9th international ABINIT developer workshop

20-22 May 2019 – Louvain-la-Neuve, Belgium

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Program (last minute changes are possible, see website for the final version)

Monday 20th May 2019		
10.30	Welcome	
Welcome/ABINIT development *(15 minutes presentation + 5 minutes discussion)*		
11.00	Welcome	X. Gonze
11.05	Overview of ABINIT development	A. Romero
11.20	Abimkdocs: the new infrastructure for writing ABINIT documentation and tutorials	M. Giantomassi
11.40	The test farm and its evolution	J.-M. Beuken
12.00	A new test system for Abinit, bottom-up approach on structured data	T. Cavignac
12.20	Discussion : Focus on test system and test farm	
12.40	Lunch	
ABINIT development *(15 minutes presentation + 5 minutes discussion)*		
14.00	Abipy - An overview	M. Giantomassi
14.20	Reducing technical debt and complexity by promoting collaborations	Y. Pouillon
14.40	Discussion : Focus on the build system	
15.00	Coffee Break	
DFPT (I) *(15 minutes presentation + 5 minutes discussion)*		
15.30	Ab-initio computation of Raman spectra within the DFPT+PAW(+U) formalism	L. Baguet
15.50	First-principles theory of spatial dispersion effects	M. Stengel
16.10	Current density at finite q for clamped-ion flexoelectricity	C. Dreyer
16.30	Spatial dispersion properties from DFPT: Dynamical quadrupoles and flexoelectric tensor	M. Royo
16.50	Break	
Flash presentations *(max. 4 slides, 8 minutes presentation + 2 minutes discussion)*		
17.20	Implementation of the LDA-1/2 method in ABINIT	F. Jollet
17.30	A unified modelization from condensed matter to plasmas	A. Blanchet
17.40	Calculation of effective interaction among different electronic shell using cRPA in ABINIT	R. Outerovich
17.50	New implementation of Chebishev filtering inside ABINIT	B. Sataric
18.00	Implementing the relaxed core PAW method into ABINIT	N. Brouwer
18.10	Speeding up the ground-state Hamiltonian application in real space	M. Torrent
18.20	News on (q)Agate	J. Bieder
19.30	Meeting of the ABINIT advisory committee	

Tuesday 21st May 2019		
Functionalities: Electronic *(15 minutes presentation + 5 minutes discussion)*		
8.30	GW density matrix with ABINIT	F. Bruneval
8.50	Implementation of "charge-only-DFT"+U and k-resolved spectral function in DFT+DMFT	B. Amadon
9.10	Extension of the computation of density to non-diagonal band occupations with the KGB parallelization	T. Cavignac
9.30	Orbital Magnetism	J. Zwanziger
9.50	Improving optical and X-Ray spectroscopy in ABINIT	N. Brouwer
10.10	Hybrids in ABINIT	X. Gonze
10.30	Break	
Functionalities: DFPT (II) *(15 minutes presentation + 5 minutes discussion)*		
11.00	Non-collinear treatment within DFPT and magnetic field perturbation	E. Bousquet
11.20	DFPT: Extending the first-order PAW Hamiltonian to GGA+SOC	M. Torrent
11.40	Computing the intrinsic mobility of electrons and holes in semiconductors *(25 minutes presentation + 5 minutes discussion)*	H. Miranda and G. Brunin
12.10	Electron-phonon coupling in naphtalene crystals	G. Antonius
12.30	Lunch + poster session (V. Brousseau-Couture; O. Gingras; W. Lafargue-dit-Hauret; F. Ricci)	
Second-principles *(15 minutes presentation + 5 minutes discussion)*		
14.00	Scale-Up: An implementation of Second-Principles DFT	J. Junquera+...
14.20	Scale-Up: An implementation of Second-Principles DFT	...+ P. Garcia-Gonzalez
14.40	The MULTIBINIT software project	J. Bieder
15.00	Construction of complex Effective Lattice Models with MULTIBINIT and Electron-Phonon Couplings combining MULTIBINIT & SCALE UP	M. Schmitt
15.20	Spin dynamics in MULTIBINIT	X. He
15.40	Discussion : Software engineering of interfacing, specifically the use of F2003 structures	
16.00	Coffee	

Potential landscapes *(15 minutes presentation + 5 minutes discussion)*		
16.30	a-TDEP: Temperature Dependent Effective Potential for ABINIT	F. Bottin
16.50	Finite temperature vibrational and thermal properties of dichalcogenides	A. Dewandre
17.00	Machine learning ab initio calculations for materials science	S. P. Ong
17.20	Materials Prediction by Random Searching Method	J.-B. Charraud
17.40	Discussion : Physics of the interfacing of first-principles calclulations to higher-level formalisms	

Wednesday 22nd May 2019		
Improving ABINIT : discussion / round tables in small groups		
8.30	Initialisation	
8.40	Discussions (round tables in small groups)	
10.30	Break	
Improving ABINIT: discussion / global		
11.00	Global discussion	
12.30	Lunch + Poster session (V. Brousseau-Couture; O. Gingras; W. Lafargue-dit-Hauret; F. Ricci)	
High-Throughput with ABINIT *(15 minutes presentation + 5 minutes discussion)*		
14.00	Why the hell did you not use VASP?" Pros and cons of ABINIT in the high-throughput world	G. Hautier
14.20	Technical aspects related to high-throughput calculations with ABINIT	M. Giantomassi
14.40	Updates on high-throughput DFPT	G. Petretto
15.00	High-throughput study of non-linear optical materials	F. Naccarato
15.20	Discussion : strategic high-throughput evolution of ABINIT	
16.00	Coffee	
Libraries + Industry *(15 minutes presentation + 5 minutes discussion)*		
16.30	Infrastructure developments for electronic structure codes in ELSI	V. Blum
16.50	Prediction and discovery of topological materials: Wannier charge centers and Z2PACK package	A. Soluyanov
17.10	Interfacing abinit with external libraries or packages: electronic structure analysis and molecular dynamics	A. Romero
17.30	Ab initio in nanoelectronics industry	M. Van Setten
17.50	Discussion : ABINIT evolution with partner projects	
19.00	Social dinner	

Abimkdocs: the new infrastructure for writing ABINIT documentation and tutorials

M. Giantomassi[1]

[1] Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium

In this talk, I will describe the new documentation system of ABINIT and the different technologies employed to facilitate the creation of new content and the automatic generation of the HTML version.
Most of the ABINIT documentation is now written in Markdown, a lightweight markup language with plain text formatting syntax. In addition to the basic markdown syntax, the ABINIT documentation supports extensions and shortcuts to ease the inclusion of hyperlinks, bibliographic citations in bibtex format as well as LaTeXequations thanks to the MathJax JavaScript library.
The website is automatically generated with MkDocs a static site generator geared towards project documentation. MkDocs employs Python-Markdown to parse the Markdown documentation and uses a single Yaml configuration file (*mkdocs.yml*) defining the organization of the pages on the website. The website uses Mkdocs-Material, a theme built using Google's Material Design guidelines. Navigation bars, header and footer are generated automatically by the framework using the Jinja template engine.
As a net result, ABINIT developers can write nice-looking documentation without having to use HTML explicitly while working in an environment that is well-integrated with the other parts of the package (the python database of input variables, the ABINIT test suite with the corresponding input and output files, the file with bibtex citations). Adding new content is straightforward: write a new page in Markdown, register the new entry in *mkdocs.yml* and finally regenerate the website with the *mksite.py* python script.

The test farm and its evolution.

Jean-Michel Beuken

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In order to keep the individual developments in line with the global objectives of the project, all contributions have to be periodically reviewed because every new development has a significant probability to break the correct behaviour of another feature. This concern has been addressed in Abinit thanks to the set-up of a test suite and a Test Farm [1]. It examines on-demand the tentative contribution of each developer. This test farm does not only build the latest contributions, but also runs the test suite and validates the results. Thanks to this tool, the contribution of each developer is validated before it is considered for merge in the the trunk.
Our Test Farm is made of two distinct parts: a series of computer platforms providing various development and running environments, and BuildBot[2], a software development continuous integration tool which automates the compile/test cycle required to validate changes to the project code base. By automatically rebuilding and testing the source tree each time something has changed, build problems are pinpointed early, before other developers are inconvenienced by the failure. By running the builds on a variety of platforms, developers will at know shortly afterwards whether they have broken the build or have encountered portability issues.
Since 2009, the Test Farm has grown and evolved. Today, twenty-one slaves with a diversity of open source and proprietary operating systems, compilers, MPI libraries and numerical libraries are provided[3].

References

[1] Y. Pouillon, J-M Beuken, T. Deutsch, M.Torrent and X. Gonze, Organizing Software Growth and Distributed Development: The Case of Abinit, Computing in Science and Engineering, vol. 13, no. 1, pp. 62-69, (2011).

[2] https://buildbot.net/

[3] https://wiki.abinit.org/doku.php?id=bb:slaves

A new test system for ABINIT, bottom-up approach on structured data

T. Cavignac[1,2] and M. Giantomassi[2], G.-M. Rignanese[2], X. Gonze[2]

[1] Ecole Centrale de Lyon
[2] UCLouvain

As a big open source project ABINIT need facilities to ensure the stability of its features. These facilities take the form of around a thousand tests checking numerical precision of a specific feature. The historic program running tests use a naive line by line algorithm comparing each floating point value on each line. This method has its advantages but also have some limitations.
During my internship at MODL/UCLouvain I have been working on a brand new system for writing and running tests in a bottom-up fashion that addresses the limitations of the old style testing method. Those tests are based on two key concepts. First, they work on structured machine-readable data written in YAML in the ABINIT output file. Second they are defined by a flexible configuration file also based on YAML.
I will present the principles of this new system and the implications on the ABINIT developer work flow. The goal is also to collect feedback from the ABINIT community. This work aims at helping improving the overall quality of ABINIT and at providing the tools for a new approach of the validation of ABINIT features.

AbiPy - An overview

M. Giantomassi[1] and the AbiPy developers

[1] Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium

AbiPy is a python package that provides a flexible scripting environment for the analysis and the post-processing of ABINIT calculations as well as tools for the automatic generation of input files and the submission of jobs on parallel architectures. Started out as a mere set of scripts to automate the typical tasks needed during software development, AbiPy evolved gradually into a much more powerful and user-friendly toolkit that has been successfully employed in different domains including high-throughput DFPT applications [1], automatic *GW* calculations [2], generation and validation of pseudopotentials [3] as well as more conventional ab-initio studies [4]. In this talk, I will give an update on the new features available in version 0.6 and a brief description of the developments planned for the forthcoming releases.

References

[1] G. Petretto *et al.*, Sci. Data **5**, 180065 (2018)

[2] M. J. van Setten *et al.*, Phys. Rev. B **96**, 155207 (2017)

[3] M. J. van Setten *et al.*, Comput. Phys. Commun. **226**, 39-54 (2018)

[4] Y. Gillet *et al.*, Sci Rep **7**, 7344 (2017)

Reducing technical debt and complexity by promoting collaborations

Y. Pouillon[1], Marc Torrent[2], Jean-Michel Beuken[3] *et al.*

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Technical debt and complexity are inevitable consequences of software growth. Most of the times, they can be mitigated by appropriate practices — such as periodic beautifications and core-developer coordination meetings — and do not necessarily become growing threats. Along the history of ABINIT, they have lead to the creation of a bunch of components and features which were solutions to specific problems at specific times: abilint, the ABINIT Fallbacks, the bindings, or the hierarchical block-structured user interface of the build system, to cite the most obvious ones. With time, the situation evolved significantly, and they stopped being adequate solutions.

Over the last few years, the build system of ABINIT has been redesigned to address the issues encountered in the current technological and social contexts of electronic structure. Its internals have been rewritten to allow non-expert developers to interact with it. This long and tedious restructuring process has lead to a noticeable simplification in the maintenance of the logical blocks of ABINIT. It has also permitted the split of the source tree and a multi-stage compilation. One of its main outcomes is a definitive end to the circular dependency that had been chaining ABINIT and BigDFT for nearly 10 years.

In the meantime, other collaborations have been established and/or strengthened to improve the overall quality of software developed within the electronic structure community and make progress on the complex topic of dependency management. Different solutions have been explored within the Electronic Structure Library (ESL) and the E-CAM Center of Excellence. Some of them, like the ESL Bundle, EasyBuild, and Spack, work together and are already used by some Electronic Structure codes. They constitute a growing number of superior alternatives to the ABINIT Fallbacks and will likely replace it in the near future.

Ab-initio computation of Raman spectra within the DFPT+PAW(+U) formalism

L. Baguet[1] and M. Torrent[2]

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The interpretation of experimental Raman spectra of materials is, in general, a difficult task. To compare these spectra with theoretical ones gives a deeper understanding of the underlying physical phenomena. Using Density-Functional Perturbation Theory, phonon modes are obtained at the second order of perturbation, giving the peak positions.
Raman intensities are computed from a third order perturbation with respect to an atomic displacement and the application of an electric field [1, 2].
Several implementations of Raman intensities exist, but they are limited to norm-conserving [1, 2], or ultra-soft pseudo-potentials [3]. Recently, Raman intensities have been obtained in DFT+U [4], which is more precise for correlated materials. Here, we present the new Abinit implementation valid for norm conserving and PAW pseudo-potentials. After a little reformulation of the PAW+U method [5], DFPT+PAW computations, including the third order, can include "+U" terms without too much implementation work.
Finally, we present how Raman intensities are computed in practice and discuss the comparison of theoretical spectra with experimental ones.

References

[1] M. Lazzeri and F. Mauri, Phys. Rev. Lett. **90**, 036401 (2003)

[2] M. Veithen, X. Gonze, and P. Ghosez, Phys. Rev. B **71**, 125107 (2005)

[3] K. Miwa, Phys. Rev. B **84**, 094304 (2011)

[4] K. Miwa, Phys. Rev. B **97**, 075143 (2018)

[5] B. Amadon, F. Jollet, and M. Torrent, Phys. Rev. B **77**, 155104 (2008)

First-principles theory of spatial dispersion effects

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Density-functional perturbation theory (DFPT) is nowadays the method of choice for the accurate computation of linear and non-linear response properties of materials from first principles. A notable advantage of DFPT over alternative approaches is the possibility of treating incommensurate lattice distortions with an arbitrary wavevector, $\mathbf{q}$, at comparable computational cost as the lattice-periodic case. In this talk I will show that $\mathbf{q}$ can be formally treated as a perturbation parameter, and used in conjunction with established results of perturbation theory (e.g. the "$2n+1$" theorem) to perform a long-wave expansion of an arbitrary response function in powers of the wavevector components. This provides a powerful, general framework to accessing a wide range of spatial dispersion effects that were formerly difficult to calculate by means of first-principles electronic-structure methods. In particular, the physical response to the spatial gradient of any external field can now be calculated at essentially no cost, by using the response functions to *uniform* perturbations (electric, magnetic or strain fields) as the only input. [1] I will also discuss special issues that need to be addressed for the calculation of the flexoelectric tensor, such as the finite-$\mathbf{q}$ generalization of the polarization [2] response and of the strain [3, 4] perturbation.

References

[1] Miquel Royo and Massimiliano Stengel, arXiv:1812.05935 (2018).
[2] Cyrus E. Dreyer, Massimiliano Stengel, and David Vanderbilt, Phys. Rev. B **98**, 075153 (2018).
[3] Massimiliano Stengel and David Vanderbilt, Phys. Rev. B **98**, 125133 (2018).
[4] A. Schiaffino, C. E. Dreyer, D. Vanderbilt and M. Stengel, Phys. Rev. B **99**, 085107 (2019).

Current density at finite *q* for clamped-ion flexoelectricity

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Current density is a fundamental quantum mechanical observable and is used in first-principles calculations of physical properties including magnetic and dielectric susceptibility, NMR chemical shifts, and EPR *g* tensors. In addition, the current density resulting from an atomic-displacement perturbation gives clamped-ion electromechanical couplings such as piezoelectricity and flexoelectricity (polarization induced by a strain gradient). We have recently developed a density-functional perturbation theory implementation to efficiently calculate flexoelectric coefficients from the current-density response to the adiabatic displacement of atoms from a long wavelength acoustic phonon [1]. In this context, determining the current is complicated because of the nonuniform (i.e., finite wavevector **q**) nature of the perturbation, and the presence of nonlocal pseudopotential operators. In this talk I will outline our methodology, including recent developments [2] combining it with the recently-developed "metric wave" approach [3].

[1] C. E. Dreyer, M. Stengel, D. Vanderbilt, Phys. Rev. B 98, 075153 (2018).
[2] A. Schiaffino, C. E. Dreyer, D.Vanderbilt, and M. Stengel, Phys. Rev. B 99, 085107 (2019).
[3] M. Stengel and D. Vanderbilt, Phys. Rev. B 98, 125133 (2018)

Spatial dispersion properties from DFPT: Dynamical quadrupoles and flexoelectric tensor

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In condensed-matter physics, spatial dispersion refers to the dependence of many material properties on the wavevector **q** at which they are probed, or equivalently on the gradients of the external field (electric, magnetic, strain...) and/or the response in real space. Remarkable examples of such gradient effects include the natural optical rotation, [1] whereby some crystals rotate the polarization plane of the transmitted light, or the flexoelectric tensor, [2] which describes the polarization response to a gradient of applied strain. The former is originated from the first-order wavevector dependence of the dielectric susceptibility tensor, while the latter can be written as the electrical current that is produced by an acoustic phonon at second-order in **q**. Density-functional perturbation theory (DFPT) appears as the ideal framework to compute these effects from first principles, but the general computational tools to deal with the long-wavelength limit are currently missing.

In this contribution we present two applications of a general formalism [3] based on an analytical long-wavelength expansion of the second-order DFPT energies that enables the direct calculation of spatial dispersion quantities. The latter are directly obtained from the uniform field linear-response functions and at essentially no additional cost. In particular, we elaborate on the specific implementation of the method for the cases of the flexoelectric tensor and the dynamical quadrupoles (the higher-order multi-polar counterpart of the Born effective charges). The flexoelectric coefficients calculated for several materials are directly benchmarked against previously published results, [4, 5] whereas the lattice sum of the PbTiO 3 quadrupole moments is shown to exactly reproduce its piezoelectric tensor, as predicted by R.M. Martin in his seminal paper. [6]

References

[1] V. I. Belinicher and B. I. Sturman Sov. Phys. Usp. 23, 199 (1980).
[2] P. Zubko, G. Catalan and A. K. Tagantsev, Ann. Rev. Mat. Res. 43, 387 (2013).
[3] M. Royo and M. Stengel, *submitted*.
[4] M. Stengel, Phys. Rev. B 93, 245107 (2016).
[5] C. E. Dreyer, M. Stengel and D. Vanderbilt, Phys. Rev. B 98, 075153 (2018).
[6] R. M. Martin, Phys. Rev. B 5, 1607 (1972).

Implementation of the LDA-1/2 method in ABINIT

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In this talk, we shall present the implementation of the LDA-1/2 method in ABINIT. We shall first mention the interest of the method to recover the band gap of semiconductors and show rapidly how it works [1]. We then shall detail the implementation in ABINIT, the keywords to be activated and the modifications introduced in the JTH table to account for this method. An example of a calculation in ABINIT will be shown at the end.

References

[1] L. G. Ferreira, M. Marques, and L.K. Teles. Approximation to density functional theory for the calculation of band gaps of semiconductors. *Phys. Rev. B*, 78:125116, 2008.

A unified modelization from condensed matter to plasmas

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During the last twenty years, Density functionnal theory has emerged mostly to describe cold condensed matter. When one wants to describe warm dense matter at high electronic temperature ($\approx$ 10 eV), plane waves DFT codes pain to get the ground state. Indeed, at these temperature ranges, one has to consider many electronic orbitals which lead to a drastic increase of the number of plane waves needed to describe the ground state wave functions. The diagonalization procedure of the Hamiltonian will be impacted by the number of plane waves, and the calculation will became numerically impossible.

To overcome this limitation, orbital free methods have been developped. Unfortunately, these methods are not able to describe matter at ambiant temperature because of the absence of orbitals. Fortunately some simplifications to this problem [1] can be applied to plane waves DFT codes, which will allow a unification of these methods, and will lead to a better understanding of warm dense matter at a quantum level.

References

[1] Shen Zhang, Hongwei Wang, Wei Kang, Ping Zhang, and X. T. He. Extended application of Kohn-Sham first-principles molecular dynamics method with plane wave approximation at high energy—From cold materials to hot dense plasmas. *Physics of Plasmas*, 23(4):042707, April 2016.

Calculation of effective interaction among different electronic shell using cRPA in ABINIT

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The calculation of the Hubbard U and Hund J parameters used in DFT+U or DFT+DMFT has been implemented in ABINIT using the constrained Random Phase Approximation in 2014 [1]. This implementation only considers intra-shell correlation (*f*-*f* in Ce for example).
We present here a work on the generalization of this implementation that allows us to perform inter-shell interaction calculation. In general, inter-shell interactions can be computed on a single atom (e.g. *f*-*d* in Ce), or on different atom site (e.g. Ni*d*-O*p* in NiO)[2]. This new implementation is based on the extension of Projected Localized Orbital Wannier functions to several atoms and orbitals, previously implemented in ABINIT[3].
The role of those inter-shell interactions has rarely been discussed in the literature, but has been proved to be non-negligible ($U^{fd} = 1.8$ eV in Ce)[2]. We hope that the ability to calculate those terms from first principle will allow us to quantitatively explain the difficulties that DFT+U or DFT+DMFT face when treating some correlated materials.

References

[1] B. Amadon, T. Applencourt, F. Bruneval, Phys. Rev. B **89**, 125110 (2014).

[2] P. Seth, P. Hansmann, A. van Roekeghem, L. Vaugier, and S.Biermann, Phys. Rev. Lett. **119**, 056401 (2017).

[3] B. Amadon, A. Gerossier, Phys. Rev. B **91**, 161103(R) (2015).

New implementation of Chebishev filtering inside ABINIT

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We consider the problem of improving the parallelization of electronic structure computations in plane-wave Density Functional Theory. In such computations, parallelism has to be found at two levels: the iterative eigensolver and the application of the Hamiltonian operator.

We show how the algorithm based on Chebyshev polynomials, implemented in ABINIT in 2015 [1], can be improved according to recent improvements made inside the LOPBCG solver [2].

Improvements include rewriting existing Chevishev filtering module using newly formed ABINIT abstract layer (Xg datatypes and functions). Xg module hides and improves OpenMP and MPI parallelization within linear and matrix algebra as well as memory management of wave functions arrays.

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Implementing the Relaxed Core PAW Method into ABINIT

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The projector augmented wave method usually treats core electrons using the frozen core approximation in order to save computational cost in comparison to all-electron codes. However, in certain cases, e. g. under warm dense matter conditions, core wave functions are expected to be altered significantly. Due to the large number of atoms and bands, that might be required under these conditions, the computational cost of all-electron codes can be prohibitive.
As an alternative Marsman and Kresse [1] developed the relaxed core projector augmented wave method (RCPAW), which relaxes the core wave functions with respect to the altered valence band electron density. In this short presentation, we will present our plans for implementing RCPAW into the ABINIT software package.

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Speeding up the ground-state Hamiltonian application in real space

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An implementation of the non-local potential in real space will be presented. This implementation is based on the well-known work of King-Smith *et al* [1]. We will show what are the necessary modifications in the code to achieve this, what approximations are introduced, and what is the expected numerical precision for this kind of calculation.
We have also explored some ways to improve the initial method, releasing degrees of freedom in optimizing the parameters.
The main application of this development lies in Molecular Dynamics calculations.

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News on (q)Agate

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The Abinit Graphical Analysis Technical Engine (Agate) is an easy-to-use utility software to post-process and analyse outputs of ABINIT. It allows to extract the physics of simulations with a convenient new graphical interface. The Qt interface (qAgate) has been rewritten from scratch with all original features available. It includes a set of tools dedicated to particular tasks like conductivity calculation, phonon at finite temperature extraction and plot of dispersion curves. The input format list has been extended to be able to read binary abinit headers and ETSF netcdf files. Importation via ssh is now included. A non exhaustive list of new features will be presented along with the new interface.

GW density matrix with ABINIT

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The *GW* approximation is a succesful approximation to the many-body self-energy that is generally used to produce band structures and band gaps of semiconductors. It has been shown to be extremely successful in do so during the last 30 years [1].

However, the *GW* approximation can give access to other physical quantities and, most noticeably, to the density matrix. The density matrix allows one to directly calculate the expectation value of any local and non-local operator, such as the kinetic energy, the electron density, the electrostatic potential, the exchange energy, etc.

We have recently derived a simple perturbative expression [2] for the GW density matrix and we have tested it for molecular systems in the Gaussian basis code MOLGW [3]. The first results are very promising.

In this contribution we present our strategy how to generalize the expression to periodic systems and how to implement it in ABINIT.

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Implementation of "charge-only-DFT"+U and k-resolved spectral function in DFT+DMFT.

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I present two developments that aim to improve the description of strongly correlated systems. First, I detail the implementation of the "charge-only-DFT"+U method proposed in Refs. [1]. It intents to improve the description of exchange in usual DFT+U. I show the benchmark of the implementation on magnetic effects on iron and I show the application of this method for properties of actinides [2]. Secondly, I present the implementation of **k**-resolved spectral function in DFT+DMFT. It requires the analytic continuation of the self energy from the imaginary frequency axis to the real frequency axis. I show the example of OmegaMaxent [3] which uses the Maximum Entropy method to do this continuation. I benchmark the implementation of spectral function in $SrVO_3$, and I show the application to α-cerium (cf Fig 1).

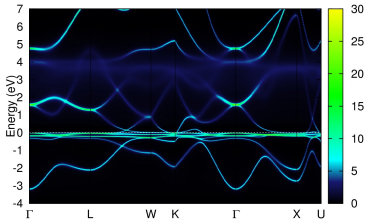

Figure 1: **k** resolved LDA+DMFT spectral function of α-cerium (U=6 eV)

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Extension of the computation of density to non-diagonal band occupations with the KGB parallelization

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As it solves a model corresponding to a perturbed Hamiltonian, DMFT produces non-diagonal occupations (in the band space) when converting the results to the DFT Kohn Sham band space. Non-diagonal occupations were an obstacle to use DMFT with the KGB parallelization because of the required mixing of Kohn Sham bands that are not available to the current MPI process. As a consequence DMFT computation were before this work only possible with the simpler and less efficient K parallelization.
My first master internship was dedicated to the extension of the existing code to solve this problem. I implemented alongside the density computation the possibility to use non-diagonal occupations even in the case where only a subset of the bands are available to a given process.
After a few reminders on the parallelization modes of Abinit and the way wave functions are distributed among processors, I will present the way I solved this problem, using natural orbitals in one case, and point-to-point communications in another case. I will then exhibit the effect of my work on computations on large systems. This work opens the door to studies of multi-atoms problems like phonons or defects with DFT+DMFT. It could also be used to implement further methods implying the use of non-diagonal occupations in Abinit.

ORBITAL MAGNETISM

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I discuss my implementation of the calculation of orbital magnetism, based on the first-order energy change due to an applied magnetic field, in an insulator. The basic formalism was derived in Ref. [1], and has been adapted to the PAW formalism by X. Gonze [2].
Because the orbital magnetism of an insulator at zero magnetic field is zero, I also implemented nuclear magnetic dipole moments as inputs and features of the ground state Hamiltonian. In the presence of an array of such moments, of fixed direction, the orbital magnetization and Chern number are both non-zero, and this provides a way to test the implementation. It is also highly relevant for experimentalists because it allows for the computation of chemical shielding, one of the observables in nuclear magnetic resonance, by the so-called "converse method" [3]. In this method the shielding σ is computed as the change in orbital magnetization as a function of dipole moment strength.
My implementation is parallelized over k points for both magnetization and Chern number, and the Chern number part can also take advantage of spatial symmetries.

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Improving Optical and X-Ray Spectroscopy in ABINIT

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The prediction and analysis of optical and X-Ray spectra of materials under warm dense matter conditions is of great scientific interest. The ABINIT implementation of the PAW formalism is well suited to treat this highly excited state of matter. One important aspect when treating optical and X-Ray spectroscopy, especially for heavier elements, is the spin-orbit coupling.
In this talk, we will present our improvments of the prtnabla option and the conducti post-processing tool, which take advantage of ABINIT's PAW spinor implementation in the calculation of optical and X-Ray spectra. Spinors are now treated correctly and an option to take spin-orbit coupling into account in the dipole matrix element as well has been added for optical spectroscopy. Furthermore, it is now possible to import spinor core wave functions provided by the new version of atompaw, which allows to predict the spin-orbit splitting and the ratio of the X-ray absorption edges correctly. In addition, we have added NetCDF and MPI support for the conducti post-processing tool. Finally, we will present our plans for the implementation of the relaxed core approximation in ABINIT.

Hybrids in ABINIT

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The status of the implementation of hybrids in ABINIT will be reviewed. The Fock exchange term, the PBE0, B3LYP and HSE functionals, are implemented both in the norm-conserving pseudopotential framework and in the PAW one, in the non-spin-polarized and spin-polarized cases. In all these cases, forces and stresses are computed. Also, the wavefunctions that are obtained in the norm-conserving case can be used as a starting point to perform GW calculations. The implementation for spinor wavefunctions is not yet available.

Work is still in progress concerning the efficiency of the calculation. The adaptively compressed exchange operator [1] is implemented, giving typically a 3-4 speedup. Fock operator k-point downsampling [2] and parallelism is available. A double-loop algorithm, including wavefunction mixing through biorthogonalization, is under development.

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Non-collinear treatment within DFPT and magnetic field perturbation

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In this talk we will first briefly present the status of the non-collinear magnetism in ABINIT for ground state calculations and related capabilities (convergence, applied Zeeman magnetic field, constrained magnetic moments).
Then we will discuss our developments regarding the extension of DFPT for non-collinear magnetism [1]. We will see that the main problem comes with the exchange-correlation (XC) potential derivatives, which are the only ones that are affected by the non-collinearity of the system. Most of the present XC functionals are, however, constructed at the collinear level such that the off-diagonal derivatives coming from the non-collinearity are absent. We will show that a good solution is to perform the non-collinear derivatives through a local collinear basis where the z axis is aligned with the magnetization. We will present the results of our implementation on phonons and electric field perturbation for LDA functional and norm-conserving pseudopotential scheme.
At last, we will discuss the development of a DFPT extension treating magnetic field perturbation acting on the spins (Zeeman field perturbation). Our implementation has been done for LDA and norm-conserving case and works for any wave-vector q, giving access to the q-dependent magnetic susceptibility or magnon spectra.

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DFPT: Extending the first-order PAW Hamiltonian to GGA+SOC

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The formalism used to generalize calculations of full phonon spectra will be derived in the case of the Generalized Gradient Approximation (GGA) with spinorial wave functions (spin-orbit coupling). This is done in the Density Functional Perturbation Theory (DFPT) formalism within the PAW approach. The main difficulty of the implementation is to correctly take into account the imaginary parts resulting from the phase and from the coupling, as well as to apply the symmetries.
A focus will be made on the on-site exchange and correlation potential implemented as a Taylor development around the spherical contribution to the density.

COMPUTING THE INTRINSIC MOBILITY OF ELECTRONS ANS HOLES IN SEMICONDUCTORS

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Computing the electronic transport from first principles is crucial for the discovery and development of new functional materials. Recently, different works have reported the *ab initio* phonon-limited mobility for various semiconductors and metals [1, 2].
We report the new developments for the ABINIT package to compute the electron self-energy due to electron-phonon coupling using a plane-wave basis set. In particular we focus on computing the lifetimes from the imaginary part of the self-energy at the Kohn-Sham energies, which we use to solve the linearized Boltzmann transport equation and obtain the phonon-limited mobility in a single ABINIT run.
In the first part of the talk we will present convergence studies for the mobility of Si and GaP and introduce different techniques used to speed up the computations and reduce the memory requirements. In the second part we will discuss technical aspects of the implementation of these techniques. These include the interpolation of the DFPT potentials, the use of symmetries, check point and restart, the tetrahedron integration, double-grid and filtering. We will finalize by outlining problems encountered during development as well as our suggested solutions.

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Electron-Phonon coupling in naphtalene crystals

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We study the effect of electron-phonon interactions in naphthalene crystals, namely, the temperature-dependent renormalization of the band gap as well as the electron and hole mobilities. We take advantage of newly implemented interpolation schemes in Abinit for the phonon coupling potential, as well as an energy panelling technique for the real part of the self-energy. We show that special care has to be taken when converging the q-points grids, as both the coarse and the fine grids can have a dramatic impact on the mobilities. Moreover, we employ a self-consistent scheme for the electron-phonon coupling self-energy and the spectral function. It allows us to compare the accuracy of the on-the-mass-shell and the off-shell calculations.

Scale-Up: An implementation of Second-Principles DFT

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Second-Principles Density Functional Density (SPDFT) [1] is a first-principles-based method designed to have an accuracy similar to DFT, at a much smaller computational cost. The resulting method, that allows for a systematical improbable approximation of DFT and that is related to self-consistent tight-binding DFT, can be used to perform simulations in large systems (typically tens of thousands of atoms) and is able to deal with metals and magnetic systems. In SPDFT a material is divided into two subsystems; the lattice, corresponding with a reference, electronic state (usually the ground state) whose energy is calculated using a force-field [2] and the electrons, that are activated to correct the results when the state of the system deviates from the reference. Here, we will focus on giving an overview of current capabilities and limitations of the method.
Scale-Up is our implementation of SPDFT and it allows obtaining many of the magnitudes that a DFT code typically provides, from the total energy or the forces to the charge or spin distribution over the atoms. This package can be used as a library by other Second Principles codes like Multibinit in order to complement these codes with extra functionality. Finally, we will devote some time to discuss how to generate electron models from first-principles simulations and the interface between Scale-Up and Siesta.

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The MULTIBINIT software project

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The atomic-scale description of mesoscopic systems at finite temperatures still remains very challenging, and significant efforts have been devoted recently to the development of second-principles effective models. These extend the capabilities of DFT calculations to larger systems and time-scales, while retaining most of the first-principles predictive power and accuracy.

The purpose of the MULTIBINIT software project is to develop a unified platform for the automatic construction of “second-principles” effective models for atoms, electrons, lattice modes and spin degrees of freedom, and for their use in mesoscopic simulations, either separately or coupled together (e.g. atoms + electrons, atoms + spins, lattice mode + spins).

In this talk, we will first provide an overview of the generic structure of MULTIBINIT and of the present status of development of the different types of models. Then, we will provide a more detailed description of the lattice part [1], providing some details of the implementation and highlighting the limitations of the present version. A few words will be said regarding the improvements of the AGATE post processing tool, and the features available for the analysis of MD runs, phonons, etc... More detailed descriptions of the electron, spin and lattice mode parts will be provided in separate presentations.

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Construction of complex Effective Lattice Models with MULTIBINIT and Electron-Phonon Couplings combining MULTIBINIT & SCALE UP

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The lattice part of MULTIBINIT relies on the construction of effective atomic models, integrating out the electronic degrees of freedom and properly mimicking the Born-Oppenheimer energy surface around a given reference configuration [1]. In practice, the energy is expressed in terms of individual atomic distortions and macroscopic strains by means of a Taylor series. MULTIBINIT automatically generate the terms allowed by symmetry up to a given order and range of interactions and then determine the values of the related coefficients from a set of first-principles data. Nonetheless, the automatic generation of models for materials with complex energy surface incorporating multiple local minima and large distortions with respect to the reference still pose significant problems. The greatest challenge is to guarantee the boundedness of the model i.e. avoid divergence of the model energy to minus infinity for large lattice distortion amplitudes in the high-dimensional space of the individual atomic distortions. Here, we present a simple algorithm that imposes the boundedness for any given effective potential while keeping its precision to a limited range of first-principles data. The successful application of this algorithm to the case of $CaTiO_3$ is discussed.
Then, it is sometimes important or even necessary to reintroduce explicitly some electronic degrees of freedom in the simulation. This can be achieved by combining the lattice part of MULTIBINIT with a second-principles model describing the relevant electronic states, while avoiding double counting as provided by SCALE-UP [2]. We will show the first implementation of a coupled electron-lattice models obtained from the combination of MULTIBINIT with the SCALE-UP module responsible for the electron treatment. The technical aspects of the implementation will be introduced and its capabilities exemplified on a simple electron-lattice model addressing fundamental questions of orbital physics in solids.

Finally, an outlook of future challenges of the joint MULTIBINIT SCALE-UP project - further integration of data structures, code licensing-distribution, integrated testing - will be made and posed to discussion.

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Spin dynamics in Multibinit

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Atomistic spin dynamics has been implemented in Multibinit for modeling large-scale spin systems. The formalism is based on a Heisenberg model, which includes exchange and Dzyaloshinskii-Moriya interactions, single ion anisotropy, dipole-dipole interaction, and an external magnetic field. The dynamics is performed using the Landau-Lifshitz-Gilbert (LLG) equation [1].

A program has been developed to handle the automatic calculation of superexchange interaction parameters J of all neighbors through a Wannier function (WF) based tight-binding Hamiltonian built from density functional theory. The spin rotation of localized WFs is treated perturbatively, allowing for the calculation of exchange parameters thanks to the spin force theorem [2].

We also discuss the ongoing development of a coupled spin-lattice dynamics. The coupling between the lattice and spin subsystems is considered, and the molecular dynamics and spin dynamics are performed simultaneously.

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a-TDEP : Temperature Dependent Effective Potential for ABINIT

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The capture of thermal effects in solid state physic is a long standing issue and several stand-alone or post-process computational codes now include the so called anharmonic effects. We show how A-TDEP can produce a large panel of temperature dependent thermodynamic quantities, from a single *ab initio* molecular dynamic trajectory and by means of a Graphical User Interface (AGATHE) very easy to use : phonon spectra, free energy, specific heat, elastic constants and moduli, Grüneisen parameter, thermal expansion, sound velocities... We start by detailing how the originally "Temperature Dependent Effective Potential" method proposed by Hellman *al.* [1] is implemented in ABINIT [2]. In particular, we present the various algorithms and schemes used to obtain the Interatomic Force Constants : self-consistency, constrained least-square method, lattice symmetries, translation or rotation invariances of the system... We also show some representative applications of A-TDEP (Ti, U, Fe, MgO, Pu...) [3], and highlight how the strong anharmonicity alters their thermodynamic properties.

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Finite temperature vibrational and thermal properties of Dichalcogenides

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Interest in the transition metal dichalcogenide materials has exploded due to their wide range of physical properties, which go from photovoltaic to thermoelectric applications. Dichalcogenides are also known to have a low out of plane thermal conductivity due to their layered structures. We present the vibrational and thermal properties of different Dichalcogenides,calculated using the Temperature Dependent Effective Potential package, linked as a library with Abinit, to calculate the finite temperature lattice dynamics. In particular we use an efficient automatic scheme for generating distorted snapshots which allows us to calculate anharmonic effects avoiding long ab-initio molecular dynamics runs.

Machine Learning Ab Initio Calculations for Materials Science

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As unprecedented amounts of materials data generated from high-throughput ab initio calculations, machine learning techniques has the potential to greatly accelerate materials discovery and design. In this talk, I will present our latest efforts at developing high-accurate surrogate models for energies, forces and materials properties by machine learning "large" ab initio data. I will discuss various representations for crystals – from undirected graphs to local atomic density functions – and demonstrate how models built on these representations – from simple linear models to state-of-the-art graph networks – can achieve near-DFT accuracy in energy, force and property predictions. [1–5] Finally, I outline how such models may be used in accessing compositional, time and length scales far beyond that accessible by *ab initio* calculations today, enabling the search for novel materials in vast compositional spaces and the study of microstructure of materials.

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Materials Prediction By Random Searching Method

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In a lot of domains, structure identification of new materials is a necessary step to the development of new devices with innovative functionalities. As an example one can mention the energy sector where new materials are searched to increase energy transportation and storage efficiency. To identify the most promising compounds and provide support for a precise characterization of their properties, experimental synthesis is not always enough by itself and has to be guided by numerical simulations. Algorithms using supercomputers and artificial intelligence have been introduced to predict crystal structures of new materials under specific physical conditions such as high pressure. These crystal structure prediction algorithms become a required element for the search of new promising materials. This talk is focused on a specific type of these methods called Ab Initio Random Structure Searching. Following the principles introduced by Pickard and Needs [**1**], it's use on supercomputers using ABINIT in conjunction with external scripts is firstly presented. This approach is driven by the search for new superconductors with possible high critical temperature that could be found in hydrogen rich alloys under pressure, called "superhydrides". It is also motivated by testing methods using Machine Learning approach. Finally the algorithm's implementation in Abinit will be discussed.

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"Why the hell did you not use VASP?" Pros and cons of ABINIT in the high-throughput world

G. Hautier[1] and G.-M. Rignanese[1]

[1] Université catholique de Louvain

High-throughput computation is an emerging area of ab initio materials design. The vast majority of high-throughput computations have been performed using VASP but the use of other plane-wave codes such as ABINIT is currently growing. A case in point is the recent building of a high-throughput phonon database using ABINIT and DFPT.

We will provide a personal view from a materials designer/user perspective on the pros and cons from different plane wave codes and especially VASP (with possible additional wrappers such as phonopy) and ABINIT. I will focus on current activities in our group targeting the use of ABINIT especially for linear and non-linear response computations (phonons, electron-phonon, non-linear optics). This general overview talk will be followed by more detailled and technical talks. It will hopefully motivate further discussion on the priority in ABINIT future developments as an additional engine to high-throughput computational design.

Technical aspects related to high-throughput calculations with ABINIT.

M. Giantomassi[1] and the AbiPy developers

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In this talk, I will present the approach employed in AbiPy to implement automatic ABINIT calculations. More specifically, I will discuss how we employ YAML and netcdf files to exchange information between Fortran and Python, the logic used in AbiPy to parallelize and optimize calculations at runtime and the protocol used to handle possible errors during the ab-initio computation. I will also discuss how to use the Fortran API of ABINIT to generate netcdf files that can interoperate seamlessly with our high-throughput infrastructure. In the last part, I will present some of the technical problems we are still facing and discuss possible approaches to address these issues.

Updates on high-throughput DFPT

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High-throughput calculations in general require a robust framework to handle the whole process from generating inputs to storing the final results. This is even more true in the case of Density Functional Perturbation Theory, where a large number of calculations should be performed to reach the final result.
The framework for high-troughput workflows with Abinit have been finalized and employed to generate full phonon band structures for more than 1500 materials in collaboration with the Materials project [1, 2]. The results will be shown along with a discussion of the problems that emerged running the calculations.

References

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High-throughput study of non-linear optical materials

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Nonlinear optical (NLO) processes, such as second harmonic generation (SHG), shift current, sum frequency generation, and others, play an important role in modern optics, especially in laser-related science and technology. They are at the core of a wide variety of applications ranging from optoelectronics to medicine. Among the various NLO materials, semiconductors are particularly important for second-order NLO properties. In particular, only crystals which are non-centrosymmetric can display a non-zero second-order NLO susceptibility. Furthermore, the semiconductors need to satisfy the so-called phase matching condition in order for NLO processes to occur with good efficiency. These two requirements drastically limit the choice of compounds and, despite recent progress, a systematic approach to design NLO materials is still lacking. In this work, we set up a high-throughput framework for computing the nonlinear susceptibility response using Density Functional Perturbation Theory. Within this approach, the effective SHG nonlinear coefficient is then calculated from the susceptibility tensor for a few hundred semiconductors, revealing new potential NLO materials. The data are also investigated to determine descriptors that play an important role in nonlinear phenomena.

Infrastructure Developments for Electronic Structure Codes in ELSI

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This talk describes the open-source infrastructure "ELSI" (https://wordpress.elsi-interchange.org/ and Ref. [1]), which provides simple access to state-of-the art solutions to the Kohn-Sham eigenvalue problem for different codes and solvers using a single uniform interface. ELSI provides a uniform solutions ranging from simple serial to large-scale massively parallel solutions, with efficient matrix conversion between dense and sparse matrix formats. Supported solvers include ELPA (massively parallel $O(N^3)$ eigenproblem solutions), PEXSI ($O(N^2)$ density-matrix based solutions including for metallic systems), NTPoly (O(N) density matrix purification), and several further, specialized solvers. ELSI is a cross-code development, now used in production versions of FHI-aims, Siesta, DFTB+, and DGDFT; additionally, ELSI is part of the broader "Electronic Structure Library" Bundle of open-source libraries for electronic structure theory. Different solvers have different use scenarios in terms of system size, system type and parallelism, assessed in a comprehensive set of benchmarks in this talk. Finally, we outline a new reverse communication interface (RCI) enabling the facile, efficient implementation of different iterative solver strategies aimed at plane wave basis sets, led by ELSI developers Yingzhou Li and Jianfeng Lu (Duke University).

References

[1] V. Yu *et al.*, Comput. Phys. Commun. **222**, 267 (2018).

PREDICTION AND DISCOVERY OF TOPOLOGICAL MATERIALS: WANNIER CHARGE CENTERS AND Z2PACK PACKAGE

Topological phases can be found in many weakly interacting crystalline materials, the electronic structure of which is easily accessible with *ab initio* software packages like ABINIT. Unlike the metal from insulator distinction accessible from the band structure – eigenvalues of the crystalline Hamiltonian, all the geometrical and topological properties of the material is stored in the eigenstates of the crystalline Hamiltonian – the Bloch states.
In this talk I will describe how this information can be extracted from standard first-principles calculations and used for prediction of topological phases hosted in insulators and metals. Time permitting, I will also describe novel software tools, applicable with ABINIT, that allow for a complete *ab initio* description of non-trivial topological phases of materials.

Interfacing abinit with external libraries or packages: electronic structure analysis and molecular dynamics

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In this talk, I will present our efforts in interfacing Abinit with two different packages.

PyProcar is a robust, open-source Python library used for pre and post-processing of electronic structure data from DFT calculations. The PROCAR file generated from DFT calculations contain the projections of the Kohn-Sham wave functions for every energy band and k-point for all the atoms in the structure also taking spin into account. PyProcar parses the energy band structure and the orbital resolved contributions and provides a set of graphical analysis including the electronic band structure with orbital, atom and spin projection, spin-texture, 3D and 2D Fermi surface with orbital, atom, spin and Fermi velocity projection, multi-band comparison, band unfolding to name a few.

Molecular Dynamics with Constraints (mdwc) package is an open source, user friendly Python program to perform constrained molecular dynamics simulations. It utilizes the Rahman-Parrinello Lagrangian to perform NPT and NVT calculations. Based on the SHAKE algorithm, mdwc can impose constraints on bond distances, angles, atomic positions, lattice parameters, angles between lattice vectors and the volume of the unit cell. Libraries from this development can be linked directly to any software that provides forces and energies. While the molecular dynamics code propagates the particles in the simulation, the energy and forces are calculated through Abinit. These calculations can be easily performed with the help of a clear set of Jupyter notebook examples.

Ab initio in nanoelectronics industry

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Various trends in the electronics industry are systematically rendering the conventional macro and mesoscopic modeling methods less effective. The dimensions of typical modules are rapidly dropping into the nanometer range requiring the need for a full quantum treatment. Good old silicon is more and more replaced by new materials. For these, the fundamental knowledge is lagging too much to provide the parameters for compact modeling. The use of flexible substrates and increasingly complex modules in the back end of line puts strict limits on the processing temperatures. These are, in most cases, well below those the are required to anneal the involved materials into the crystalline phases. Fundamental knowledge of the resulting amorphous phases is however even less well developed.

Ab initio modelling can provide the needed intel to use a base for compact modeling and improve the needed fundamental understanding needed for real progress. The application of ab initio methods in this fields however also pushes the current implementations to their limits.

In this presentation an overview and a series of examples is presented to make academic developers more aware of the needs from and the challenges faced in industry.