Introduction to

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Thanks to > 50 ABINIT contributors …

The ABINIT project

What is ABINIT ?

http://www.abinit.org

ABINIT is a software suite to calculate the optical, mechanical, vibrational and other observable properties of materials. Starting from the quantum equations of **density functional theory** (DFT), you can build up to advanced applications with **perturbation theories** based on DFT and many-body Green's functions (GW and DMFT).

ABINIT can calculate molecules, nanostructures, and solids with any chemical composition and comes with several complete and robust tables of **atomic potentials**

The ABINIT software project

Ideas (1997) :

1) Softwares for first-principles simulations are more and more complex : needs a worldwide collaboration, of specialized, complementary, groups
2) Linux software development : 'free software' model

Now (2019) :

>2000 registered people on the forum
800 kLines of F90 + many python scripts (abipy)
1000 automatic tests
about 50 contributors to ABINITv8

Last release v8.10 used in this school
http://www.abinit.org

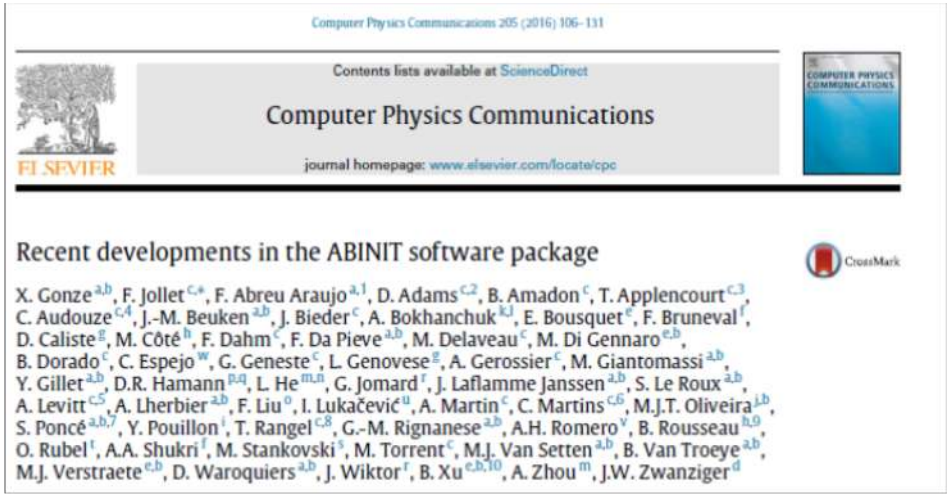
Avaialable freely
(GPL, like Linux)

ABINIT milestones

- Precursor : the Corning PW code (commercialized 1992-1995 by Biosym)
- 1997 : beginning of the ABINIT project
- Dec 2000 : release of ABINITv3 under the GNU General Public License (GPL)
- Nov 2002 – May 2017 : 8 international ABINIT developer workshops
  (between 40 and 60 participants each)
- Jan 2010 : launch of the Forum

Major active contributors:

- Université Catholique de Louvain la Neuve (UCL)
- CEA Bruyères le Châtel
- Université de Liège (ULG)
- …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Recent developments in the ABINIT software package

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The “Free” software concept

Free for freedom (also price ...)

- freedom 1 : unlimited use for any purpose
- freedom 2 : study and modify for your needs (need source access !)
- freedom 3 : copy
- freedom 4 : distribute modifications

From copyright to freedom (“copyleft”)

- copyright allows licensing
- licenses grants freedom

ABINIT pioneered the use of the GPL « Free software license » in the computational condensed matter community (2000)

ABINIT is tested and can be installed on many OS

Lecture:
Installation of ABINIT
Monday afternoon

Distributive developments

- How to secure existing capabilitites despite the development efforts (by rather diverse groups) and the associated bug generation ?

- Around 1000 automatic tests have been set up, and new ones are added for securing each new feature
  - in general, each last a dozen of seconds on a PC
  - they examine “all” capabilities of ABINIT
  - the output is automatically compared to a reference file
  - these tests can be used as examples for beginners

- A « farm » of platforms is used for testing thanks to nightly builds

- The code is developped using « git ». Coding rules are to be respected.

Density-functional theory (DFT)

ABINIT solves the Schrödinger equation in the frame of the DFT.

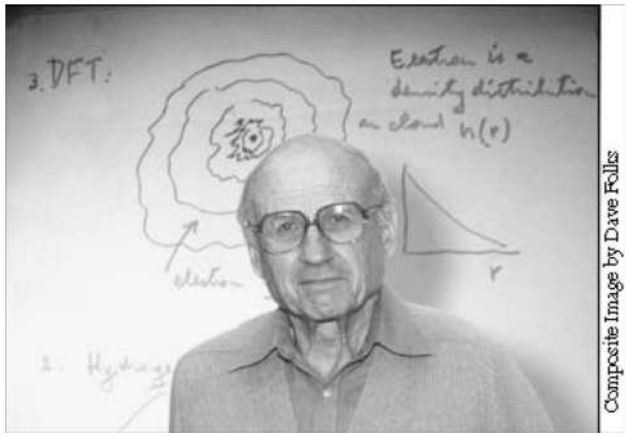
Quantum objects : wavefunctions
for interacting particles

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,...,\mathbf{r}_N,t)$$

Hohenberg & Kohn (1964), Kohn & Sham (1965) :

DFT : set of wavefunctions
for non-interacting particles

$$\psi_1(\mathbf{r},t),\psi_2(\mathbf{r},t),...\psi_N(\mathbf{r},t)$$



W. Kohn, chemistry Nobel prize 1998

The Kohn-Sham orbitals and eigenvalues

Non-interacting electrons in the Kohn-Sham potential :

$$\left(-\frac{1}{2}\nabla^2 + V_{\rm KS}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\,\psi_i(\mathbf{r})$$

Density $n(\mathbf{r}) = \sum_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r})$

$$V_{\rm KS}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int \frac{n(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}|}\,d\mathbf{r}_1 + \frac{\delta E_{\rm xc}[n]}{\delta n(\mathbf{r})}$$

Hartree potential Exchange-correlation potential

To be solved self-consistently !

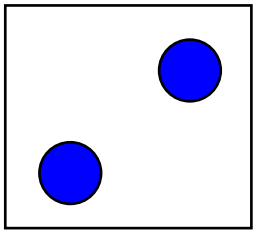
Lecture:
Plane wave based DFT
Tuesday morning

ABINIT capabilities

The ABINIT capabilities: basis

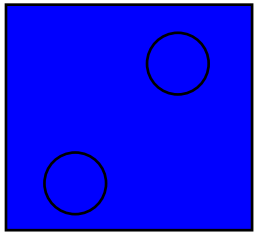
Wavefunctions ψ can be developped on a basis which is…

Localized



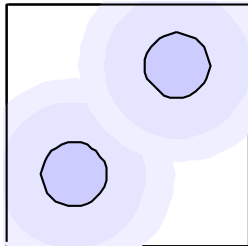
Spherical Harmonics, gaussians,…

Delocalized



Plane waves, …

Adaptive



Wavelets, …

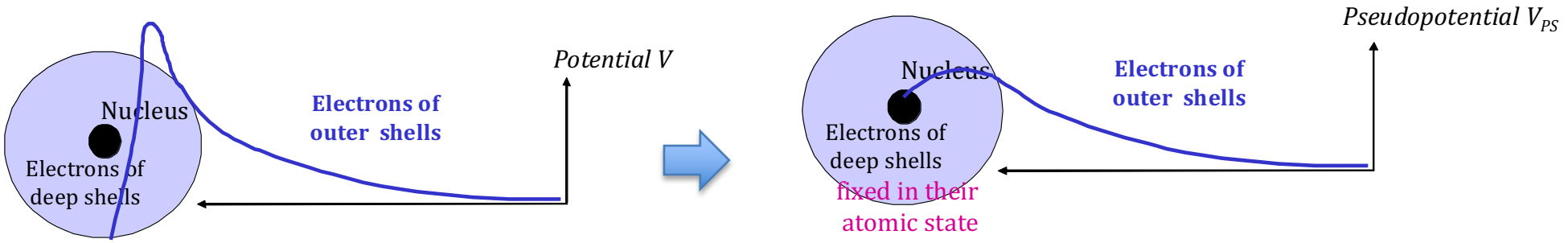
All-electron approaches

- ✓ Small number of elements in the basis
- ✓ All the electrons can be
- ✓ Results are accurate, calculations are « heavy »
- ✓ The basis moves with the atoms

Pseudopotential approaches

- ✓ Large number of elements in the basis to account for localised wavefunctions
- ✓ Convergency is easily controlled
- ✓ Approached results as the core electrons are « pseudized »

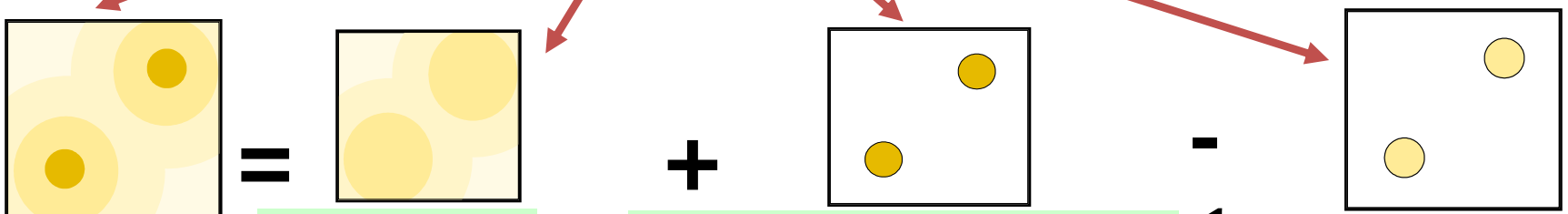
The ABINIT capabilities: pseudopotentials



- 1979-1982: pseudos BHS (Bachelet,Hamann, Schlüter)
- 1982: pseudos KB (Kleinman ,Bylander)
- 1990: pseudos MT (Martins, Troullier)
- 1991: ultrasoft pseudos (Vanderbilt)
- 1994: Projector Augmented-Wave PAW (P. Bloechl)

Lecture:
Plane wave based DFT
Tuesday morning

$$|\psi_n\rangle = |\tilde{\psi}_n\rangle + \sum_i \left(|\phi_i\rangle - |\tilde{\phi}_i\rangle \right) \langle \tilde{p}_i | \tilde{\psi}_n \rangle$$



plane waves ~ All-electron « on-site » part 1 Pseudized on-site part ~1

The ABINIT capabilities: magnetism

When the spin of the electron is taken into account,

$|\Psi_n\rangle$ becomes $|\Psi_n^\alpha\rangle = \begin{pmatrix} |\Psi_n^1\rangle \\ |\Psi_n^2\rangle \end{pmatrix}$ H becomes $H^{\alpha\beta} = \begin{pmatrix} H^{11} & H^{12} \\ H^{21} & H^{22} \end{pmatrix}$

The wave equation becomes: $\sum_\beta H^{\alpha\beta} |\Psi_n^\beta\rangle = \varepsilon_n O |\Psi_n^\alpha\rangle$

The density becomes: $n^{\alpha\beta}(r) = \sum_n \Psi_n^{\alpha *}(r) \cdot \Psi_n^\beta(r)$

Lecture:
Magnetism
Tuesday afternoon

In the case of colinear magnetism: $\alpha = \uparrow, \downarrow$ $H^{12} = H^{21} = 0$

$n = n^\uparrow + n^\downarrow$

- Two independent systems
- parallelisation over the spins, at the same level of the k points ($\times 2$)

The ABINIT capabilities: parallelism

Electronic density formula:

$$\rho(\vec{r}) = \sum_{\substack{n \\ Bands}} \left[\int_{\substack{\vec{k} \\ Reciprocal \\ space}} \left(\left| \sum_{\substack{\vec{g} \\ Plane \\ waves}} \left(C_{n,k}(\vec{g}) \cdot e^{i \cdot (\vec{k}+\vec{g}) \cdot \vec{r}} \right) \right|^2 \cdot d\vec{k} \right) \right]$$

3 parallelisation/distribution levels

Bands

k vector & spin

Plane waves

Parallelisation over k points: easy and available from a long time

interesting for metals

Parallelisation over plane waves: requires a parallel 3-dim FFT

Parallelisation over bands: requires a block eigensolver

Lecture:
parallelism
Wednesday morning

ABINIT v8 capabilities (I)

Pseudopotentials/Plane Waves

+ Projector Augmented Waves (for selected capabilities)

Many pseudopotential types, different PAW generators

(ATOMPAW is shipped with ABINIT)

+ Wavelets (BIGDFT effort)

Density functionals : LDA, GGA (many : PBE and variations, HCTH, ...),

LDA+U (or GGA+U), Van Der Waals corrected functionals (Grimme),

hybrid functionals + some advanced functionals (exact exchange + RPA or ...)

LR-TDDFT for finite systems excitation energies (Casida)

GW for accurate electronic eigenenergies

(4 plasmon pole models or contour integration ; non-self-consistent / partly self-consistent / quasiparticle self-consistent ; spin-polarized)

Bethe-Salpeter for accurate optical properties calculations

DMFT for correlated orbitals

Lecture:
Advanced features
Thursday afternoon

ABINIT v8 capabilities (II)

Insulators/metals - smearings : Fermi, Gaussian, Gauss-Hermite ...

Collinear spin / non-collinear spin / spin-orbit coupling

Forces, stresses, automatic optimisation of atomic positions and unit cell parameters (Broyden and Molecular dynamics with damping)

Molecular dynamics (Verlet or Numerov), Nosé thermostat, Langevin dynamics

Path-Integral Molecular Dynamics, String / NEB method for saddle points

Susceptibility matrix by sum over states

Optical (linear + non-linear) spectra

Polarization, finite electric field calculations

Electric field gradients, magnetic shielding (NMR)

Positron lifetime

Symmetry analyser (database of the 230 spatial groups and the 1191 Shubnikov magnetic groups)

Lecture:
Structural relaxatio
Molecular dynamics
Wednesday afternoon

ABINIT v8 capabilities (III)

Density-Functional Perturbation Theory :

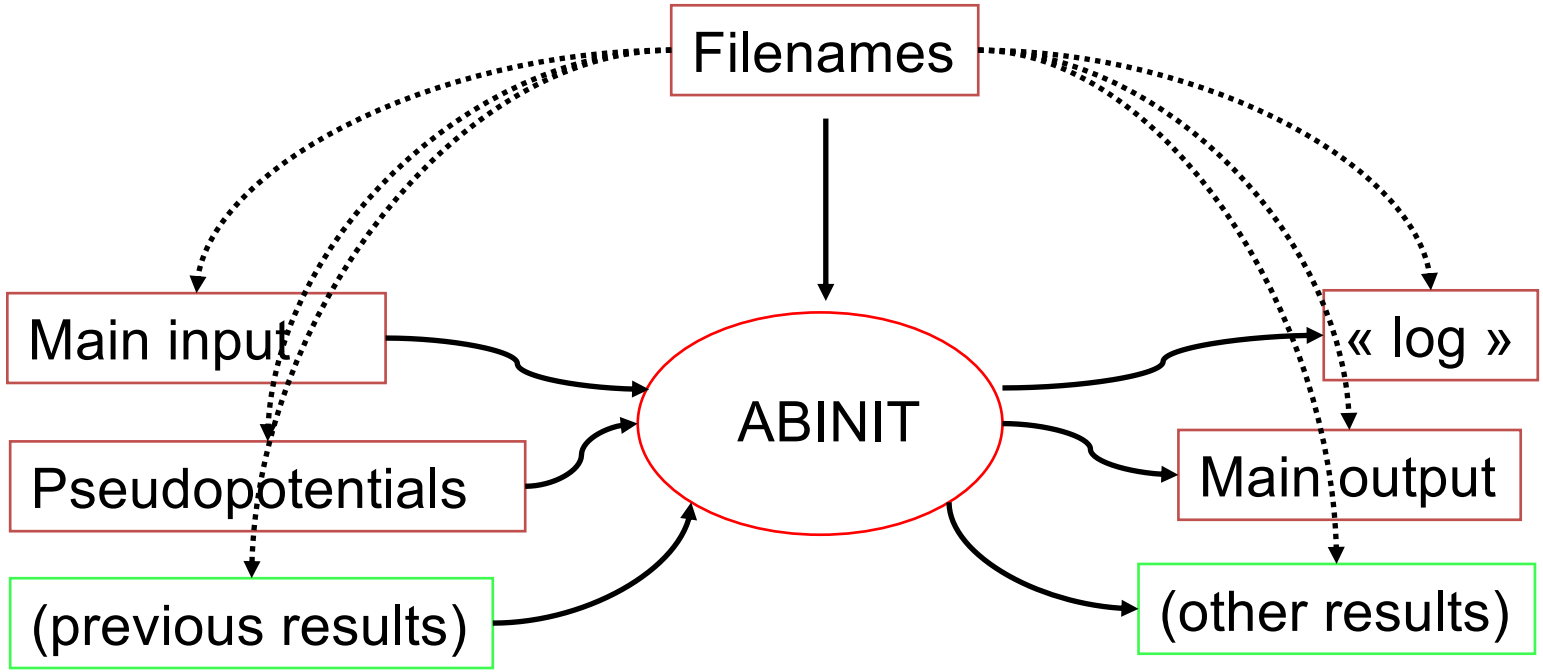
- Responses to atomic displacements, to static homogeneous electric field, to strain perturbations

- Second-order derivatives of the energy, giving direct access to :
  dynamical matrices at any q, phonon frequencies, force constants ;
  phonon DOS, thermodynamic properties (quasi-harmonic approximation) ;
  dielectric tensor, Born effective charges ;
  elastic constants, internal strain ;
  piezoelectric tensor ...
- Matrix elements, giving direct access to :
  electron-phonon coupling, deformation potentials, superconductivity
- Non-linear responses thanks to the 2n+1 theorem - at present :
  non-linear dielectric susceptibility; Raman cross-section ;
  electro-optic tensor

Lecture:
Advanced features
Thursday afternoon

Structure and documentation

External files in a ABINIT run



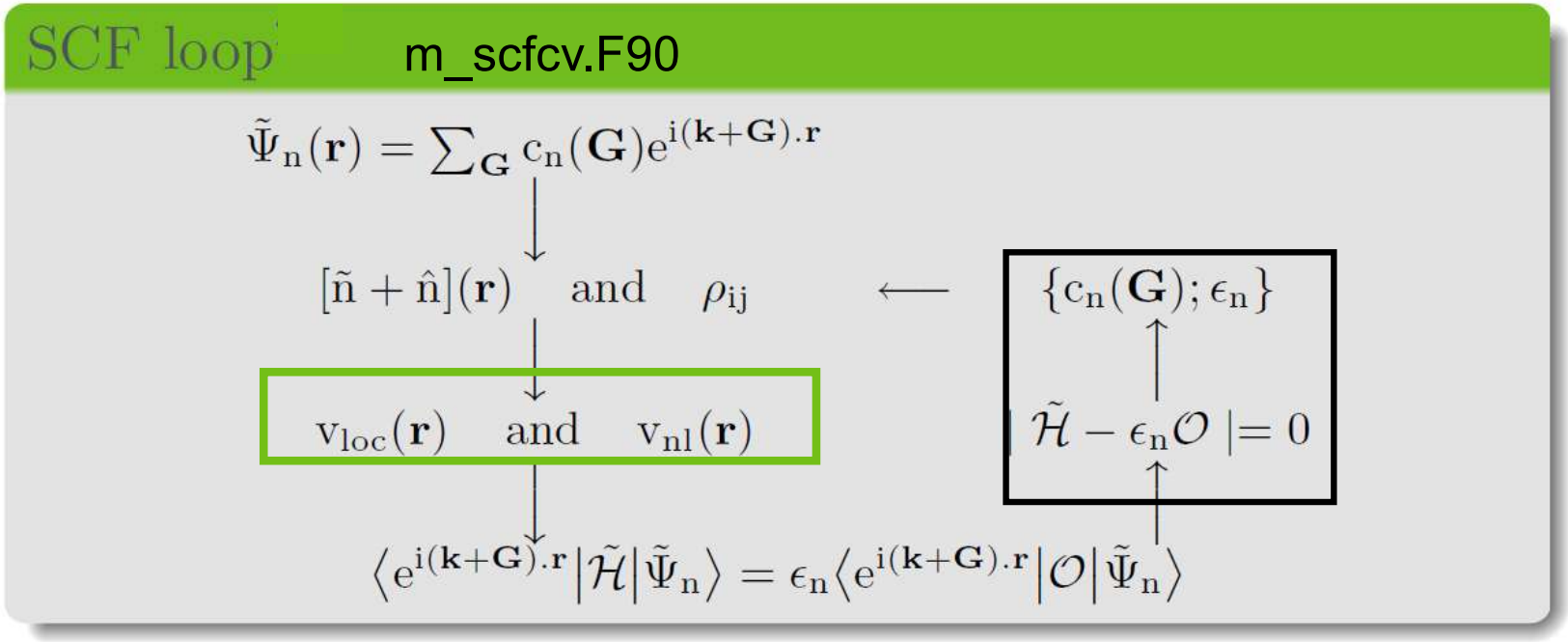
Results : density (_DEN), potential (_POT),
wavefunctions (_WFK), ...

Lecture:
Post-processing and analysis
Thursday morning

The SCF cycle

Resolution of a general eigenvalue problem $\tilde{H}\left|\tilde{\Psi}_n\right\rangle = \varepsilon_n O\left|\tilde{\Psi}_n\right\rangle$

In case of plane wave basis (PAW):



Lecture:
Efficient use of ABINIT
Thursday morning

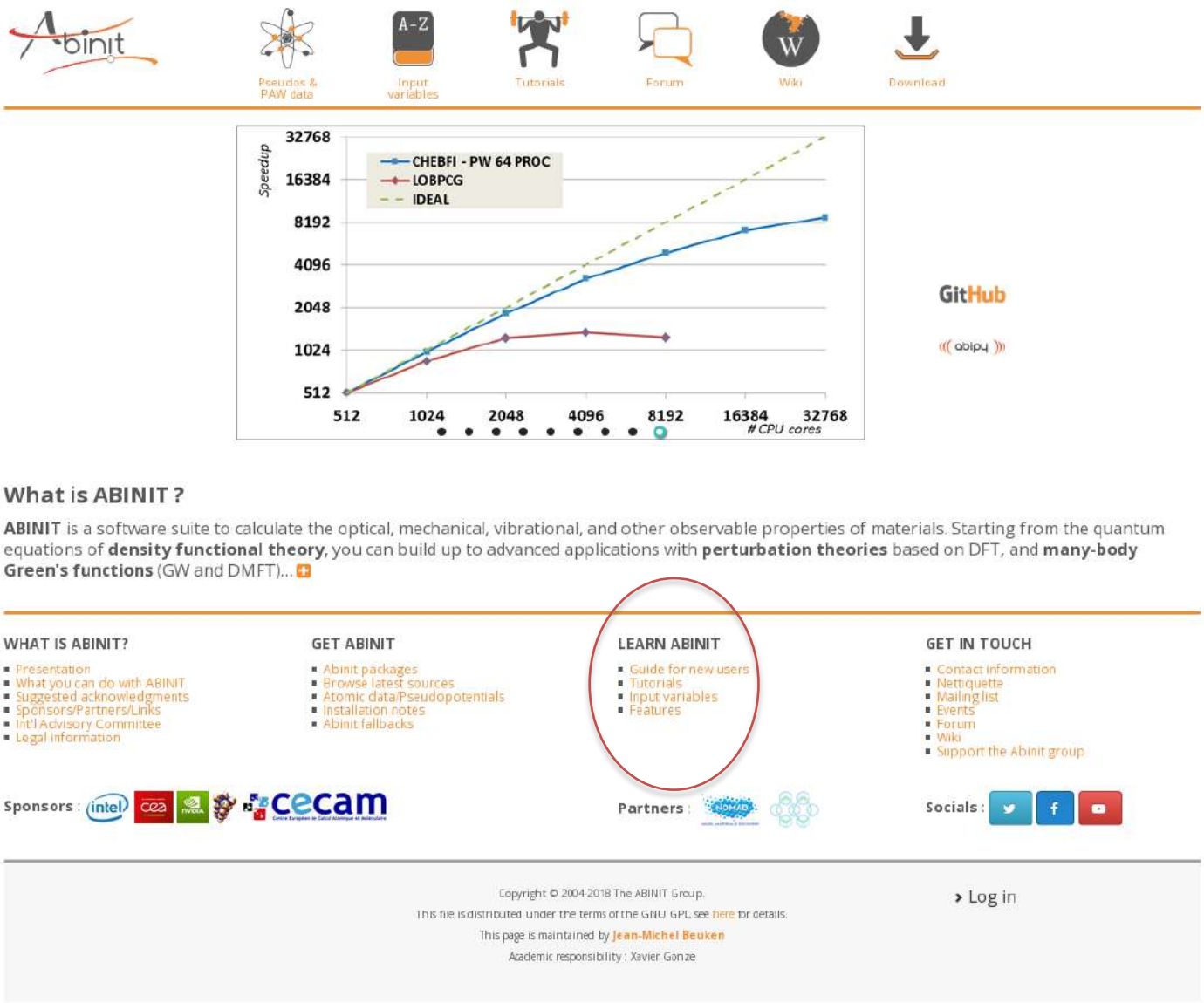
A basic input file : dihydrogen (I)

```
# H2 molecule in a big box

# Definition of the unit cell
acell 10 10 10              # The keyword "acell" refers to the
                            #  lengths of the primitive vectors (default in Bohr)
# Definition of the atom types
ntypat 1                    # There is only one type of atom
znucl 1                     # The keyword "znucl" refers to the atomic number of the
                            # possible type(s) of atom. The pseudopotential(s)
                            # mentioned in the "filenames" file must correspond
                            # to the type(s) of atom. Here, the only type is Hydrogen.
# Definition of the atoms
natom 2                     # There are two atoms
typat 1 1                   # They both are of type 1, that is, Hydrogen
xcart                       # This keyword indicate that the location of the atoms
                            # will follow, one triplet of number for each atom
  -0.7 0.0 0.0              # Triplet giving the cartesian coordinates of atom 1, in Bohr
   0.7 0.0 0.0              # Triplet giving the cartesian coordinates of atom 2, in Bohr
```

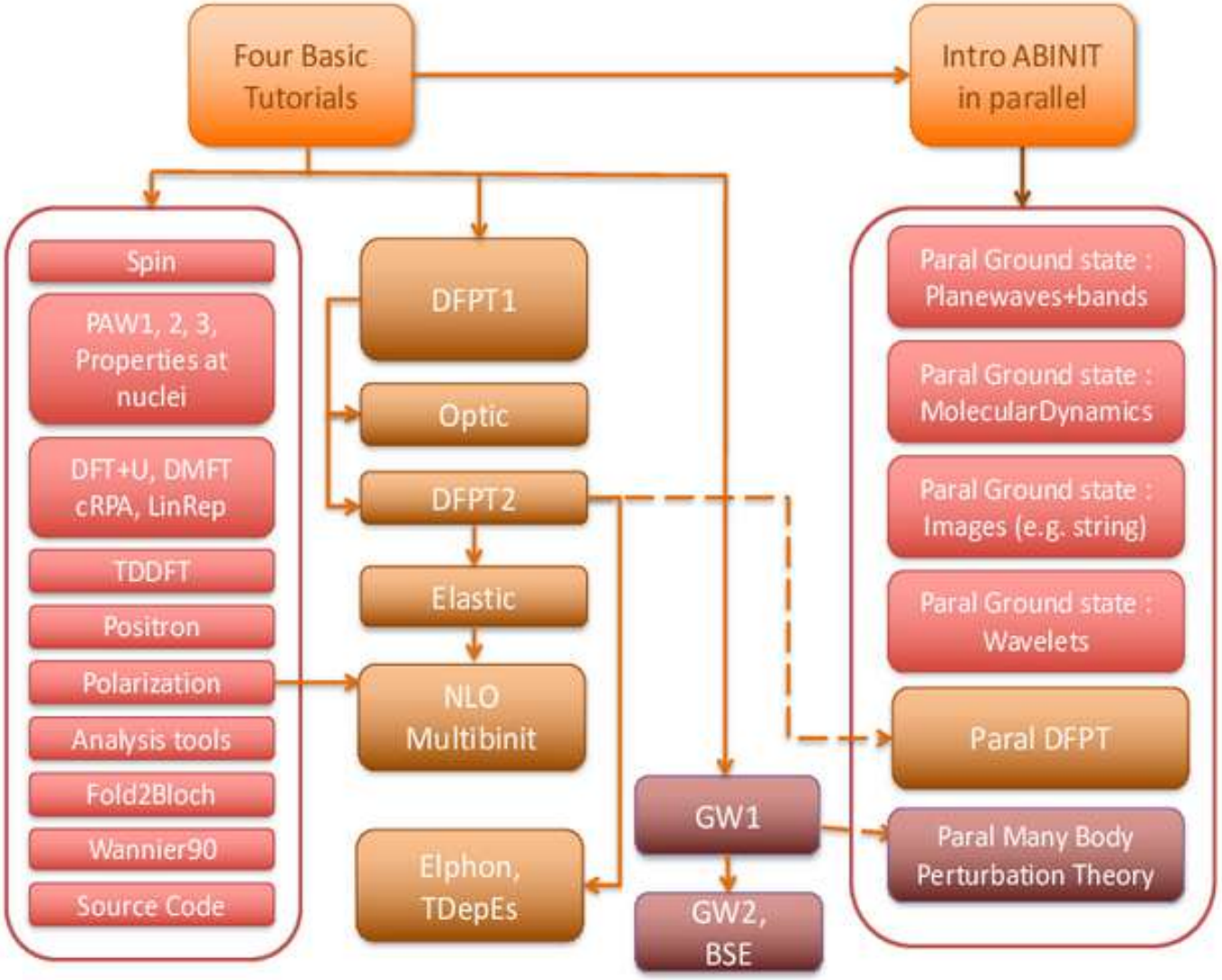
A basic input file : dihydrogen (II)

```
# Definition of the planewave basis set
ecut 10.0          # Maximal plane-wave kinetic energy cut-off, in Hartree

# Definition of the k-point grid
kptopt 0           # Enter the k points manually
nkpt 1             # Only one k point is needed for isolated system,
                   # taken by default to be 0.0 0.0 0.0

#Definition of the SCF (self-consistent field) procedure
nstep 10           # Maximal number of SCF cycles
toldfe 1.0d-6      # Will stop when, twice in a row, the difference
                   # between two consecutive evaluations of total energy
                   # differ by less than toldfe (default in Hartree)
diemac 2.0         # Although this is not mandatory, it is worth to
                   # precondition the SCF cycle. The model dielectric
                   # function used as the standard preconditioner
                   # is described in the "dielng" input variable section.
                   # Here, we follow the prescriptions for molecules
                   # in a big box
```

Documentation



ABINIT tutorial : layout + dependencies



A few references

- Description of the ABINIT project and ABINIT capabilities

  X. Gonze et al, Comput. Mat. Science 25, 478 (2002)

  X. Gonze et al, Z. Kristallogr. 220, 558 (2005)

  X. Gonze et al, Comp. Phys. Comm. 180, 2582 (2009)

  X. Gonze et al, Comp. Phys. Comm. 205, 106 (2016)

- Software engineering and management techniques used in ABINIT

  Y. Pouillon et al, Computing in Science and Engineering 13, 62 (2011)

- Focused papers on specific implementations within ABINIT

  (e.g. PAW, parallelism)

  M. Torrent et al, Comput. Mat. Science 42, 337 (2008)

  F. Bottin et al, Comp. Mat. Science 42, 329 (2008)

More references in the other parts of this tutorial ...