Report on the 4thinternational ABINIT developer workshop

Autrans (France)

24th– 27thMarch 2009

Psi$_k$ network, GdR-DFT and Scienomics

P. Blaise, D. Caliste*, T. Deutsch, L. Genovese and V. Olevano

`http://wwwold.abinit.org/2009-Abinit`

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.

This year, the number of participants reached 56 people including four invited speakers from different other communities. This opening to developers outside ABINIT and their interesting contributions show the maturity of this software. These invited contributions were done in the field of post-ground state calculations with the talk about Yambo, a software for Many-Body calculations in solid state and molecular physics (A. Marini). The second talk in this field was about the capability to compute the Maximaly Localized Wannier Functions for accelerated band structure calculations with the help of the Wannier90 library (A. Mostofi). In these both cases, ABINIT is used as the fundamental tool to compute the ground state of the system. The second axis of the invited talks was about the improvement of ABINIT with the help of outside contributions. On one hand this was done with the presentation of a Linux distribution packager point of view about the package and its distribution (D. Berkholz) and on the other hand by the presentation of the XC library initially developped for Octopus software but on the way for inclusion inside ABINIT (M. Marquès).

Beside these outside contributions, different labs implied in the development of ABINIT presented their contributions. One should remember two main axis. The first was about the ongoing effort to implement the missing functionnalities in the PAW formalism in comparison with the functionnalities of norm-conserving pseudo-potentials. This includes the non-colinear magnetism, the spin orbit coupling and the DFPT formalism (M. Torrent) ; but also the capability to simulate Mössbauer spectra and to compute the response to an electric or a magnetic field within the PAW formalism (J. Zwanziger) ; or also the development of the local exact exchange (F. Jollet). The second main axis was in the field of the GW approximation and its improvements (better paralllelism, method for fewer empty bands...) as presented by F. Bruneval and M. Giantomassi. Besides these two axis, several other points were discussed. One can cite the effort to port ABINIT to super-computers, with massively parallel network (F. Bottin), hybrid architectures (L. Genovese) or distributed computational power (M. Oliveira). Finally, several applications of the ABINIT program were presented, like the key exploration done by M. Mikami for warm-white led engineering, the *ab initio* explanation of the structure of GeMn nano-columns (E. Arras) or temperature dependance of the band energy in semiconductors (P. Boulanger).

The workshop was also the place for several discussions about the development of the ABINIT software. Among these talks, the documentation and user oriented tutorials and information were discussed around the availability and improvement of the new web site. One other discussion session was dedicated to the required decisions to continue the development of ABINIT with the same level of quality with an always growing software base and contributors. Indeed, ABINIT will need to enforce its coding standards and current code through a beautification phase to go to version 6 that will allow to continue to easily and safely add new functionnalities.

With all these diverse contributions, external, physics and software engineering, the meeting was considered by all the attendees as a very good working session resulting in several achievements. The full program is available on-line at `http://wwwold.abinit.org/2009-Abinit` as the list of the participants.

Programme

		Tuesday 24th	Wednesday 25th	
Morning			Methodological developments: ■ L. Genovese (25') ■ M. Mancini (25') ■ A. Lherbier (A) (10') ■ A. Romero (A) (10')	9.00 10.15
			Tea/coffee break	
			Links with communities: ■ D. Caliste (25') ■ M. Marques (25') ■ A. Mostofi (25')	10.45 12.00
			Scienomics ■ X. Krokidis (30')	12.30
		Lunch time	Lunch time	
Afternoon	14.00	Introduction + SWOT Ch.: X. Gonze, T. Deutsch & G.-M. Rignanese	Software engineering: Ch.: M. Côté ■ X. Gonze (25') ■ J.-M. Beuken (25')	14.00 14.50
	14.30 15.50	PAW session: ■ M. Torrent (25') ■ J. Zwanziger (25') ■ G. Jomard (A) (10') ■ A. Jacques (10' + 10')	Discussion (30') Mod.: M. Côté An.: X. Gonze, J.-M. Beuken & A. Jacques ■ Merge/testing	15.20
		Tea/coffee break	Tea/coffee break	
	16.20 17.20	Correlated electrons: ■ B. Amadon (25') ■ F. Jollet (25') ■ D. Adams (A) (10')	Software engineering: Ch.: M. Côté ■ Y. Pouillon (25') ■ T. Deutsch (15')	15.50 16.30
			Discussion (30') Mod.: M. Côté An.: T. Deutsch & Y. Pouillon ■ Build system	
	17.30 18.00	Discussion (30') Mod.: J.-M. Beuken ■ Web	Software engineering: Ch.: M. Côté ■ D. Berkholz (25')	17.00 17.25
			Discussion (25' + 25') An.: A. Jacques, D. Berkholz & G.-M. Rignanese ■ Packaging ■ SWOT	
	19.00	Poster session	Advisory board	18.15

		Thursday 26th	Friday 27th	
Morning	9.00	Perturbation: Ch.: R. Caracas ■ P. Boulanger (25') ■ M. Torrent (25') ■ M. Verstaete (25') ■ F. Da Pieve (A) (10')	Applications: Ch.: J. Zwanziger ■ S. Blackburn (20') ■ P. Blaise (20') ■ E. Arras (20')	9.00
	10.25			10.00
		Tea/coffee break	Tea/coffee break	
	10.55	■ J. Zwanziger (25') ■ P. Hermet (A) (10')	■ R. Caracas (20') ■ M. Mikami (20')	10.30
	11.30	Discussion (40') Mod.: R. Caracas An.: X. Gonze, Y. Pouillon & M. Giantomassi ■ Beautification	Discussion (80') Mod.: J. Zwanziger An.: X. Gonze & Y. Pouillon ■ ABINIT6 ■ Debriefing	11.10
	12.10			12.30
		Lunch time	Lunch time	
Afternoon	14.00	GW+BS: Ch.: M. Torrent ■ F. Bruneval (25') ■ M. Giantomassi (40') ■ T. Rangel (25') ■ M. Cazzaniga (A) (10')		
	15.40			
		Tea/coffee break		
	16.10	■ A. Marini (25')		
	16.35	High performance: ■ F. Bottin (25') ■ M. Oliveira (25') ■ J. Laflamme (A) (10')		
	17.35	Discussion (HPC) (55') Mod.: M. Torrent An.: F. Bottin, L. Genovese, M. Oliveira & M. Côté ■ GPU ■ Multi-parallelism		
Evening		Social diner		

Talks

Plane wave based electronic structure calculations using DMFT and projected local orbitals

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The description of realistic strongly correlated systems has recently advanced through the combination of density functional theory in the local density approximation (LDA) and dynamical mean field theory (DMFT). This LDA+DMFT method is able to treat both strongly correlated insulators and metals. Several interfaces between LDA and DMFT have been used, such as (N^{th} order) linear muffin-tin orbitals or maximally localized Wannier functions. Such schemes are, however, either complex in use or additional simplifications are often performed (*i.e.*, the atomic sphere approximation). We present an alternative implementation of LDA+DMFT, which keeps the precision of the Wannier implementation, but which is lighter [1]. It relies on the projection of localized orbitals onto a restricted set of Kohn-Sham states to define the correlated subspace. The method is implemented within the projector augmented wave and within the mixed-basis pseudopotential frameworks. This opens the way to electronic structure calcula-

tions within LDA+DMFT for more complex structures with the precision of an all-electron method. In this presentation, we will briefly present the theoretical framework, discuss practical details and prospects of the implementation, and give some examples of applications.

References

[1] B. Amadon, F. Lechermann, A. Georges, F. Jollet, T. O. Wehling, and A. I. Lichtenstein Phys. Rev. B 77, 205112 (2008)

Computational investigation of the atomic structure of Mn-rich nanocolumns: comparison with a possible GeMn ordered compound

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High curie temperature ($> 400K$) GeMn alloys have recently been grown by means of low temperature molecular beam epitaxy. The samples exhibit Mn-rich nanostructures embedded in a nearly pure germanium matrix. The composition of theses nanostructures is close to Ge_2Mn but their atomic structure is still puzzling. A recent Extended X-Ray Absorption Fine Structure (EXAFS) study reveals that these nanostructures present a complex local structure that does not correspond to any known stable GeMn compound [2]. Based on electronic structure calculations we have investigated both magnetic and structural properties of a possible GeMn ordered compound found in similar transition-metal metalloid systems. The comparison is based on both magnetic properties of the relaxed compounds as well as their simulated EXAFS spectra. This methodology was first validated on the Ge_3Mn_5 compound and then applied to other ordered compounds. Moreover the Curie temperature is calculated by means of coupled KKR-Monte Carlo calculations for the compounds that exhibit a stable ferromagnetic ordering.

References

[1] M. Jamet , A. Barski, T. Devillers, V. Poydenot, R. Dujardin, P. Bayle-Guillemaud, J. Rothman, E. Bellet-Amalric, A. Marty, J. Cibert, R. Mattana, and S. Tatarenko, Nat. Mater. **5**, 653 (2006).
[2] M. Rovezzi, T. Devillers, E. Arras, F. d'Acapito, A. Barski, M. Jamet, and P. Pochet, Appl. Phys. Lett. **92**, 242510 (2008).

How to be a distribution-friendly project

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Getting ABINIT integrated into Linux distributions will help to increase its adoption and to ensure that users have ABINIT well-integrated into their systems and kept up-to-date easily. ABINIT is already packaged in Gentoo Linux, and Donnie will share his experience creating and maintaining ABINIT's Gentoo package and offer suggestions for improvement. Technical and philosophical questions that determine how easy or difficult it is for distribution packagers to work with ABINIT developers will be discussed. Technical issues include the basic metaphor that ABINIT's build and installation process is an API to distribution packages – it should be changed carefully and purposefully, and changes should be well-documented. In addition, Donnie will describe the level of control and system integration desired by packagers. Philosophical issues, including user expectations and licensing requirements, differ between distributions and can cause major conflicts with upstream developers. Finally, Donnie will discuss developments toward the future of distribution packaging so that ABINIT developers can consider how this fits into the future of ABINIT.

Superconductivity near a lattice phase transition: the case of NbN

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We report the study of the electron-phonon coupling in $NbC_{1-x}N_x$ crystals in the rocksalt structure. The Kohn anomaly associated with the topology of the Fermi surface greatly increases the electron-phonon coupling and induces a structural instability when the electronic density of states reaches a critical value. We develop a model of the Eliashberg spectral function where the effect of the unstable phonons is set apart. We show that this model within the McMillan formula can reproduce the increase of T_c near the structural phase transition.

From application-centric to data-centric computation: use of *ab initio* methods in applied research

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We present some results in applied electronics obtained with ab initio methods: computation of realistic band offsets of a high-K MOS gate stack, using a combination of Siesta (DFT/LDA) and Abinit (G_0W_0), calculation of electronic levels useful for future development of flash memories. A more general discussion will follow about crucial differences when one uses ab initio methods for fundamental or applied research. Some perspectives will be drawn about the embedding of an application like Abinit in a typical workflow for e-science.

Ab initio calculation on three levels of parallelization

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Three levels of parallelization [1] are now available in the ABINIT code package. Indifferently, these ones can be used separately or coupled the ones with the others. To the parallelization on k-points, previously introduced into the code, we add two others of them acting on bands and plane waves. These two last levels of parallelization are based on two algorithms previously introduced in the code: on one hand, a three-dimensional Fast Fourier Transform (3dim-FFT) [2], which allows a parallelization on plane waves, and on the other hand, a blocked eigensolver (LOBPCG) [3], in order to perform a band parallelization. First, we briefly recall the implementation and the efficiency of this parallelization. In particular, we indicate the last implementations carried out in the code and the new features which are now available. Then we focus on various sudies, involving a large number of CPUs (up to one thousand), bands (a few thousands), atoms (a few hundreds) and/or plane waves [4], in order to illustrate the use of this parallelization. For each system we indicate the CPU time needed to perform such a calculation.

References

[1] F. Bottin, S. Leroux, A. Knyazev, and G. Zerah, Comput. Mater. Sci. 42, 329 (2008).
[2] S. Goedecker, M. Boulet and T. Deutsch, Comput. Phys. Comm. 154, 105 (2003)
[3] A. Knyazev, SIAM Journal on Scientific Computing 23, 517 (2001).
[4] S. Mazevet, F. Lambert, F. Bottin, G. Zerah and J. Clerouin, Phys. Rev. E 75, 056404 (2007); F. Bottin and G. Zerah, Phys. Rev. B 75, 174114 (2007)

Temperature Dependance of the band energies of semiconductors

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The band energies of semiconductors are known to exhibit significant shifts and broadening with the variation of temperature. At constant volume, this dependance is a consequence of the renormalization of band energies due to electron-phonon interactions. This effect was first fully described in a formalism developed by Cardona and coworkers[1] within a semi-empirical context.
We have reanalyzed this formalism in a density functional perturbation theory approach (DFPT). This new formalism includes an extra term, the non-diagonal Debye-Waller term, which can be calculated with the help of DFPT. We have studied the importance of this contribution on diatomic molecules using frozen phonon and DFPT calculations. For the H_2 molecule, it contributes to up to 15% of the total temperature dependence. This formalism might help explain the discrepancy still found between calculations and experiments for solids[2].
In this presentation, the details of this implementation in the Abinit package will be discussed and examples on how it can be used will be given.

References

[1] P.B Allen and M. Cardona, Physical Review B 23, 1495 (1981)

[2] D. Olguin, M. Cardona and A. Cantarero, Solid State Communications 122, 575 (2002); M. Cardona, Solid State Communications 133, 3 (2004)

Fast GW approximation with only a few empty states

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The GW approximation to the electronic self-energy yields band structures in excellent agreement with experimental data. Unfortunately, this type of calculation is extremely cumbersome even for nowadays computers. The huge number of empty states required both in the calculation of the polarizability and of the self-energy is a major bottleneck in GW calculations. We propose an almost costless scheme, which allows to divide the number of empty states by about a factor of five to reach the same accuracy. The computational cost and the memory requirements are decreased by the same amount, accelerating all calculations from small primitive cells to large supercells. I will describe how this method has been implemented in Abinit.

Parser and visualisation: how to link ABINIT and V_Sim?

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Dealing with developments around the main ABINIT loop, this talk will focus on two linked topics. The first one will present how the input file parser has been extracted and is now exposed to third party developers. The second topic will deal with the visualisation capabilities of V_Sim [1] developed these last two years and specifically these related to ABINIT.
Either before the calculation for checking purposes or after the calculation for analysis and sorting purposes, one would like to access the ABINIT input file easily and independently from the language one uses. The ABINIT parser is a quite complex object that would be useless to duplicate and which has interesting capabilities like the unit parameters, the array notation, the data sets... A Fortran90 module has thus been created linking with the ABINIT own routines. The purpose of this module is to expose an object oriented interface to be able to bind easily in scripting languages like Python. This part of the talk will present the available interfaces in Fortran90, C and Python.
The development of V_Sim [1] has tightly followed the development of computational softwares around ABINIT. Indeed, using the C bindings of the ABINIT parser, one can now visualise directly whatever step of a data set directly loading the input file. Beside that, several capabilities have been added, like the box duplication that allows to clearly understand the atomic relations from a file describing a primitive cell; or the density mapping, the interactive geometry modifications...

References

[1] visit `http://inac.cea.fr/L_Sim/V_Sim` or download Debian packages `http://packages.debian.org/sid/v-sim`.

High-pressure study of water ices VII-VIII-X

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We study high-pressure solid H_2O ice: the lattice dynamical properties of ice X and the transition path between molecular ices VII/VIII and the ionic ice X with first-principles calculations using density functional theory in the ABINIT implementation. Our work [1] defines the dynamical stability of ice X between about 120 GPa up to about 400 GPa. Based on phonon band dispersion we show that the phase transition sequence at low temperature and high pressures in ice is ice VIII - disordered ice X - ice X - ice Pbcm. The disordered ice X is due to a phonon collapse in the whole Brillouin zone at pressures below 120 GPa, phonon that corresponds to hydrogen atoms bouncing back and forth between every two oxygen neighbors in a double well potential. Post-ice X is orthorhombic Pbcm and appears due to phonon instability in M at pressures higher than 400 GPa that distorts the bcc cubic sublattice of oxygen atoms into a hcp-like structure. Our calculations validate earlier theoretical predictions for a phase transition to a post-ice X structure in H_2O [2]. We also identify and discuss the (meta)stability of several intermediate phases between ice VIII and ice X and try to explain some new experimental data.

abilint: python script to help developers

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The python script abilint is used to generate automatically interfaces from Fortran routines and dependencies in the build system. This script was developed to help developers with the goal to be ignored. Due to the diversity of developers, this objective was achieved by developing a Fortran parser!
In this talk, I will present the main characteristics of abilint and gives some ideas for its future use to improve modularity and quality of the ABINIT code.

ab initio simulation of large systems in complex environments : the BigDFT project

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The european BigDFT project has developed an *ab initio* Density Functional Theory code based on Daubechies wavelets. Such functions have features which make them a powerful and promising basis set for application in materials science. These are a compact support multiresolution basis, and form one of the few examples of systematic real space basis sets. For these reasons they are an optimal basis for expanding localised information. The real space description they provide allows to build an efficient, clean method to treat systems in complex environments, like surfaces geometries or system with a net charge. The mathematical properties of the formalism are optimal to build a robust, highly optimised code, conceived for systems of few hundred atoms, with excellent efficiency on parallel computers. During this talk we will illustrate the main features of the code, its actual performances and capabilities. We will then conclude by outlining the planned developments and the potentialities of this powerful formalism in the context of electronic structure calculations.

Gathering the contributions of the ABINIT developer : the whole story.

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Over the years, many different people have submitted contributions to the ABINIT project. Despite their diversity, the vast majority of these contributions have been successfully integrated into ABINIT, without ABINIT falling apart... I will survey the reasons, the tools and software techniques that have made this possible. This will give justification to the presence of the rules to be followed by developers, concerning automatic tests, structure of the files, requested documentation, etc. , and, I hope, also more motivation to follow them!

Local exact exchange in the Projector Augmented-Waves framework: Implementation in the ABINIT code, validation, and application to actinide compounds

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Exact exchange is used to describe correlated orbitals in the Projector Augmented Waves (PAW)framework. As suggested recently in another context [1], Hartree-Fock exchange energy is used for strongly correlated electrons only inside the PAW atomic spheres. This is done thanks to the PBE0 exchange-correlation hybrid form functional. This method is tested on NiO and results well agree with already published results and LDA+U calculations. It is then applied to UO_2 and PuO_2 for which the results well agree too with LDA+U calculations, but without adjustable parameter.

References

[1] P. Novak et al., Phys. Status Solidi B 243, 563 (2006)

MAPS - A flexible modeling environment for efficient delivery of Open Source code

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The Materials And Processes Simulations Platform (MAPS) is a molecular modeling environment offering a variety of tools allowing the building of molecular models (finite and periodic), the access to simulation codes, job management and analysis of results. Today the technology in MAPS covers the areas of quantum, classical, mesoscale and chemical engineering simulations. Moreover, MAPS offers full Python scripting capability that allows the creation of customized graphical user interfaces and simulation scenarios.
Scienomics likes to promote the MAPS platform as a key tool to help open source solutions to become more popular in the scientific community. The plugin based architecture of MAPS and its robust Application Programming Interfaces (APIs) toolbox make MAPS an excellent tool for developing graphical user interfaces for simulation engines. The usage of a simulation code within MAPS is facilitated even for non expert users since they can benefit also of all auxiliary technology in MAPS (builders, visualization, analysis and other simulation engines). This is particularly important for industrial users who usually perform multi-scale modeling.
MAPS includes an interface to ABINIT and to other open source or free simulation engines. In particular ABINIT users can easily build their models and perform some of the sophisticated calculations allowed by ABINIT with a few steps guided by the graphical user interface. Moreover, the results can be visualized and analyzed within the framework of MAPS.
However, in order to increase efficiency a close collaboration with the communities developing the open source tools and Scienomics is required to deliver (a higher) high end technology to the industrial community.

A Recursion method in abinit

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Classical Abinit simulations are limited to temperatures up to approximately 10eV as a consequence of the very rapid growth of the number of electronic states when solving the Mermin-Kohn-Sham effective Schrödinger equation. The recursion method is based on a direct evaluation of the density matrix in the real space representation. This allows for an orbital free computation of the charge density in the Kohn-Sham formalism at finite temperature whose numeric complexity increases linearly with the size of the system (order N method). In our implementation, the density matrix is computed by a recursion method based on the Trotter formula which allows simulation up to very high temperatures. We present the Recursion method and its Abinit implementation, its advantages (high temperature simulations, good parallelization properties) and limitations (low temperature performance, no yet non-local potential). We illustrate the assessment with numerical tests performed to the computation of the Hugoniot curve of cryogenic Helium using two different pseudo-potentials, and we compare our results with Path Integral Monte Carlo simulations and experimental data.

An *ab initio* tool for excited state calculations

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Yambo[1] aims to be a combination of several projects devoted to the device of new theoretical and/or numerical tools for calculating, *ab initio*, the excited state properties of electronic systems. In practice, Yambo is a mixed Fortran/C code composed of a core part and many extensions. These extensions are pieces of code embodied in the main Yambo trunk, that can be isolated or joint together. The result is one source but many possible executables. The core of yambo calculates quasiparticle energies and optical properties within the framework of many-body perturbation theory and time-dependent density functional theory, and it is released under the GPL license. Quasiparticle energies are calculated within the GW approximation for the self-energy. Optical properties are evaluated either by solving the Bethe-Salpeter equation or by using the adiabatic local density approximation. However yambo features are very much extended by the different projects that cohabit in the code: total energy, electron-phonon coupling, surface spectroscopy, non equilibrium time-dependent dynamics, and so on. Yambo is a plane-wave code that, although particularly suited for calculations of periodic bulk systems, has been applied to a large variety of physical systems. Yambo relies on efficient numerical techniques devised to treat systems with reduced dimensionality, or with a large number of degrees of freedom. The code has a user-friendly command-line based interface, flexible I/O procedures and is interfaced to Abinit, PWscf and with the "ETSF file format"[2]. In this talk I will outline the history of the code and its philosophy. I will briefly describe some of the code's features and specific numerical tools. I will also present the projects that cohabit in the code and some of the most recent and intriguing results[3] we have obtained thanks to yambo.

References

[1] Yambo: "an *ab initio* tool for excited state calculations", arXiv:0810.3118. Yambo web site `http://www.yambo-code.org`

[2] European Theoretical Spectroscpy Facility(ETSF) Standardization Project, ETSF standardisation page `http://www.etsf.eu/resources/software/standardization_project`

[3] See Yambo publications `http://www.yambo-code.org/publications.html`

libxc - a library of exchange and correlation functionals

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The central quantity of density functional theory is the so-called exchange-correlation energy functional. Many approximations exist for it (probably of the order of 150-200), and they are usually arranged in families (LDA, GGA, meta-GGAs, etc.) In spite of these theoretical advances, most computer codes only include a very limited quantity of functionals, typically around 10-15. This choice usually contains the most popular variants, like the Perdew-Zunger or the Perdew-Wang LDAs, or the PBE or BLYP GGAs, but misses many of the old functionals (that are important to reproduce old results) or some of the most recent developments. With this in mind, we have developed libxc, a library of exchange and correlation functionals. This library already includes more than 100 functionals, is available under the LGPL license, and can be easily called both from C and Fortran. Furthermore, it also particularly adapted not only for ground-state calculations, but also for response calculations, as it includes higher derivatives of the exchange-correlation energy

New Phosphors for White LEDs : Theory and Experiment

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A trend to search for new phosphors for white LEDs has been acceralating, because white LEDs are highly expected as one of the most promising light sources with much less energy consumption (less CO_2 gas exhaustion) than conventional light sources such as incandescent lamp. In this presentation, we will present how our nitride/oxynitride phosphors have been developed by close cooperation between theory and experiment. In particular, it will be stressed that ABINIT computation was greatly helpful for the discussion on the feasibility of phosphor synthesis as well as the determination of crystal structures. Outlook and issues will be discussed for possible "*ab initio* design" of phosphor materials.

The Wannier90 Project: Design, Developments, Directions

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Wannier90[1] is a code for obtaining maximally-localised Wannier functions[2] (MLWF) in a post-processing procedure following an electronic structure calculation. Written in modern, modular FORTRAN, independence from the basis set and methodology used for the underlying electronic structure calculation is a fundamental design feature of the code. Its structure and current scientific functionality will be presented, with particular emphasis on the elements required for a seamless interface to an electronic structure program of choice. Time permitting, some recent developments will be discussed and directions and challenges for the future will be highlighted.

References

[1] A. A. Mostofi et al., Comput. Phys. Commun., 178, 685 (2008)
[2] N. Marzari et al., PRB 56, 12847 (1997); I. Souza et al., PRB 65, 035109 (2002)

Running ABINIT in a GRID environment

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GRID computing facilities are becoming widely available, as they allow research institutions to share their computational resources in an effective and efficient way. Nevertheless, up to now, usage of GRID facilities to run ab-initio codes, like ABINIT, has not been very popular. One of the reasons for this was the deficient MPI support. Indeed, GRID facilities were initially designed having in mind large amounts of small serial jobs, but this is now changing, as support for MPI jobs started to become widely available. In this talk we will present our experience in running ABINIT in a GRID using the GLite software, both in serial and parallel modes. We will discuss the problems encountered, as well as how these were solved. A short introduction to GRID concepts will also be presented.

The mutation of Abinit

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During the five last years Abinit has undergone a comprehensive mutation at various levels, including a complete restructuring of the source code and the website, the introduction of enhanced management tools, as well as a substantial increase in terms of size, versatility, visibility and user base. The lifespan of Abinit 5 has moreover let us know much better about the needs of the community and how to drive a sustainable growth.
In addition to improving the development workflows and the conformance of the source code to modern standards, the roles of the various contributors, *i.e.* end-users, developers and maintainers, have been clarified. Previously, everyone was modifying the source and build system, while further advances required more specialization in the community, *e.g.* the management of external libraries - in growing number - which has to be done by skilled maintainers.
To address the issues raised by Fortran compilers, and because the ABINIT developers are mostly scientists, it was decided to provide support beyond the GNU Autotools (nowadays the paradigm for binary/package generation) by developing a new build system on top of it, while keeping backward-compatibility with the features present in Abinit 4 as long as possible. Though it has permitted a smoother transition, the latter constraint has also led to a certain number of limitations. Solutions will be proposed to set Abinit 6 free from them.

The ABINIT-Wannier90 interface.

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The numerous applications of the Maximaly-Localized Wannier Functions (MLWFs) have motivated many people to work on the development of an interface between ABINIT [1] and Wannier90 [2]. The implementation was first started by Bernard Amadon, and François Jollet some years ago [3]. From the beginning, the interface was developed to work with Projected Augmented Waves (PAW) and Norm Conserving pseudopotentials.
As a first improvement to this existing interface, we have provided a variety of possible initial guess for the MLWFs. Indeed, the choice of this initial guess can considerably speed up the convergence of the localization procedure. In particular, for the conduction bands, the convergence cannot be achieved starting with at random.
More recently, we have extended this interface in order to use it in the framework of Many-Body Perturbation Theory (MBPT) for GW calculations. First, the MLWFs can be used to obtain the complete bandstructure based on the GW corrections computed only for a set of special k-points, hence providing a very efficient interpolation scheme. Second, the MLWFs can also be obtained for the quasiparticle wavefunctions when self-consistent GW calculations are performed [4].
As a result of these developments, ABINIT 5.7 has a very robust and user-friendly interface with Wannier90 which can be used with PAW and Norm Conserving pseudopotentials for ground state and GW calculations.

References

[1] `http://www.abinit.org`, ABINIT web site
[2] `http://www.wannier.org`, Wannier web site
[3] B. Amadon, et al., Phys. Rev. B 77, 205112 (2008)
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Non-collinear magnetism and spin-orbit coupling within PAW

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On top on existing implementation of non-collinear magnetism in ABINIT, we have generalized it to the case of the Projector Augmented-Wave (PAW) formalism. Introduction of wave-functions as spinors was necessary in the PAW part of the code, as well as imaginary "on-site" potentials and densities. I will present first the internal representation of each PAW objects, especially on-site densities, occupation matrix and pseudopotential strengths. In the second part of the presentation, I will detail the implementation of spin-orbit coupling in the PAW on-site terms. I will discuss some PAW specifc aspects of the implementation:

- the application of symmetries on PAW objects,
- the problem of the time-reversal symmetry. Then I will present some recent applications of these implementations, and, as conclusion, detail the practical use of the non-collinear/spin-orbit features.

Implementation of the DFPT in the framework of PAW: computation of phonons

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Two years ago, I presented the formulae derived to apply the Density-Functional Perturbation Theory (DFPT) approach in the framework of the Projector Augmented-Wave (PAW) method. I will briefly recall the key points of the formalism and present some recently published novelties [1]. Then I will restrict the presentation to the implementation of phonons (response of the system to an atomic displacement) and detail the internal representation of first-order perturbed PAW objects and the content of some new PAW routines. A focus on two specific aspects will be done:

- the generalized conjugate gradient algorithm used to solve the generalized Sternheimer equation,
- the case of metals.

As a conclusion, I will show the first calculations done with the DFPT+PAW and compare them with results obtained with the norm-conserving pseudopotential approach.

Finite temperature phonons and the stability of phases

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The usefulness and implementation in ABINIT of a finite temperature ("self consistent") phonon scheme, invented by Souvakis *et al.* in PRL 100 095901, is presented. In many crystallographic phase transitions, the high temperature phase presents imaginary phonon modes at low temperature. This precludes the use of the *ab initio* vibrational spectrum to calculate thermodynamical properties. Increasing the electronic temperature is usually not enough: it is the phonon frequencies themselves which change with (ionic) temperature. This is exemplified by the transition of Ti, Zr, or Hf to a BCC structure at high temperatures, while the 0K phonons present imaginary modes. Starting from the ground state phonons and a (typically 4x4x4) supercell of atoms, the atomic forces, normal mode displacements, and phonon frequencies are solved for self-consistently, accounting for the desired temperature in the statistical occupation of the modes. In this way the high temperature phase phonons can be stabilized, and compared properly to experiments. First examples on Aluminium present encouraging results.

Perturbations in the PAW Formalism: DDK, Electric, and Magnetic Fields

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Building on the general PAW DFPT scheme being implemented, we are working to add response functions to electric and magnetic fields within the PAW formalism. This project is in the development and implementation stages. Earlier work by Umari, Gonze, and Pasquarello (PRB 69, 235102 (2004)) showed how to treat both the DDK and static electric field perturbations in the ultrasoft pseudopotential case, and the DFPT PAW equations are very similar (though their implementation is more complex). I will discuss current progress in implementing these perturbations in abinit, including the additional nonlocal potentials required and the unusual asymmetric derivatives of the projectors. Then I will discuss recent work of Xavier Gonze, Marc Torrent, and myself on implementing the response to a static magnetic field. This has required significantly more new theoretical development, and will ultimately represent a substantial step forward as compared to finite-difference methods for treating this perturbation as present in CASTEP and PWSCF

Properties at the Nuclei: Electric Field Gradients and Mössbauer Isomer Shifts in the PAW Formalism

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Key observables in Mössbauer spectroscopy include the isomer shift and the electric field gradient at each nucleus. The electric field gradient is also observable in nuclear magnetic resonance and nuclear quadrupole resonance. Since the last workshop Marc Torrent and I have implemented the EFG in abinit, and recently I have implemented the Fermi-contact interaction, which is proportional to the isomer shift. I will briefly describe the theory of both these interactions, and show results on various compounds. In particular, I will show how the EFG acts as a useful probe of electron correlation effects in the Mott-Hubbard insulator $LaTiO_3$, and I will show a variety of results on Mössbauer spectra, including the effect of pressure on on Fe and ZnO.

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