broader group of people. Second, it appeared that compared to other softwares, one of the drawbacks of ABINIT is the absence of a default PAW pseudopotential table. A working group has consequently been defined to build a full table of tested PAW pseudopotentials. Finally, and without being exhaustive, let us mention that it was also decided to upgrade the WEB site (WIKI style) and to investigate the possibility to convert the present mailing list system (so successful that it is generating too many messages for the users) into a more efficient WEB based system.

Finally the IADW was also the opportunity of the bi-annual meeting of the advisory committee. A new chairman has been elected: Gian-Marco Rignanese from UCL (Belgium). New members have been proposed for the committee. Suggestions have also been made concerning the next ABINIT School and the next IADW. Positions have also been discussed concerning recent requirement from the industry.

Program

MONDAY 29

• 13:57 WELCOME address Ph. Ghosez (3 mins)

• 14:00-15:30 SESSION 1 : Software engineering : build system and software analysis tools (Chair D.C. Allan)

Y. Pouillon *The build system of ABINIT 5 [30'+10']*

T. Deutsch *Helping robustness of ABINIT code: Interfaces and abilint [12+5]*

S. Pesant *Graphical interface for the creation of input files for Abinit [20+10]*

• 15:30-16:00 Coffee break

• 16:00-18:00 SESSION 2 : Parallelism (Chair G.M. Rignanese)

S. Goedecker *Efficient parallelization of multiple 3-dim FFT's [20+10]*

F. Bottin *Band FFT parallelisation of Abinit [20+10]*

T. Hoefler *Optimization of a parallel 3D-FFT with non-blocking collective operations [20+10]*

P. Plaenitz *Enhancing Parallelizing Capabilities of ABINIT [20+10]*

• 18:45-… POSTERS (with food & drinks)

TUESDAY 30

• 9:00-9:50 SESSION 3 : Software engineering : file formats (Chair M. Mikami)

V. Olevano *Specifications for the Nanoquanta-ETSF NetCDF file format [20+10]*

D. Caliste *ETSF_IO, a new library to access electronic structure calculation files [15+5]*

• 9:50-10:20 Coffee break

• 10:20-12:00 SESSION 4 : PAW (Chair G. Zerah)

F. Jollet *Implementation of PAW in ABINIT and PAW atomic data file generation [20+10]*

M. Torrent *Implementation of the linear response in PAW [20+10]*

B. Amadon *LDA+U method in PAW [15+5]*

S. Mazevet *Electrical conductivity calculations within the PAW formalism [15+5]*

• 12:00-14:15 Lunch

• 15:15-15:50 SESSION 5 : Speed-up (Chair S. Goedecker)

P.M. Anglade *SCF Preconditioners within Abinit [20+10]*

M. Torrent *Several aspects of the SC cycle mixing in Abinit [20+10]*

D. Caliste & L. Genovese *Introducing wavelet basis sets inside ABINIT via the BigDFT project [25+10]*

• 15:50-16:15 Coffee break

• 16:15-18:00 SESSION 6 : Advanced use of ABINIT (Chair Ph. Ghosez)

M. Mikami *Virtual Crystal Approximation for Heterovalent Ions [20+10]*

J. Zwanziger *Zero Stress Optic Glass without Lead [20+5]*

D. Sangalli *Implementation and applications of Casida TDDFT approach to electronic excitations, for spin-polarized collinear systems [10+5]*

R. Caracas *Elastic and spectroscopic properties of Earth and planetary materials [15+5]*

• 18:00-19:00 Discussions

• 19:15 Conference Dinner

WEDNESDAY 31

• 9:00-9:50 SESSION 7 : Electron-phonon interaction (Chair M. Coté)

M. Verstraete *The electron-phonon coupling in ABINIT* [20+10]

M. Giantomassi *Electron-phonon calculations with ABINIT* [15+5]

• 9:50-10:20 Coffee break

• 10:20-12:10 SESSION 8 : Phonons, electric field and Wannier functions (Chair D. Hamann)

X. Wang *Perturbation treatment of response properties of insulators in finite electric fields* [20+10]

A. Romero *Anisotropic thermal expansion coefficients in wurtzite semiconductors* [20+10]

P. Hermet *First-principles modelling of experimental phonon spectra* [15+5]

J. Bhattacharjee *Bonding and polarization analysis using localized orbitals* [20+10]

• 12:10-14:00 Lunch

• 14:00-15:30 SESSION 9 : GW (Chair L Reining)

F. Bruneval *Self-Consistent GW Electronic Structure of Solids* [20+10]

R. Shaltaf *Speeding up the GW code : Parallelism + PPM models* [20+10]

M. Giantomassi *The GW code of ABINIT: present status, new features and future developments* [20+10]

• 15:30-16:00 Coffee break

• 16:00-17:30 Discussions (chair : G. Zerah & M. Coté)

• 17:30 Closing remarks (X. Gonze)

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