FIRST-PRINCIPLES STUDIES OF MATERIALS : HOW TO ORGANIZE THE SOFTWARE DEVELOPMENT ?

The state-of-the-art is in constant progression ...
(the following list is not exhaustive, and is biased towards pseudopotentials)

- 1985 Car-Parinello technique

- 1985 GW calculations

- 1987 Linear-response approach to phonons, dielectric tensor ...

- 1991 Ultrasoft pseudopotentials

- 1992 Berry phase approach to polarization

- 1994 Projector Augmented Waves

- 1996 Time-dependent DFT for excited states

- 1997 Maximally-localized Wannier functions

- 1998 Bethe-Salpether equation

- 2002 Treatment of finite electric fields

... not even mentioning other advances for which one cannot clearly isolate a date (parallelism, order(N) scaling, DMFT, ...).
Obviously, the frontier of research has moved a lot.
This trend will continue !
In order to stay up-to-date, softwares will have to include more and more "basics".

✔ Software engineering concepts are needed.

✔ Collaborative effort of groups is needed.

ABINIT : A PROJECT THAT FAVOURS DEVELOPMENT AND COLLABORATION

(http://www.abinit.org)

① The group

An international collaboration ...

② Open source

GNU General Public License ...

③ Reliable

More than 500 automated tests ...

④ Portable

Easy and frequent installation on more than 10 platforms ...

⑤ High-level coding and documentation

Explicit coding style, self-documentation, ...

⑥ Many capabilities

Ground state, response functions, excited states ...

⑦ Easy to learn and use

Tutorial, examples, input metalanguage ...

ABINIT : 1. THE ABINIT GROUP

Since the beginning of the project, in 1997, several groups have shown a clear commitment to the ABINIT project:

- ✔ J.-M. Beuken, X. Gonze, G.-M. Rignanese, L. Sindic ... (Université Catholique de Louvain, Belgium)

- ✔ G. Zerah, F. Jollet, M. Torrent, G. Jomard, A. Roy, V. Recoules, ... (Commissariat Energie Atomique, Bruyeres, France)

- ✔ M. Mikami (Mitsubishi Chemical Corp., Japan)

- ✔ Ph. Ghosez, J.-Y. Raty (Université de Liege, Belgium)

- ✔ L. Reining, V. Olevano, G. Onida, R. Godby (contributors to the GW part of ABINIT, from Ecole Polytechnique Palaiseau (France), U. Roma (Italy), U. of York (UK), U. Grenoble)

- ✔ D. Vanderbilt, D. Hamann (Rutgers U., USA)

- ✔ M. Coté (U. de Montréal, Canada)

Many others have contributed to development and testing efforts (more than 200 persons on the developpers mailing list), including :
D.C. Allan, S. Goedecker, T. Deutsch, Y. Pouillon, M. Verstraete, F. Bruneval, ...

An international collaboration, self-organized ...

ABINIT : 2. OPEN SOURCE

- Is the use of ABINIT subject to an agreement ?

- Are the sources available ?

- Could I modify them, and redistribute them ?

Starting with ABINITv3.0 (released in December 2000), the distribution of ABINIT is under GNU General Public Licence (GPL), see http://www.gnu.org/copyleft/gpl.html .

"The licences for most softwares are designed to take away your freedom to share and change it. By contrast, the GNU GPL is intended to guarantee your freedom to share and change free software – to make sure the software is free for all its users."

You have the freedom to :

➥ run the program, for any purpose

➥ modify the program to suit your needs

➥ redistribute copies

➥ distribute modified versions (if they are advertised to be so)

... Others have the same rights as you !
... If one delivers binaries one must also deliver the sources !
... Can be used in another package only if that package is GNU GPL !

GNU GPL acts like a computer virus.
Sharing of code is guaranteed.

ABINIT : 3. RELIABLE

How to secure existing capabilities despite heavy development efforts and the associated bug generation ?

More than 500 automatic tests have been set up.

➡ in general, each last a dozen of seconds on a PC, or less

➡ they examine "all" capabilities of ABINIT

➡ the output is automatically compared to a reference file

➡ PERL scripts drive the procedure

➡ these tests can be used as examples for beginners

➡ portability concerns have been solved (see next slide)

The analysis of output files is multilevel :

- for each test a few lines are produced if everything went right, and these are summarized in a unique file for each batch of 100 tests

- if there is a problem, a "diff" file can be consulted, for each test

- a detailed "log" file contains specific error handling messages, for each test

Implementation of the "self-testing" software concept.

ABINIT : 4. PORTABLE

- Is ABINIT platform-dependent ?

- How difficult is it to install ABINIT on a platform ?

The installation procedure is based on the autotools, and might be as simple as "configure ; make".
In the worst case, one machine-dependent file must be set up once, and will work for the next installations on the same machine.
It contains the compiler name and options, library locations ...

Over the years, ABINIT has been installed on :

✔ Intel - Pentium under Linux (IFC, PGI, g95, Pathscale, Fujitsu, NAG compilers)

✔ Intel - Pentium under Windows NT, Windows 98

✔ Opteron

✔ Itanium 2

✔ Compaq - alpha EV68, EV67, EV6, EV56, under UNIX + Linux

✔ SGI - Origin 200/2000, Altix/Itanium II, under UNIX

✔ IBM - Power IV, III+, Power II, under UNIX

✔ Sun - Ultrasparc III and II, under UNIX

✔ FUJITSU - VPP, under UNIX

✔ NEC - SX4, SX5, under UNIX

✔ MAC - Power G5, under MacOS X

ABINIT: 5. CODING AND DOCUMENTATION

Is it easy to become familiar with the ABINIT source files, understand what each routine is doing, and begin additional development ?

The ABINIT source files are especially clear :

The (F90) routines follow explicitly stated coding rules (ABINIT style), with a special format that allows processing by ROBODOC (http://www.xs4all.nl/˜rfsber/Robo/robodoc.html).

➡ Uniformity of style

➡ For each routine, documentation is locally available

➡ Many comments are forced by the ABINIT style
(e.g. every argument of a routine is described in a comment)

➡ Input or output intent is specified

➡ Automatic generation of "parent" and "children" subroutine lists, and automatic enforcement of coding rules

➡ On-line sources (HTML format, thanks to ROBODOC)

➡ Automatic creation of subroutine interfaces, allowing for deep analysis by the F90 compiler.

Additional documentation files describe the global structure of the code, the testing environment, the installation procedure ...

To a large extent, implementation of the "self-documentation" software engineering concept

ABINIT : 6. MANY CAPABILITIES

Features available in version 5.2 (or planned for 2007) :

- representation of wavefunctions : Plane Waves; Projector-Augmented Waves (the latter is not available for all capabilities)

- LDA, GGA, spin-DFT (many functional forms)

- band structure, DOS, charge density, total energy

- many pseudopotential types : availability of Troullier-Martins and Hartwigsen-Goedecker-Hutter pseudopotentials for the full periodic table, interface with different pseudopotential codes, including FHI98PP, and N. Holzwarth PAW pseudo generator. Generation of alchemical pseudo-atoms.

- finite systems as well as insulators and metals (smearings : Fermi, Gaussian, Gauss-Hermite, Marzari modifications)

- automatic k-point sampling of the irreducible Brillouin zone

- symmetry analyser (includes a database of the 230 spatial groups, and a database of the 1191 Shubnikov magnetic groups)

- forces, stresses, automatic optimisation of atomic positions and unit cell parameters (Broyden and Molecular dynamics with damping; soon, delocalised internal coordinates)

- molecular dynamics (Verlet or Numerov), Nose thermostat, Langevin dynamics

- spin-orbit coupling soon compatible with spin-polarisation

- responses to atomic displacements (even at non-zero wavevectors, without need of supercells !) and to homogeneous electric fields, within Density-Functional Perturbation Theory:

  dielectric tensor, Born effective charges, dynamical matrices at any wavevector, phonon frequencies, force constants phonon density of states, thermodynamic properties in the quasi-harmonic approximation

- responses to strain perturbations: elastic constants, piezoelectric coefficients.

- non-linear responses thanks to the 2n+1 theorem of perturbation theory : at present, electro-optic coefficients, Raman cross-sections.

- susceptibility matrix by sum over states

- excited states of atoms and molecules within Time Dependent-DFT or Delta SCF

- frequency-dependent conductivity in the RPA (Kubo-Greenwood)

- exact exchange and RPA+ calculation of total energies (one k-point, post-LDA or post-GGA, not yet available for spin-polarized systems or spinor wavefunctions)

- GW calculation of excited states, soon available for spin-polarized systems, not yet available for spinor wavefunctions

- MPI parallelisation of ground-state and response-function calculations over k-points, spins and bands, MPI parallelisation of FFT grid and planewave operations

ABINIT : 7. EASY TO LEARN AND USE

How difficult is it to learn to use ABINIT,
and then, to use it for daily work ?

The concept of self-learning is central to the ABINIT project :
at his fingertips, the user will find all the information he/she needs to
learn to use ABINIT

➥ Tutorial : four basic lessons of 2 hours each (used to teach classes),
and twelve specialised lessons

➥ On-line help files, and on-line list of input variables

➥ The input files used in the automatic tests show how to use all the
functionalities of ABINIT (more than 500 files).

➥ ... no need to attend a school !

The daily use has also been at the center of development efforts :

➥ Pseudopotentials are available for all the elements, in LDA, or can
be generated for the GGA

➥ Input by keywords and default values

➥ Metalanguage for chaining different datasets

➥ Automatic renaming of output files for bookkeeping