Research Networking Programmes

Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

***Proposal Title**: Abinit Developer's Workshop 2015*

Application Reference N°: 5735

1) Summary (up to one page)

ABINIT is an open-source software (http://www.abinit.org) for the atomistic modeling of the properties of periodic solids from first principles techniques (Density Functional Theory, Molecular Dynamics, etc). Initiated by Xavier Gonze (UCL, Belgium) in 1997, ABINIT rapidly became a renowned international code with more than 1000 users and more than 50 active developers.

The 7th ABINIT developer workshop has been organized in Liège by M. Verstraete, E. Bousquet, J-Y. Raty, Ph. Ghosez and Stefaan Cottenier from April 28th to May 1st 2015. Such an international ABINIT developer workshop was held in 2002 for the first time with a periodicity of about two years. It constitutes a very important event for the ABINIT community since it brings together most of the active developers of the code from all over the world (about 50 persons nowadays) in order to present the main achievements of each contributor and to organize the future evolution of the code.

52 persons from 7 different countries attended the workshop (see the list below in section 3) with diverse oral presentations going from technical code developments to practical applications. This 7th workshop edition has been the opportunity to extensively discuss the future major version of ABINIT (version 8) in view to coordinate the evolution of the code structures such as file formats, libraries, parallelization, etc. All the slides of the presentations are accessible for downloading from the workshop website. (https://sites.google.com/site/abinitworkshop2015/home).

2) Description of the scientific content of and discussions at the event (up to four pages)

The workshop has been divided into 5 main sessions:

- Benchmarking, pseudopotentials and PAW session,
- High throughput and large systems session,
- Correlations session,
- DFPT session,
- Applications session,

forming a total of 33 oral contributions, 5 discussion sessions and 1 advisory board meeting. For this 7th edition a coding party was organized in order to form working groups that aim at code improvements, outreach, and debugging. Two social dinners have also been organized during the event, to favor interactions and collaborations between the participants.

As in the previous editions, the workshop has been a unique occasion for most of the active developers and many young newcomers to get a general overview of the main code breakthroughs realized over the past two years. Indeed, ABINIT is a many-faceted software with several independent and diverse modules (Norm-Conserving, PAW, GW, DFPT, BigDFT, etc). This time, a particular highlight has been made on the high-throughput evolution of the materials community, as well as code and data validation, championed by Prof Cottenier (UGent). The workshop is thus the occasion for everyone to keep a global view on the project and stay up to date with the most recent advanced capabilities of the code. Going beyond the usual vicarious email or forum discussions, the ABINIT workshop is the opportunity for the developers to meet physically and interact directly, which is extremely useful to speed up interactions and to take collective decisions.

In the first session (Benchmarking, pseudopotentials and PAW), the focus was set on the assessment of the quality of the results produced by ABINIT, and a systematic comparison with other codes (WIEN2K, VASP, etc…). The evolution of the performance of Abinit was compared to that of other codes, emphasizing the necessity to standardize the pseudopotentials (resp. PAW datasets) with their validation against specific criteria (beyond simple elemental solids). The ability to interface ABINIT with the new CECAM electronic structure library (esl.cecam.org) was presented and discussed.

The second session presented the recent progress in 'high throughput' calculations. These are made available in ABINIT thanks to standard pseudopotential tables, improved distribution of tasks among processors, and extensive python scripts (in particular the abipy package) based on the materialsproject infrastructure, which provide workflows for many different calculations, handle job arrays etc…

The correlations session presented new technical methods in computing quantities influenced by electron-electron correlation. In particular the 'U' parameter from the Hubbard model can now be computed using different self-consistent and many-body-based schemes, and efficient numerical recipes can be used to solve the Bethe-Salpeter equation. Self-consistent van der Waals calculations based on planewave and/or Wannier function basis sets have been presented, as well as new developments of D3-type functionals that generalize the semi-empirical Grimme D2 approach.

In the DFPT session, the extension of ABINIT to the computation of anharmonic electron-phonon coupling and band gap renormalization, non-collinear magnetism and Nuclear Magnetic Resonance was presented.

The final 'application session' had a broader scope. It was an opportunity for some younger ABINIT community members to present their contributions to the field. It was also the occasion to present some more exotic applications of ABINIT (path integral molecular dynamics or electron-positron annihilation, for instance). The development of a user-friendly, powerful and complete graphical user interface was also presented (including job submission and some post-processing).

A full account of the scientific presentations can be found in the workshop abstract booklet.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

Besides advertising the new features and developments to the community, the workshop has established guidelines for the developments to be made in the coming years. It was clearly important to decide about standards for various aspects, i.e. pseudopotential performance, electronic structure results databasing, or file formats. These aspects have become crucial as the 'high-throughput' type of calculations are developing, scanning huge numbers of structures/compositions and assessing/sorting the results based on the adequacy of specific properties with selected criteria. These massive calculations should not suffer from the trade-off between quality, reliability and speed. Therefore the production of standard libraries and tools is essential.
It was also important for the community of developers to gather to decide over a unified framework for the coding and interfacing with the outside world (database, repositories, user interfaces, other post-processing tools). Many needs for new developments were identified such that the community of developers can address these in priority. The ABINIT community has continuously contributed to standardization and "librarification" efforts over the past decades, in particular through Psi-k and CECAM, and will continue to do so in a synchronized way thanks in large part to coordination achieved in the biannual developers' meeting.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

AM: Benchmarking, pseudopotentials and PAW session
- 9:00 Stefaan Cottenier “Benchmarking codes and theory: the delta factor and beyond”
- 9:25 Kurt Lejaeghere “DFT and experiment: a match made in heaven or in hell?”
- 9:50 Marc Torrent "PAW atomic datasets: A 71 element validated table in the XML format ; and the libPAW project"
- 10:15 coffee break
- 10:45 Don Hamann “The ONCVPSP method, code, and performance”
- 11:10 Michiel Van Setten and Matteo Giantomassi "Pymatgen, abipy, and the oncvpsp periodic table"
- 11:35 Micael Oliveira “ABINIT links to the CECAM Electronic Structure Library”
- 12:00 Recap - discussion

12:30 Lunch

PM: High throughput and large systems session
- 14:00 Edoardo di Napoli "The inner workings of the Simulation Laboratory "ab initio": algorithm development, parallel computing and performance efficiency”
- 14:25 Antoine Levitt "Abinit on 10,000 processors”
- 14:50 Aldo Romero “The PyChemnia package and its interface with ABINIT”
- 15:15 John Rehr "Corvus and ABINIT"
- 15:30 coffee break
- 16:00 Gian-Marco Rignanese “A high-throughput framework for ABINIT”
- 16:25 Michiel Van Setten “High throughput GW”
- 16:50 Jean-Michel Beuken “The test farm and its evolution”
- 17:05 Luigi Genovese "BigDFT order N calculations"
- 17:30 Recap - discussion

- 19:00 Social Dinner at the restaurant "l'Industrie"

Wednesday 29 April:

AM: correlations session
- 9:00 Bernard Amadon “DFT+DMFT in Abinit: Wannier functions, calculation of U and spin orbit coupling”
- 9:25 Francois Jollet “PAW and Hartree-Fock in ABINIT”
- 9:50 Yannick Gillet “Efficient Trilinear Interpolation Technique for Bethe-Salpeter Calculations of Optical Spectra"
- 10:15 coffee break
- 10:45 Camilo Espejo Pabon “Van Der Waals calculations in abinit”
- 11:10 Benoit Van Troeye “Van der Waals and phonons”
- 11:35 Yann Pouillon "Building and enhancing Abinit 8: a new paradigm"
- 12:00 Recap - discussion
- 12:30 Lunch

PM: DFPT session
- 14:00 Alexandre Martin “PAW and DFPT: elastic constants and external fields”

- 14:25 Jonathan Laflamme Janssen “Accurate effective masses from first principles”
- 14:50 Samuel Poncé “Temperature dependence of the electronic structure: the Allen-Heine-Cardona formalism and beyond”
- 15:15 coffee break
- 15:45 Gabriel Antonius “Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the band structure”
- 16:10 Fabio Ricci “Non collinear magnetism in DFPT”
- 16:30 Joe Zwanziger "PAW calculation of response properties at the nucleus"

- 16:55 Strategic discussion with everyone, presentation of new logo, etc...

- 17:45 Advisory Board meeting

- 18:30 – Social Dinner at Brasserie Curtius

Thursday 30 April:

AM: applications session
- 9:00 Grégory Geneste “Path-Integral Molecular Dynamics”
- 9:25 Marc Torrent 2 "Doppler broadening of annihilating electron-positron pairs”
- 9:50 Razvan Caracas “ABINIT on Mars via WURM”
- 10:15 Vincent Gosselin "Von Linden Horsh plasmon pole model within GW"
- 10:20 coffee break
- 10:45 Jordan Bieder “Finite temperature properties derived from second principles models"
- 11:10 Anton Bokhanchuk “Unfolding the band structure of supercells with fold2Bloch”
- 11:35 Yannick Gillet “AbinitGUI : what's up, doc ?"

- 12:00 Discussion and closing

- 13:00 Lunch

PM: groups and coding party
- 15:30 coffee break

Friday: coding party in Sart Tilman

Annex 4b: Full list of speakers and participants

A total of 52 participants have attended the workshop, 31 from Belgium, 6 from Canada, 1 from Colombia, 9 from France, 1 from Germany, 1 from Spain and 3 from USA.

First Name	Name	Institution	Address	Country
Bernard	Amadon	CEA	CEA Département de Physique Théorique et Appliquée Bruyères-le-Châtel 91297 Arpajon Cedex	France
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Razvan	Caracas	CNRS	CNRS	France

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Michel	Côté	Université de Montréal	Département de physique Pavillon Roger-Gaudry, A-406 Université de Montréal C.P. 6128, succ. Centre-ville Montréal Québec H3C 3J7 Canada	Canada
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antoine	dewandre	ULg	rue des carmes 15, 4000 liège	Belgium
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Gregory	GENESTE	CEA	CEA, DAM, DIF, F-91297 Arpajon, France	France
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