3rd International ABINIT Developer Workshop

Liège (Belgium), 29-31 January 2007

www.abinit.org

Proposal for partial funding by the ESF Psi-k programme 2007

Workshop organizing committee

- Prof. Philippe GHOSEZ (ULg, BELGIUM)
- Dr. Jean-Yves RATY (ULg, BELGIUM)
- Prof. Xavier GONZE (UCL, BELGIUM)
- Prof. Michel COTE (Université de Montréal, CANADA)
- Dr. Masayoshi MIKAMI (Mitsubichi Chemicals, JAPAN)

Scientific committee

- Dr. Masayoshi MIKAMI (Mitsubichi Chemicals, JAPAN)
- Prof. Xavier GONZE (UCL, BELGIUM)
- Prof. Gian-Marco RIGNANESE (UCL, BELGIUM)
- Prof. Philippe GHOSEZ (ULg, BELGIUM)
- Dr. Gilles ZERAH (CEA-Bruyère, FRANCE)
- Dr. François JOLLET (CEA-Bruyère, FRANCE)
- Prof. Lucia REINING (Paris VI, FRANCE)
- Prof. Michel COTE (Université de Montréal, CANADA)
- Prof. Nicola SPALDIN (UCSB, USA)
- Dr. Douglas ALLAN (Corning Inc., USA)
- Prof. Steven ERWIN (NRL, USA)
- Dr. Don HAMANN (Rutgers, USA)

1. Scientific summary

Abstract

This workshop has the aim to bring together the community of people actively working at the development of the ABINIT software, in order to discuss the global structure of the package and its possible evolution, to present the formalism and technical details of the most recent implementations, to discuss and synchronize short-term future developments, to discuss long-term strategy and developments, to highlight recent advanced use of ABINIT , to identify new needs and weaknesses.

Detailed proposal

ABINIT is an open-source software (www.abinit.org) for the atomistic modeling of the properties of periodic solids [1,2]. Initiated 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. Capabilities of ABINIT include DFT computation of total energy (Pseudopotential/PlaneWaves as well as Projector Augmented Waves), its first-, second- and third- derivatives (e.g. phonon band structure calculations, Raman efficiencies, piezoelectricity, ...), molecular dynamics, GW and TDDFT calculations.

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, or thanks to common file formats (wavefunction files, pseudopotential files ...) : CASINO, DP, EXC, FHIPP, OCTOPUS, SELF, SIESTA, WAN-T, ...

The developer workshops form a series of events, crucial for the community of ABINIT developers, organized every two years (Louvain-la-Neuve 2002, Paris 2004). Schools are also organized (Santa Barbara 2005, CECAM Lyon 2006). The developer workshops bring together the community of people actively working at the development of the software, in order to

(i) discuss the global structure of the package and its possible evolution,

(ii) present the formalism and technical details of the most recent implementations,

(iii) discuss and synchronize short-term future developments,

(iv) discuss long-term strategy and developments

(v) highlight recent advanced use of ABINIT

(vi) identify new needs and weaknesses.

The workshop is mainly on personal invitation. Nevertheless, expert users of ABINIT are also welcome to participate and will be allowed to contribute to session A and P (Posters). In any case, the number of participants will be limited to about 50-60 people in order to favor the interactions and discussions.

Practical informations will be available at : www.abinit.org/workshop

[1] First-principle computation of material properties: the ABINIT software project.
X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty, and D.C. Allan.
Comput. Materials Science 25, 478-492 (2002).

[2] A brief introduction to the ABINIT software package.
X. Gonze, G.-M. Rignanese, M. Verstraete, J.-M. Beuken, Y. Pouillon, R. Caracas, F. Jollet, M. Torrent, G. Zérah, M. Mikami, Ph. Ghosez, M. Veithen, J.-Y. Raty, V. Olevano, F. Bruneval, L. Reining, R. Godby, G. Onida, D.R. Hamann, and D.C. Allan.
Zeit. Kristall. 220, 558-562 (2005)

2. (Preliminary) Meeting program

MONDAY 29

- **14:00-15:30 Session 1a : Software engineering : File format and analysis tools [1:30]** (chair : D. Allan)
    - Y. Pouillon (ABINITv5, Autotool build system of ABINIT) [30'+15']
    - T. Deutsch (abilint) [15'+5']
    - S. Pesant (GUI) [20'+10']
- **15:30-16:00 COFFEE BREAK**
- **16:00-17:30 Session 1b : Software engineering : File format and analysis tools [1:30]** (chair : M. Mikami)
    - V. Olevano (ETSF file format / interfacing with DP code and EXC code) [20'+10']
    - X. Gonze (use of Netcdf and XMLF90 libraries) [15'+10']
    - J. Junquera (pseudopotential file format) [20'+10']
- **17:30-18:30 DISCUSSIONS (topic and chair : to be defined)**
- **19:00 DINNER**

TUESDAY 30

- **8:30-10:00 Session 2: Electron-phonon coupling and bulk transport properties [1:30]** (chair : M. Coté)
    - M. Verstraete (application to Al and Pb nanowires) [20'+10']
    - M. Giantomassi (formalism + applications) [20'+10']
    - J.-P. Crocombette (transport Eliashberg function) [20'+10']
- **10:00-10:30 : COFFEE BREAK**

- **10:30-12:40 Session 3 : Responses, finite electric field and Wannier functions [2:10]** (chair : Ph. Ghosez)
    - D. Hamann or X. Wu (piezoelectricity/internal strain) [20'+10']
    - D. Vanderbilt or X. Wang (phonons in finite field) [20'+10']
    - A. Romero (neutron scattering cross sections) [15'+5']
    - P. Hermet (IR, Raman and neutron spectra) [15'+5']
    - J. Battacharjee (Wannier functions) [20'+10']
- **12:30-14:00 : LUNCH**
- **14:00-15:30 Session 4a : PAW [1:30]** (chair : G. Zerah)
    - Gerald Jomard (pseudo – GS) [20'+10']
    - Ch. Audouze (response function : theory) [20'+10']
    - M. Torrent (response function : implementation) [20'+10']
- **15:30-16:00 COFFEE BREAK**
- **16:00-17:00 Session 4b : PAW [1:00]** (chair : D. Hamann)
    - F. Jollet (LDA+U) [20'+10']
    - P. Hermet (Berry phase) [20'+10']
- **17:00-18:00 Session A : Short talks [1:00]** (chair : S. Erwin)
    - to be defined (advanced use of ABINIT)
- **18:30-… Session P : Posters (with food & drinks)**

<u>WEDNESDAY 31</u>

- **9:00-10:30 Session 5 : SCF and wavelets [1:30]** (chair : N. Spaldin)
    - PM Anglade (Thomas-Fermi-Von Weiszacker) [20'+10']
    - M Torrent (Pulay SCF) [20'+10']
    - D. Caliste (current status of implementation of wavelets in ABINIT) [20'+10']
- **10:30-11:00 COFFEE BREAK**

- **11:00-12:30 Session 6 : Parallelism [1:30]** (chair : G.-M. Rignanese)
    - G. Zerah (band-by-band parallelism and LOBPCG algorithm) [20'+10']
    - T. Hofler (FFT parallelism) [20'+10']
    - P. Plaenitz or R. Jaenisch (perturbation parallelism) [20'+10']
- **12:30-14:00 LUNCH**
- **14:00-15:30 Session 7 : GW [1:30]** (chair : L. Reining)
    - F. Bruneval (self-consistency, no plasmon pole models) [20'+10']
    - R. Shaltaf (parallelism, two more plasmon pole models, interfaces) [20'+10']
    - Applications (to be defined) [20'+10']
- **15:30-16:00 COFFEE BREAK**
- **16:00-17:30 DISCUSSIONS & CODING PARTY** (chairs : G. Zerah & X. Gonze)
- **17:30 CLOSING REMARKS**

3. (Brief) Curriculum Vitae of Scientific Organiser

The brief CV of the contact organiser for ESF, X. Gonze, is given below.
More information can be found at
http://www.pcpm.ucl.ac.be/people/people.php?id=200 .
Information on other organisers can be found at
http://www.phythema.ulg.ac.be/Personnes/ghosez.htm
http://www.recherche.umontreal.ca/English/researchers/cote_michel.html

Brief CV X. Gonze

Present position :
- Professor (Professeur, Université Catholique de Louvain - UCL, Belgium).

Academic degrees :
- BSc in Engineering - Applied Physics ("Ingénieur civil physicien" - UCL June 1984).
- BSc in Physics ("Licencié en Physique" - UCL June 1985).
- PhD in Applied Sciences (UCL May 28, 1990).

Present research activities :
- Study of dynamical, thermodynamical, dielectric and electronic properties of the crystalline state and nanostructures within density-functional theory : band structure, phonons, thermal expansion, dielectric tensor, non-linear properties. Application to silicas, ferroelectrics (e.g. $BaTiO_3$) ...
- Excited states and Van der Waals interaction within Density-Functional Theory.
- Study of SiO_2 and high-permittivity dielectrics
- Software development and numerical techniques : coordinator of the ABINIT software project, iterative techniques for electronic structure calculations ...

Scientific output :
- 141 publications
- 271 contributions to professional meetings (58 personal invited communications).
- 35 invited seminars
- over 3000 citations in the litterature.

Academic activities :
- teaching : lectures at the Université Catholique de Louvain
- supervision of 7 PhD students and 7 students in engineering since 1992

Services :
- director of the « Institute for High Performance Computing and Mass Storage » of the UCL
- member of 18 PhD examination boards since 1993
- organizer or member of the program committee of 20 meetings since 1993.

Five most relevant publications during the last five years

First-principles study of structural, electronic, dynamical, and dielectric properties of zircon.
G.-M. Rignanese, X. Gonze and A. Pasquarello.
Phys. Rev. B 63, 104305 :1-7 (2001)

First-principle computation of material properties: the ABINIT software project.
X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty, and D.C. Allan.
Comput. Materials Science 25, 478-492 (2002).

First-principles study of the electrooptic effect in ferroelectric oxides.
M. Veithen, X. Gonze, and Ph. Ghosez. Phys. Rev. Lett. 69, 187401 :1-4 (2004)

A brief introduction to the ABINIT software package.
X. Gonze, G.-M. Rignanese, M. Verstraete, J.-M. Beuken, Y. Pouillon, R. Caracas, F. Jollet, M. Torrent, G. Zérah, M. Mikami, Ph. Ghosez, M. Veithen, J.-Y. Raty, V. Olevano, F. Bruneval, L. Reining, R. Godby, G. Onida, D.R. Hamann, and D.C. Allan.
Zeit. Kristall. 220, 558-562 (2005)

Projector Augmented-Wave Approach to Density-Functional Perturbation Theory
Ch. Audouze, F. Jollet, M. Torrent, and X. Gonze.
Phys. Rev. B 73, 235101 : 1-18 (2006)

4. Provisional list of proposed speakers

From outside Europe :

1. M. Mikami (Mitsubichi Chemicals, JAPAN)
2. A. Romero (MEXICO)
3. J. Battacharjee (JNCASR, Bengalore, INDIA)
4. M. Coté (U. Montréal, CANADA)
5. S. Pesant (U. Montréal (CANADA)
6. D. Hamann (Rutgers, USA)
7. N. Spaldin (Santa Barbara, USA)
8. S. Erwin (NRL, USA)
9. D. Allan (Corning Inc, USA)
10. D.Vanderbilt or X. Wang (Rutgers, USA)

From Europe :

11. G. Jomard (CEA-Bruyère, FRANCE)
12. Ch. Audouze (CEA-Bruyère, FRANCE)
13. M. Torrent (CEA-Bruyère, FRANCE)
14. F. Jollet (CEA-Bruyère, FRANCE)
15. G. Zerah (CEA-Bruyère, FRANCE)
16. V. Olevano (U. Grenoble, FRANCE)
17. T. Deutsch (CEA-Grenoble, FRANCE)
18. J.-P. Crocombette (CEA-Saclay, FRANCE)
19. F. Bruneval (Lugano, SWITZERLAND)
20. M. Verstraete (U. York, UK)
21. T. Hofler (Chemnitz, GERMANY)
22. P. Plaenitz or R. Jaenisch (Chemnitz, GERMANY)
23. J. Junquera (U. Cantabria, SPAIN)
24. Y. Pouillon (San Sebastian, SPAIN)

From Belgium

25. P. Hermet (ULg, BELGIUM)
26. Ph. Ghosez (ULg, BELGIUM)
27. R. Shaltaf (UCL, BELGIUM)
28. M. Giantomassi (UCL, BELGIUM)
29. X. Gonze (UCL, BELGIUM)
30. G. M. Rignanese (UCL, BELGIUM)