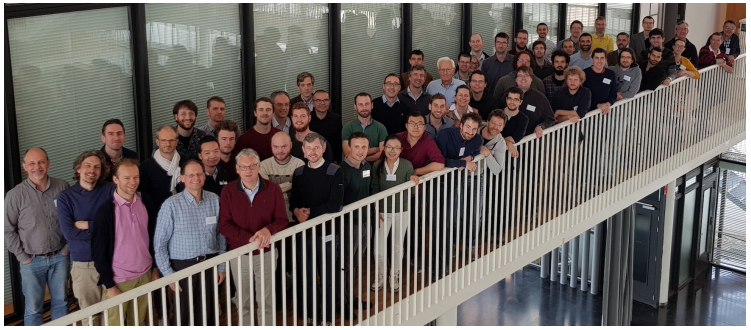
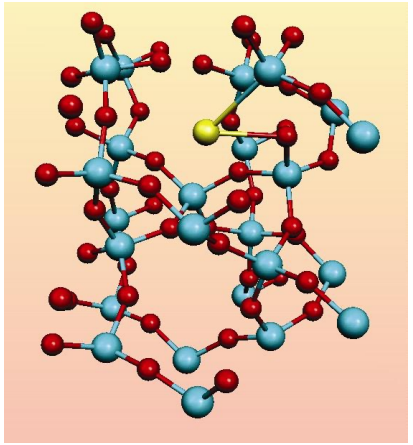
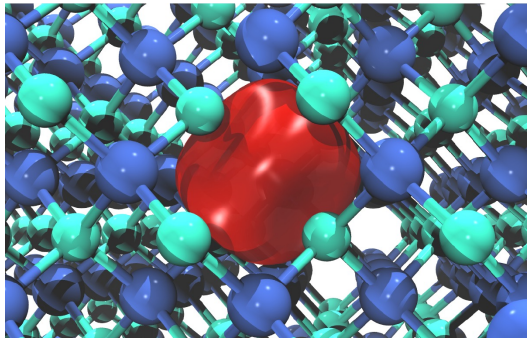
Introduction to

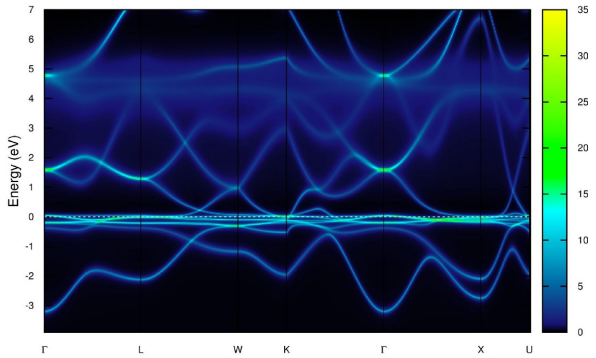
Overview

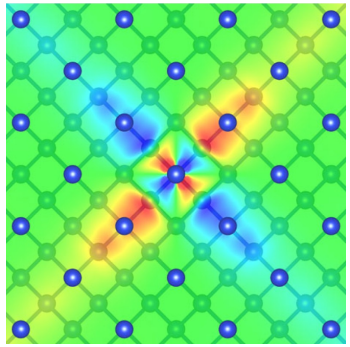


1. The ABINIT software project
2. ABINIT basics
   - Plane waves
   - Sampling the Brillouin Zone
   - Pseudopotentials / PAW
3. Running ABINIT : basics
4. HPC computing









ABINIT software project

Ideas (1997) – pioneered by **Xavier Gonze** :

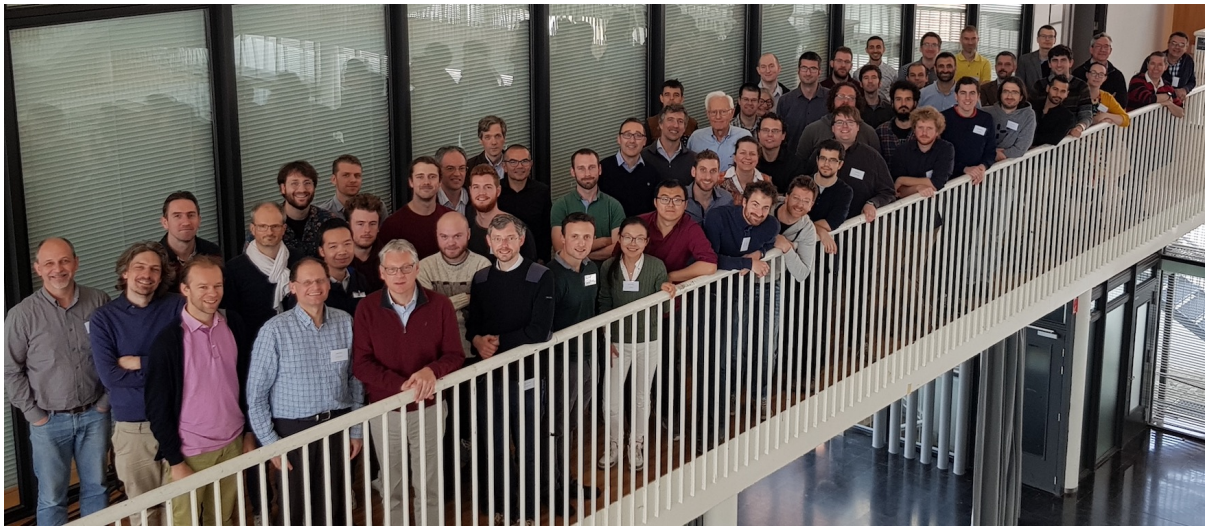
1) Software for first-principles simulations are more and more complex : needs a worldwide collaboration, of specialized, complementary, groups
2) Linux software development : ‘free software’ model

Now (2026) :

> 1 200 000 lines of F90
> 50 python scripts
about 60 contributors to ABINITv8/v9/v10

Last release 10.4
very soon 10.6,
http://www.abinit.org

Available freely
(GPL, like Linux).



ABINIT v10 capabilities (I)

Methodologies

Pseudopotentials/Plane Waves

+ Projector Augmented Waves (for selected capabilities)

Many pseudopotential types, different PAW generators

Density functionals :

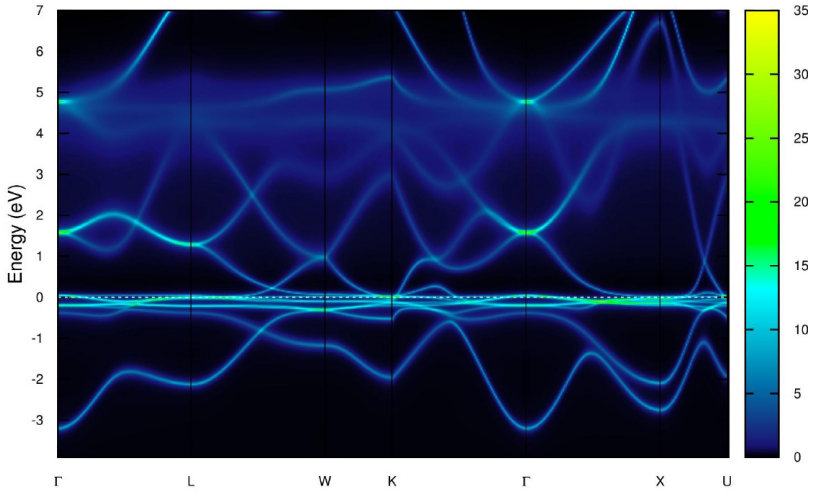
- LDA
- GGA (PBE and variations, HCTH, ...),
- LDA+U (or GGA+U)
- hybrid functionals + …

LR-TDDFT for finite systems excitations

GW for accurate electronic eigenenergies

Bethe-Salpeter for accurate optical properties

Dynamical mean field-theory (DMFT)



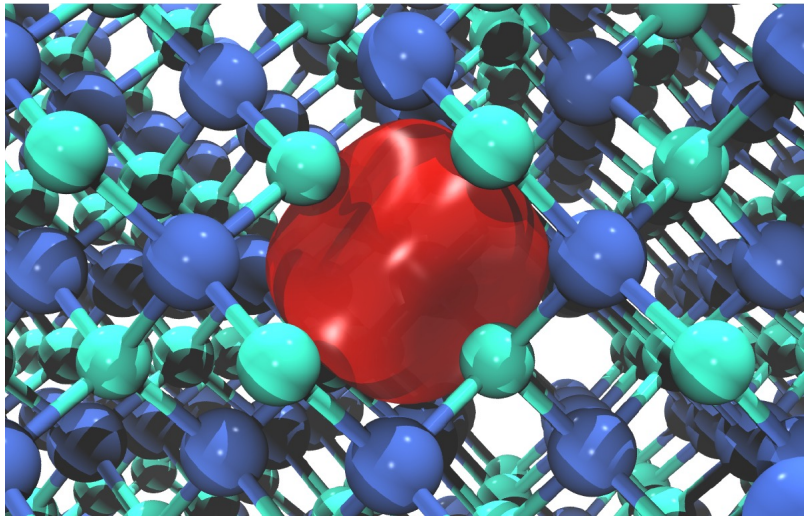
alpha-Cerium from DMFT

ABINIT v10 capabilities (II)

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

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

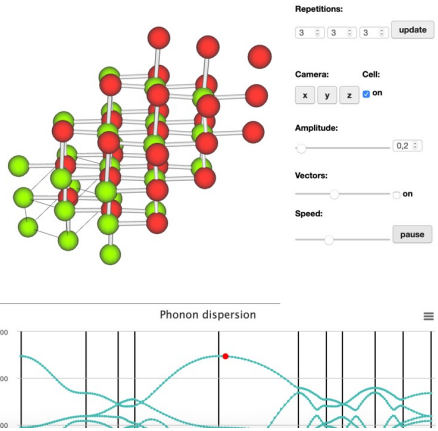
Molecular dynamics, Nosé thermostat, Langevin dynamics
Path-Integral Molecular Dynamics, String / NEB method for saddle points



Susceptibility matrix by sum over states
Optical (linear + non-linear) spectra
Polarization, finite electric field
Electric field gradients
Positron lifetime

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

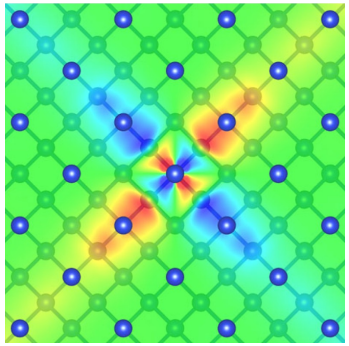
ABINIT v10 capabilities (III)



Density-Functional Perturbation Theory (DFPT) :

- Responses to atomic displacements, to static homogeneous electric&magnetic field, to strain, to long-wave 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, dynamical quadrupoles ;
  elastic constants, internal strain ...;
  piezoelectric tensor, flexoelectric tensor ... ,
- Matrix elements, giving direct access to :
  electron-phonon coupling (mobility, Seebeck, superconductivity)
  temperature-dependence of the electronic structure
- Non-linear responses thanks to the 2n+1 theorem - at present :
  non-linear dielectric susceptibility; Raman cross-section ;
  electro-optic tensor



Quality control : test suite + test farm

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

Test suite : >1200 automatic tests (+ new added for each capability)

Test farm : 7 active servers (12 to 96 cores)

with 4 compilers (gfort, Intel, NAG, NVhpc) => over 20 ‘builders’

Name	CPU Type *GPU Type*	#Cores (#THD)	RAM (GB)	OS	Compiler	MPI	Math	Misc
alps	Xeon 6230	2×20 (80)	64	Rocky-9.5	gcc9.5 NAG-7.2 oneAPI 2024 oneAPI 2025	mpich-3.3 openmpi-4.0.5	OpenBLAS MKL 2020 ELPA	py3.12
atlas	Xeon E5-2623	2×8 (16)	64	Fedora-41	gcc14.2 oneAPI 2025	openmpi-4.0.5	MKL 2025	py3.12
bob	Xeon E5-2603	2×6 (12)	16	Fedora-39	gcc13.2		Atlas 3.10	py3.12
eos	AMD 7643 $2*A30$	2×48 (192)	256	Ubuntu-22.04	nvhpc23.9 oneAPI 2023 gnu 11.3	openmpi-3 mpich-3.1	Atlas 3.10 Magma1.5 GSL1.14	cuda-12 py3.10
minimac	Apple M1 Ultra	16+4	64	macOS-15.5	gcc12	openmpi-3.1 mpich-3.2	OpenBLAS	py37 conda
scope	AMD 7502	2×32 (128)	96	Ubuntu-18.04	gnu10.2/12.2 gnu13.2	openmpi-4 mpich-3.3	MKL 2020	py36
manneback	Milan,EPYC,7763	40	2	Rocky 8	gnu 14.2	OpenMPI 4	MKL	py 3.11
haicgu	ARM Kunpeng 920	20	110	Rocky 8	gnu 14.1	OpenMPI 4	MKL	py 3.11

https://github.com/abinit/abinit_web/blob/main/docs/servers.md

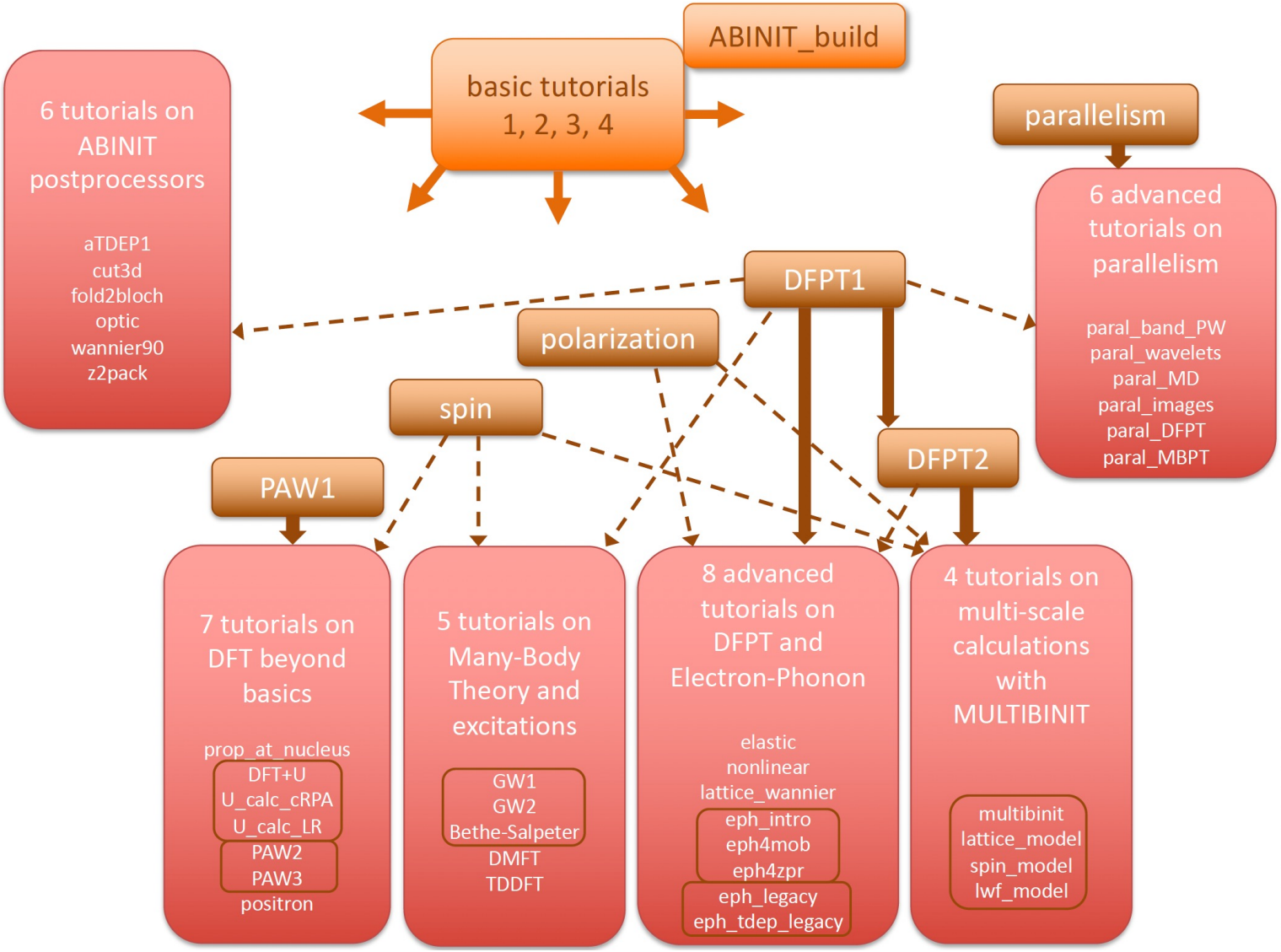
Basic Documentation

Web site http://www.abinit.org ; http://docs.abinit.org

- User's guides
- Installations notes
- List of input variables + description
- List of topics = a hub to input variables, files, tutorial, bibrefs
- Over 1000 example input files
- >30 tutorial lessons (each 1-2 hours)
  https://docs.abinit.org/tutorial

+ Forum Web site https://discourse.abinit.org
(old forum http://forum.abinit.org with more than 2000 registered members)

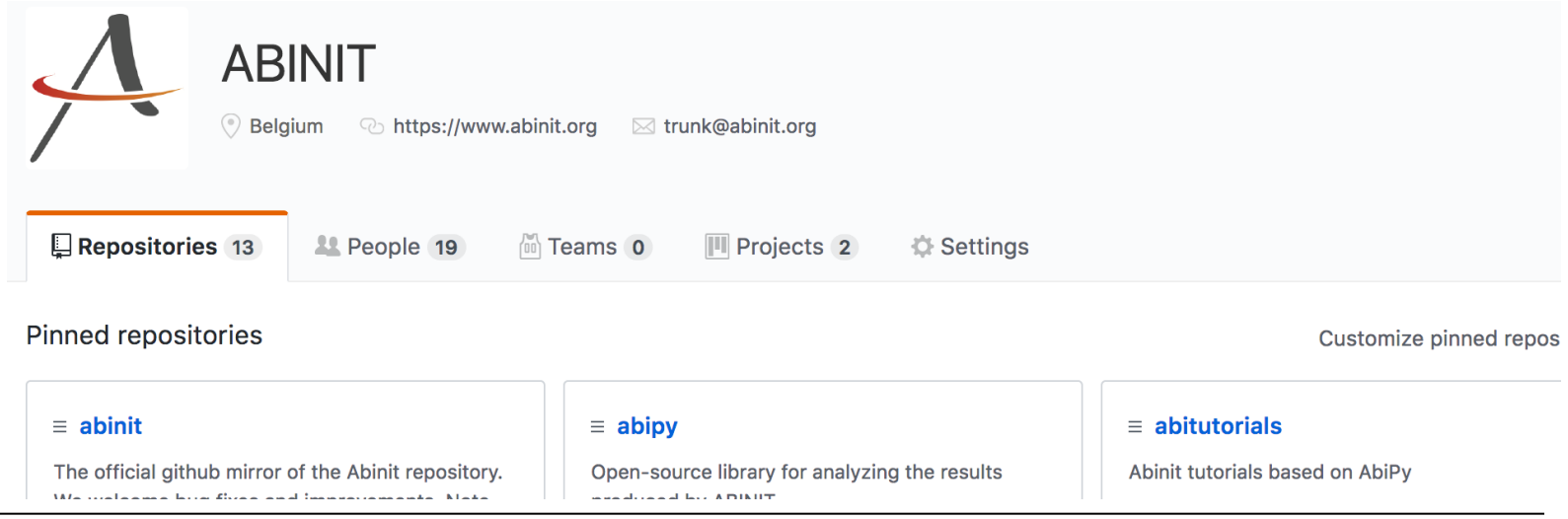
ABINIT tutorial : layout + dependencies



ABINIT + python : Abipy, Abitutorials …

ABINIT organization on GitHUB https://github.com/abinit

Abipy : python library for launching ABINIT jobs,
and analysing/plotting the results http://pythonhosted.org/abipy
=> e.g. connecting ABINIT with tools for high-throughput calculations developed in the Materials Project context (like Pymatgen, Fireworks).
Abitutorials : tutorial based on Jupyter notebooks ABINIT+python



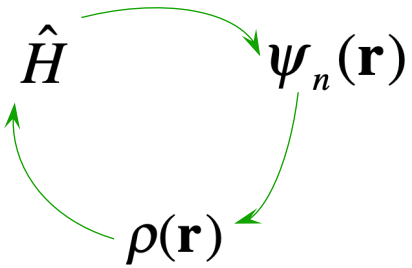
ABINIT : basic concepts

- Density Functional Theory (DFT)
- Plane wave basis
- K-points
- Pseudopotentials

Basic equations in DFT

Solve self-consistently the Kohn-Sham equation

$$\begin{cases} \hat{H}\left|\psi_n\right\rangle = \varepsilon_n\left|\psi_n\right\rangle \\ \hat{H} = \hat{T} + \hat{V} + \hat{V}_{Hxc}[\rho] \\ \rho(\vec{r}) = \sum_n^{occ} \psi_n^*(\vec{r})\psi_n(\vec{r}) \end{cases}$$



or minimize

$$E_{el}\{\psi\} = \sum_n^{occ}\left\langle\psi_n\left|\hat{T} + \hat{V}\right|\psi_n\right\rangle + E_{Hxc}[\rho]$$

with

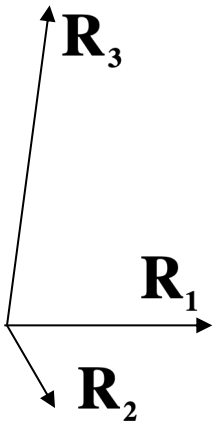
$$\hat{V}(\vec{r}) = \sum_{a\kappa} -\frac{Z_\kappa}{\left|\vec{r} - \vec{R}_\kappa^a\right|}$$

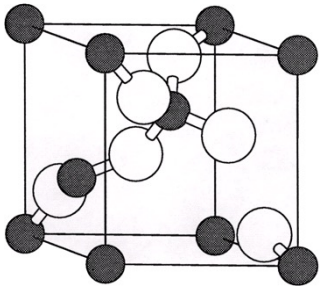
Plane waves and periodicity

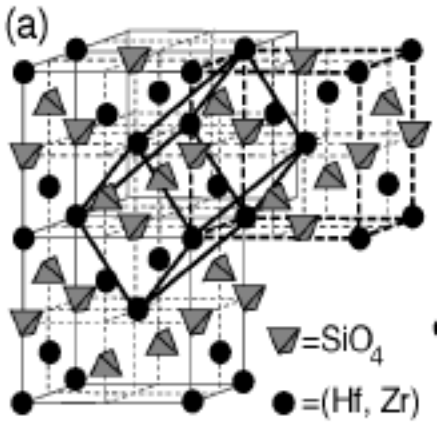
ABINIT : a periodic code

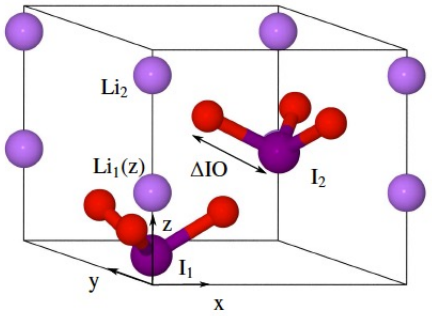
Crystalline solids: Primitive vectors $\mathbf{R}_j$, primitive cell volume Ω_0

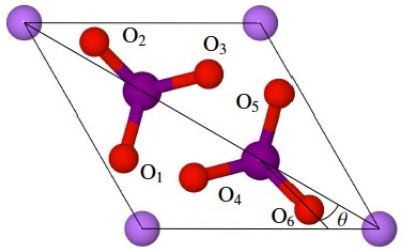
Need periodic boundary conditions.







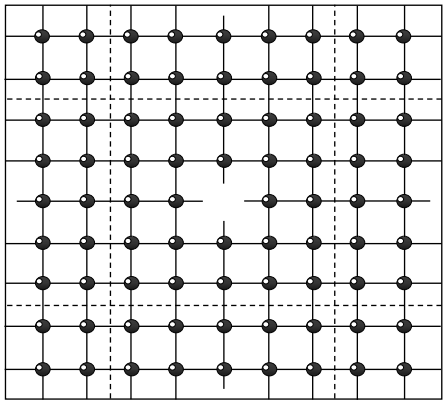




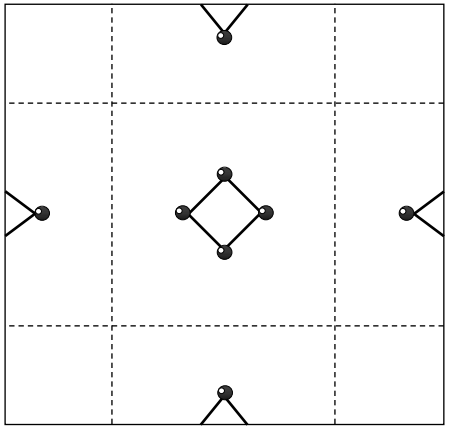
Plane waves e^{iKr} : particularly simple and efficient (when used with pseudopotentials), but infinite spatial extent.

The supercell technique

For surfaces, defects, polymers, nanotubes, finite systems

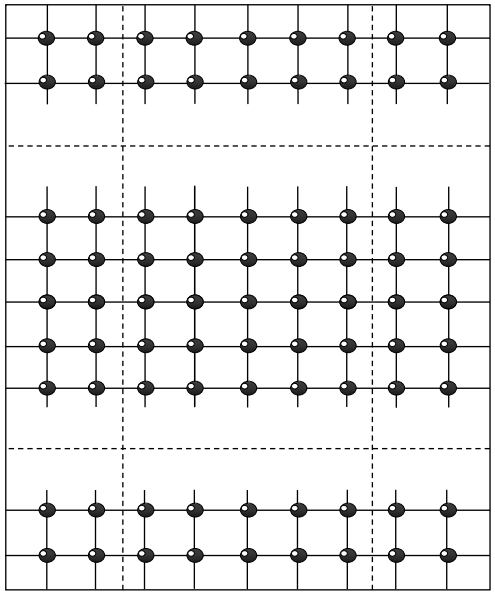


Point defect
in a bulk solid



Molecule,
cluster

Surface and interface:
treatment of a slab



The supercell must be sufficiently big : convergence study

The plane wave basis set

Periodic boundary conditions imply that

- The potential, the density, and the wavefunctions can be represented by a discrete Fourier series (plane waves)
- Wavefunctions are characterized by a wavevector (**k**)

Plane waves representation of the wavefunctions:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \left(N\Omega_0\right)^{-1/2} \sum_{\mathbf{G}} u_{\mathbf{k}}(\mathbf{G})\, e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}$$

Selection of plane waves determined by a cut-off energy E_{cut} (**ecut**) which is a convergence parameter

$$\frac{(\mathbf{k}+\mathbf{G})^2}{2} < E_{cut}$$

Plane wave sphere

Sampling the Brillouin zone

From discrete states to Brillouin zone

Discrete summations over states (e.g. the density) :

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

In the periodic case : summation over energy bands + integration over the Brillouin zone

$$n(\mathbf{r}) = \sum_n \frac{1}{\Omega_{0\mathbf{k}}} \int_{\Omega_{0\mathbf{k}}} f(\varepsilon_F - \varepsilon_{n\mathbf{k}})\psi_{n\mathbf{k}}^*(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

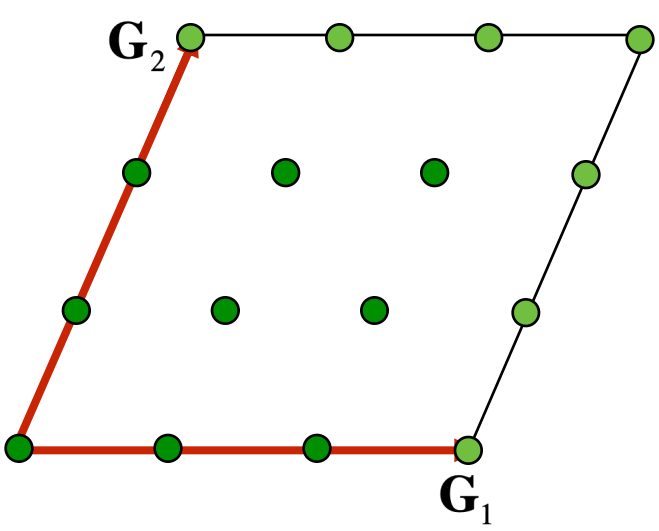
Discretize the BZ integration

$$\frac{1}{\Omega_{o\mathbf{k}}} \int_{\Omega_{o\mathbf{k}}} X_{\mathbf{k}}\, d\mathbf{k} \Rightarrow \sum_{\{\mathbf{k}\}} w_{\mathbf{k}} X_{\mathbf{k}} \qquad [\text{ with } \sum_{\{\mathbf{k}\}} w_{\mathbf{k}} = 1 \,]$$

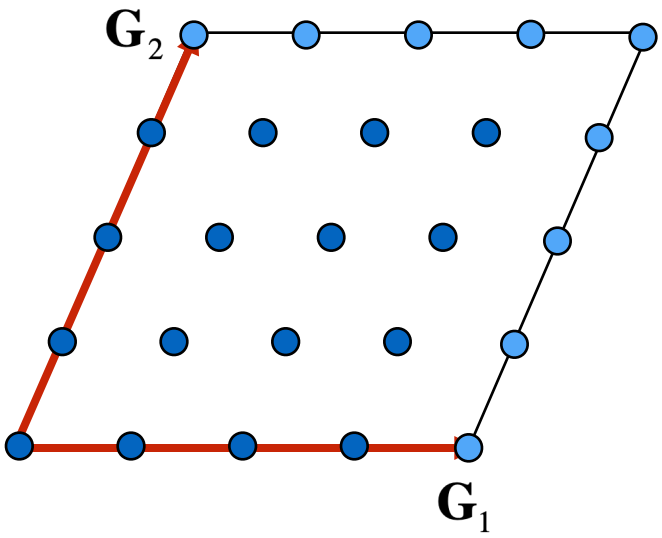
Use **symmetries** to reduce the number of k-points and assign weights $w_{\mathbf{k}}$

BZ integration : Monkhorst-Pack grid

- Uniformly spaced grid of $n_{k1} \times n_{k2} \times n_{k3}$ points in the first Brillouin Zone
  [Monkhorst & Pack, Phys. Rev. B 13, 5188 (1976)]



$n_{k1} = n_{k2} = 3$

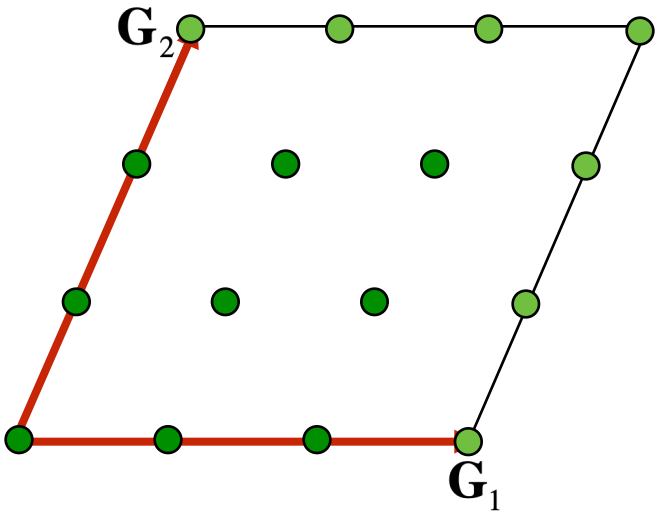


$n_{k1} = n_{k2} = 4$

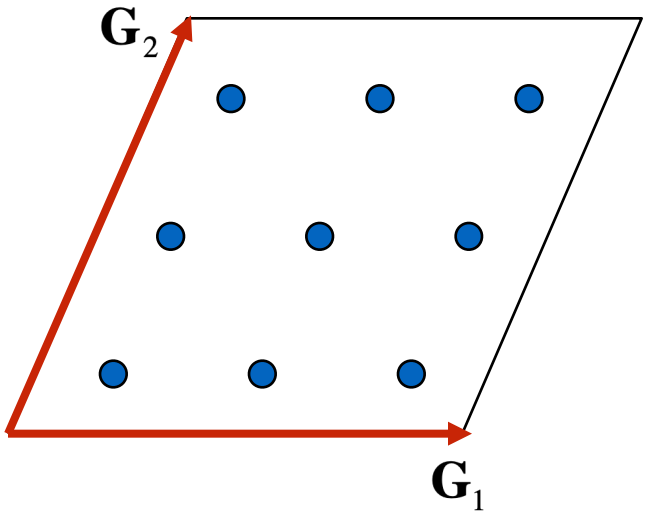
`ngkpt` nk1 nk2 nk3

Unshifted and shifted grids

- k-points grid can be chosen to be shifted : not centered at Γ.
- Advantage : comparable accuracy can be obtained with fewer k-points in IBZ (especially for highly symmetric cases)



$n_{k1} = n_{k2} = 3$
unshifted

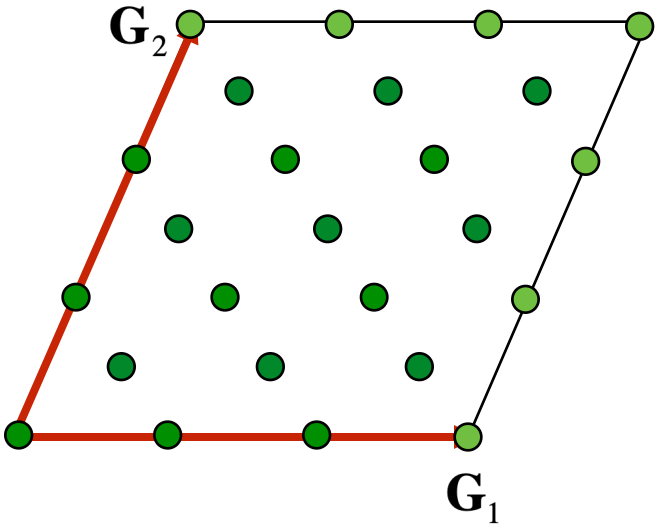


$n_{k1} = n_{k2} = 3$
shifted by (1/2,1/2)

```
ngkpt nk1 nk2 nk3
shiftk sk1 sk2 sk3   (defaut: 0.5 0.5 0.5)
```

Combining grids with various shifts

- k-points grid with various shifts can also be combined.



combining unshifted
and shifted by (1/2,1/2)
for $n_{k1} = n_{k2} = 3$

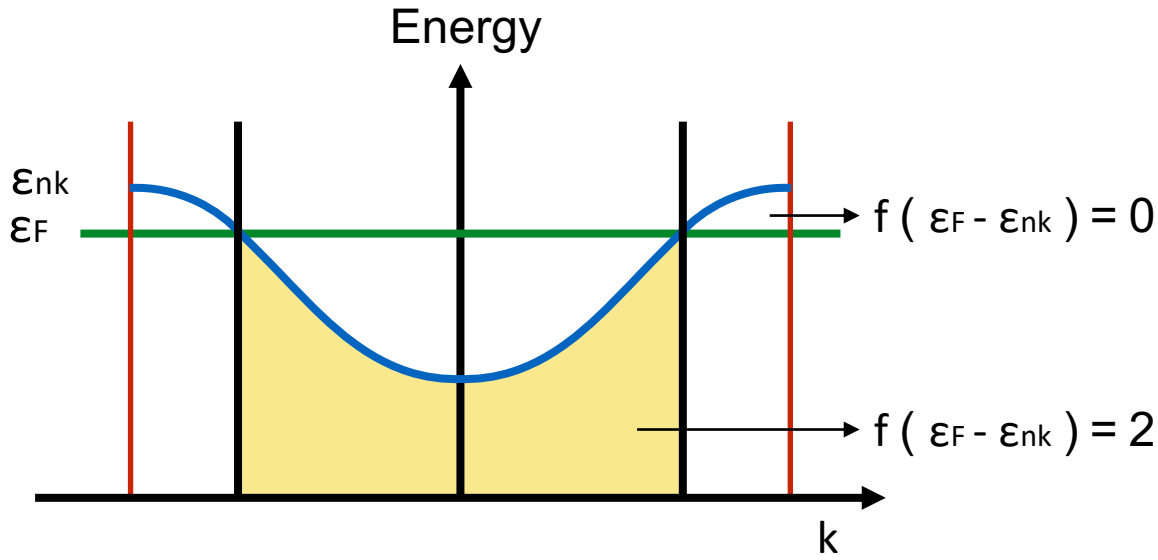
```
ngkpt nk1 nk2 nk3
nshiftk nsk
shiftk sk1(1)   sk2(1)   sk3(1)
       sk1(2)   sk2(2)   sk3(2)
       …        …        …
       sk1(nsk) sk2(nsk) sk3(nsk)
```

Treatment of metals

$$f(\varepsilon_{n\mathbf{k}}) = \frac{1}{1+e^{(\varepsilon_{n\mathbf{k}}-\varepsilon_F)/kT}}$$

f goes from 0 to 2 in an energy range $\sigma = k_B T$

At T=0, occupation factor varies abruptly at the Fermi level
=> Too many k-points needed to reach convergence!

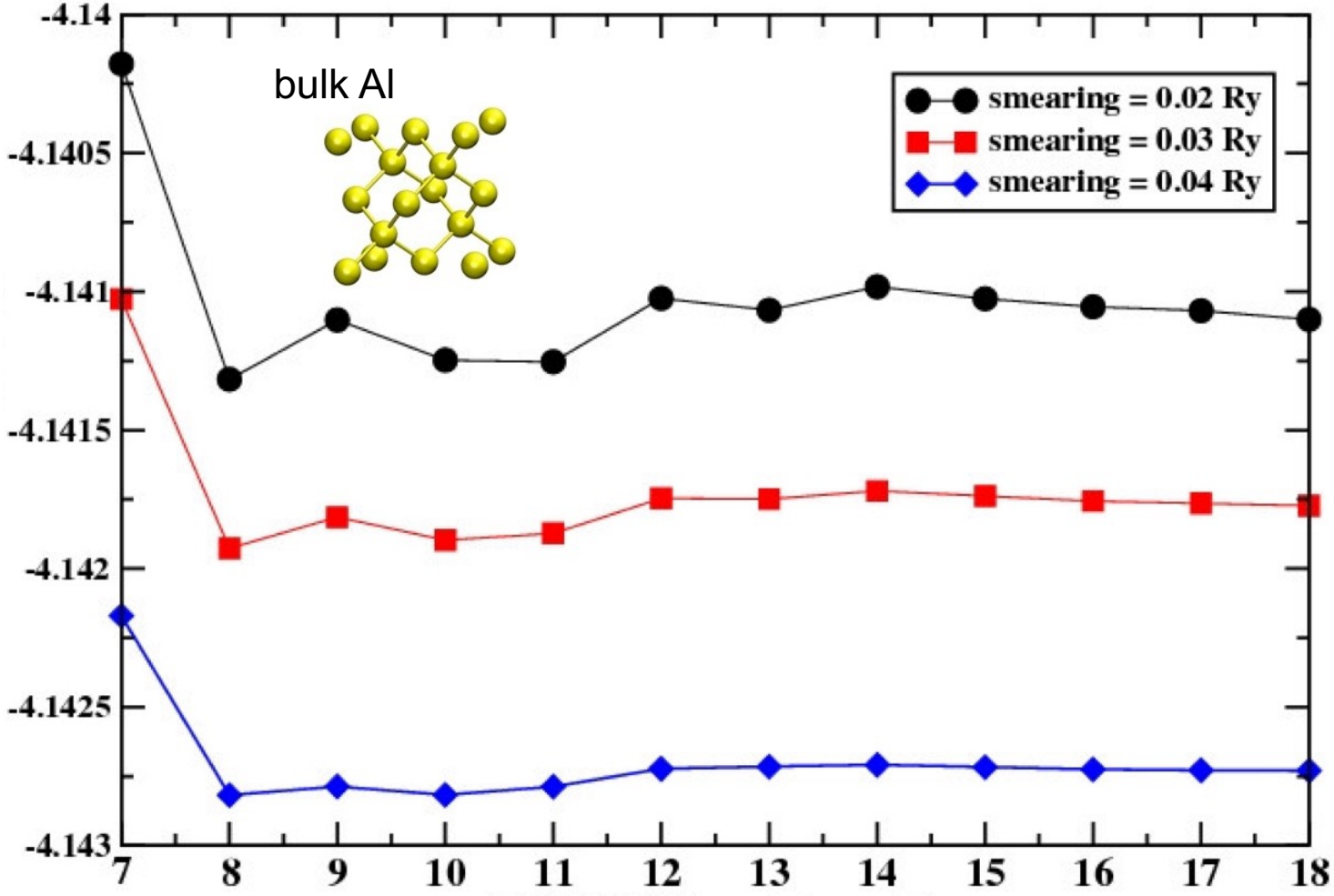


Solution: Use a **smearing scheme** with smearing temperature `tsmear` σ

- Fermi-Dirac smearing (inefficient) `occopt 3`
- Gaussian smearing (recommended) `occopt 7`
- Gauss-Hermite smearing `occopt 6`
- Cold Smearing `occopt 4/5`

Convergence wrt k-points and smearing

Total energy (Ry)



Courtesy of S. Narasimhan

Pseudopotentials

Core / valence partitioning

Core electrons occupy orbitals that are « frozen » regardless of the atomic environment

For some elements, the core / valence partitioning is obvious.

F atom : $(1s)^2$ + $(2s)^2(2p)^5$

IP 1keV 10-100 eV

For some others, it is not, and we have a choice to make!

Ti atom : $(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(4s)^2(3d)^2$ small core

$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(4s)^2(3d)^2$ large core

IP 99.2 eV 43.3eV

Choice of partitioning will affect the accuracy of the calculation

The concept of a pseudopotential

The potential of the nucleus + the frozen core electrons

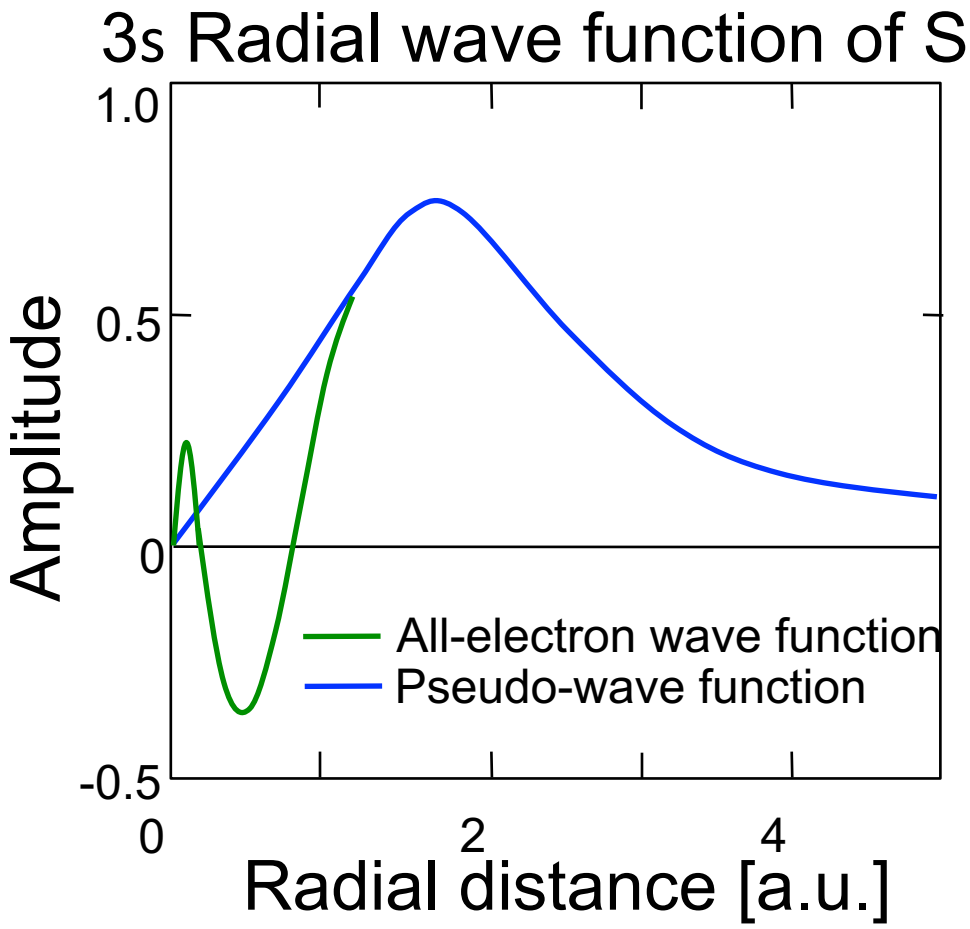
Solving the Schrödinger equation with a pseudopotential produces a **pseudo-wavefunction** with the **same eigenvalues** as the valence electrons

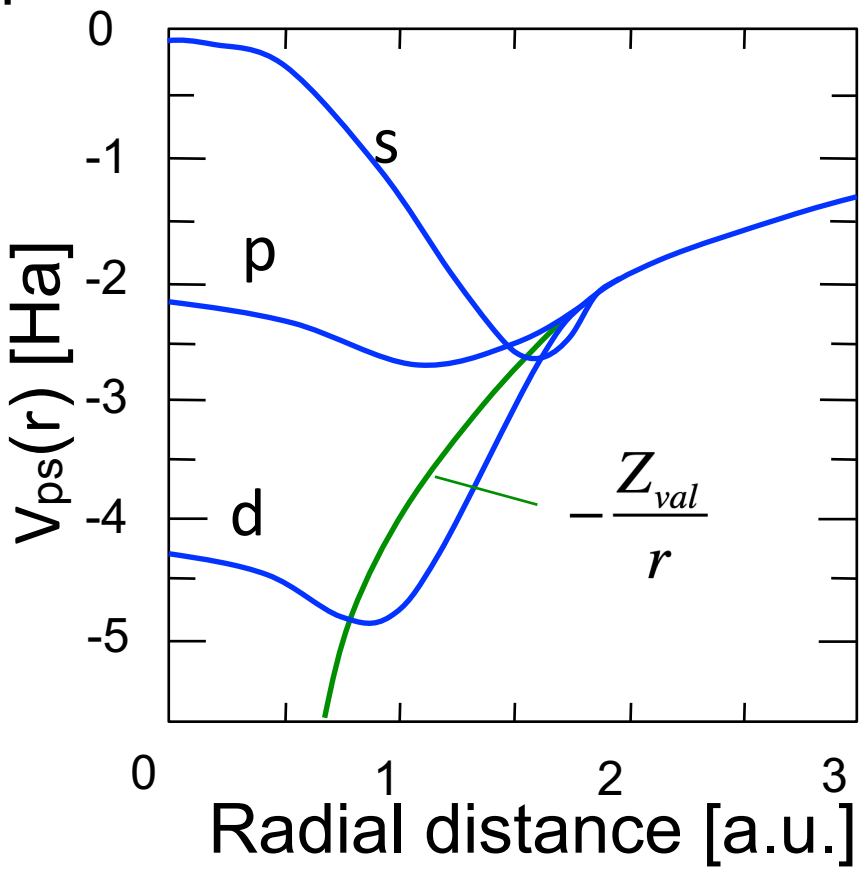
Has a cutoff radius $\mathbf{r_c}$ beyond which the pseudopotential corresponds to the real potential, and the pseudo-wavefunctions correspond to the real wavefunctions.

Different types of pseudos, depending on the constraints:

- Norm-conserving pseudopotentials (NCPP)
- Ultra-soft pseudopotentials (USPP)
- Projector-augmented plane waves (PAW)

Example of pseudopotential



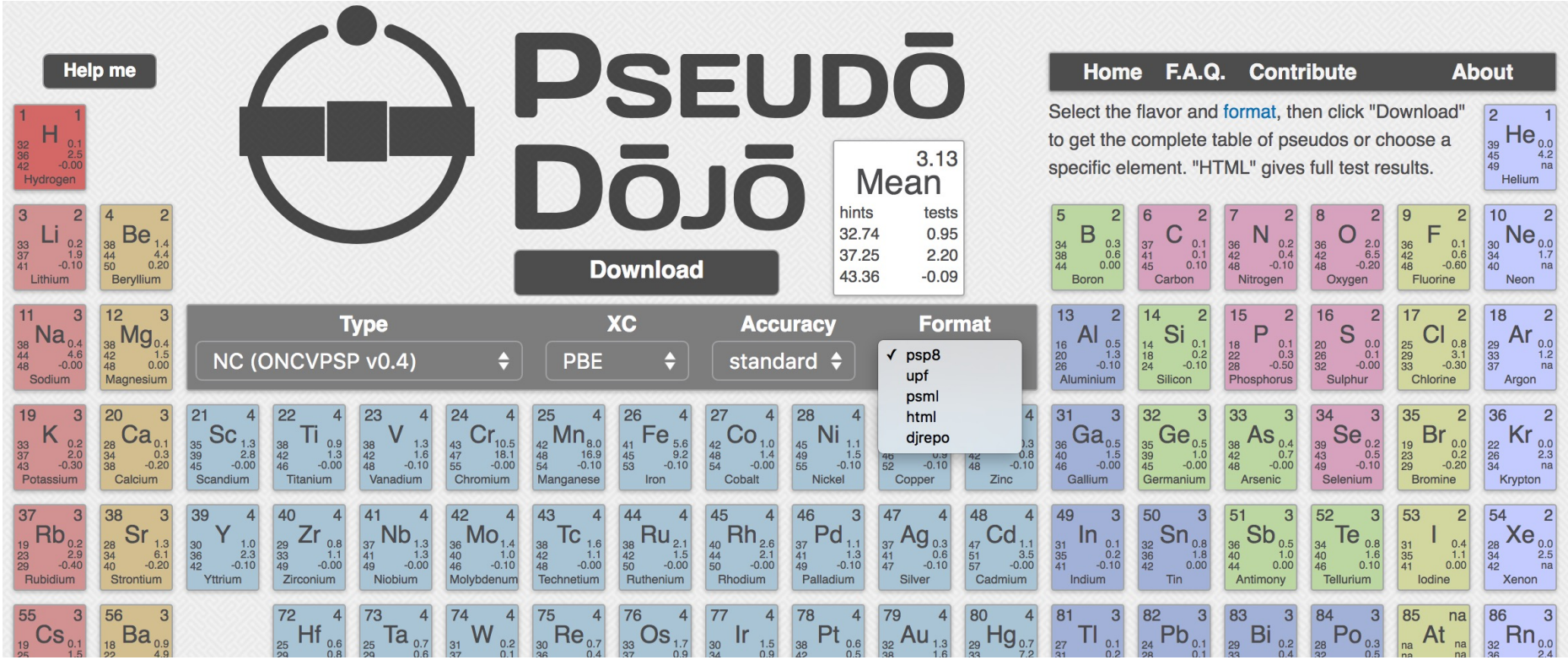


Pseudopotentials/PAW data in ABINIT

- Norm-conserving pseudos : pseudo-dojo approach

  Van Setten et al , Computer Physics Comm. 226, 39 (2018)

  https://www.pseudo-dojo.org

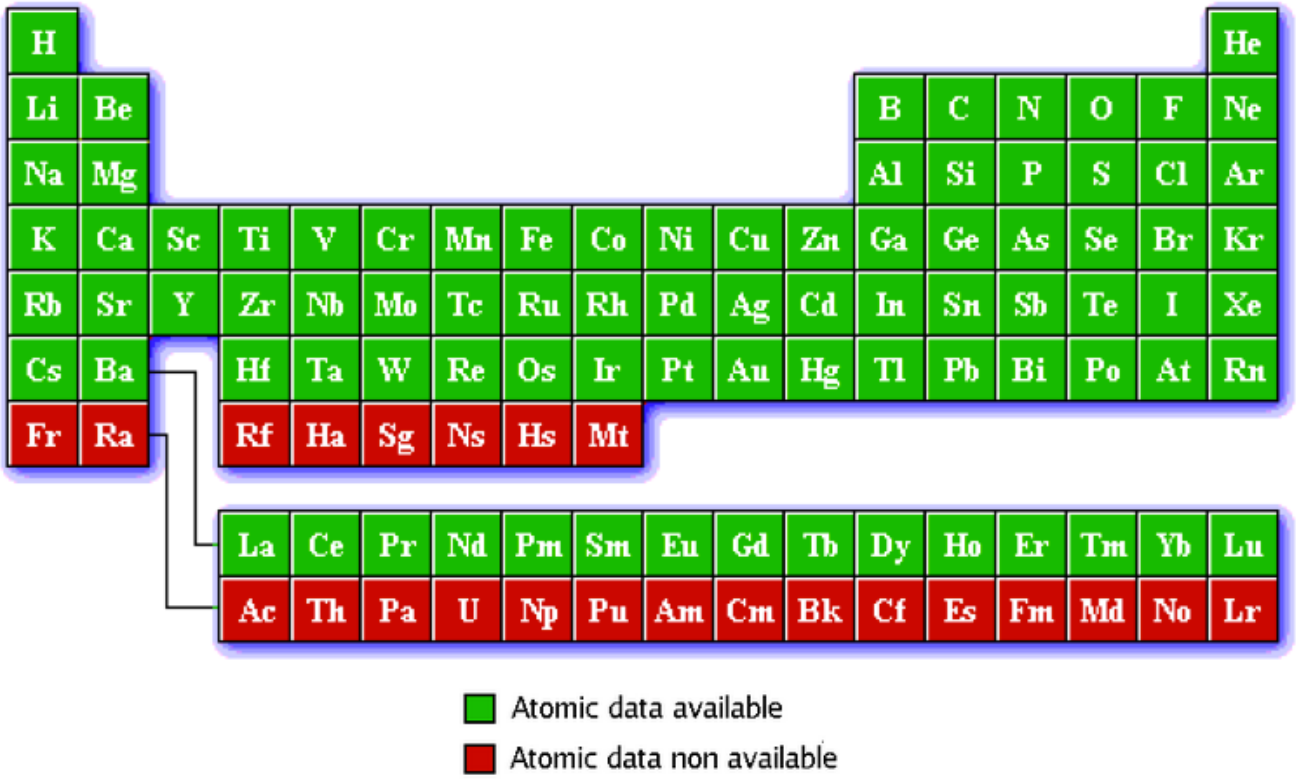


Pseudopotentials/PAW data in ABINIT

- Preferred PAW atomic dataset table : JTH

Jollet, Torrent, Holzwarth, Computer Physics Comm. 185, 1246 (2014)

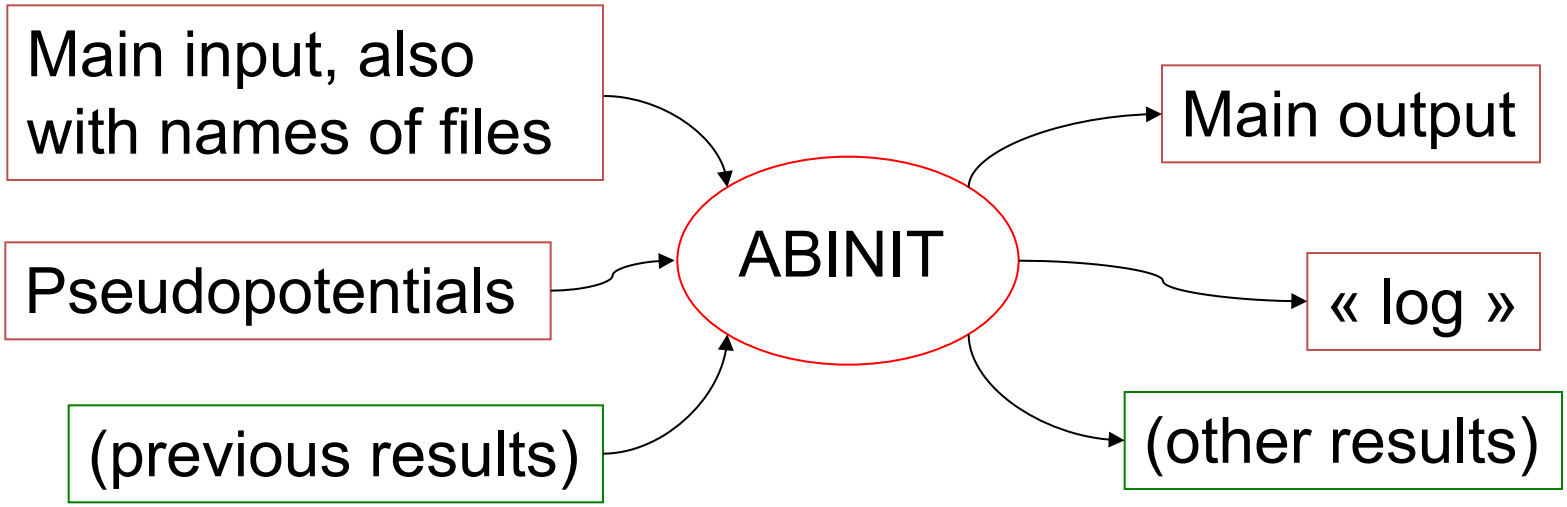
https://www.abinit.org/psp-tables



Also, possibility to use : GPAW table, GBRV v1.0 table, or norm-conserving pseudopotentials (e.g. ONCVPSP pseudo generator), or many others

Running ABINIT : basics

External files in a ABINIT run



Results :

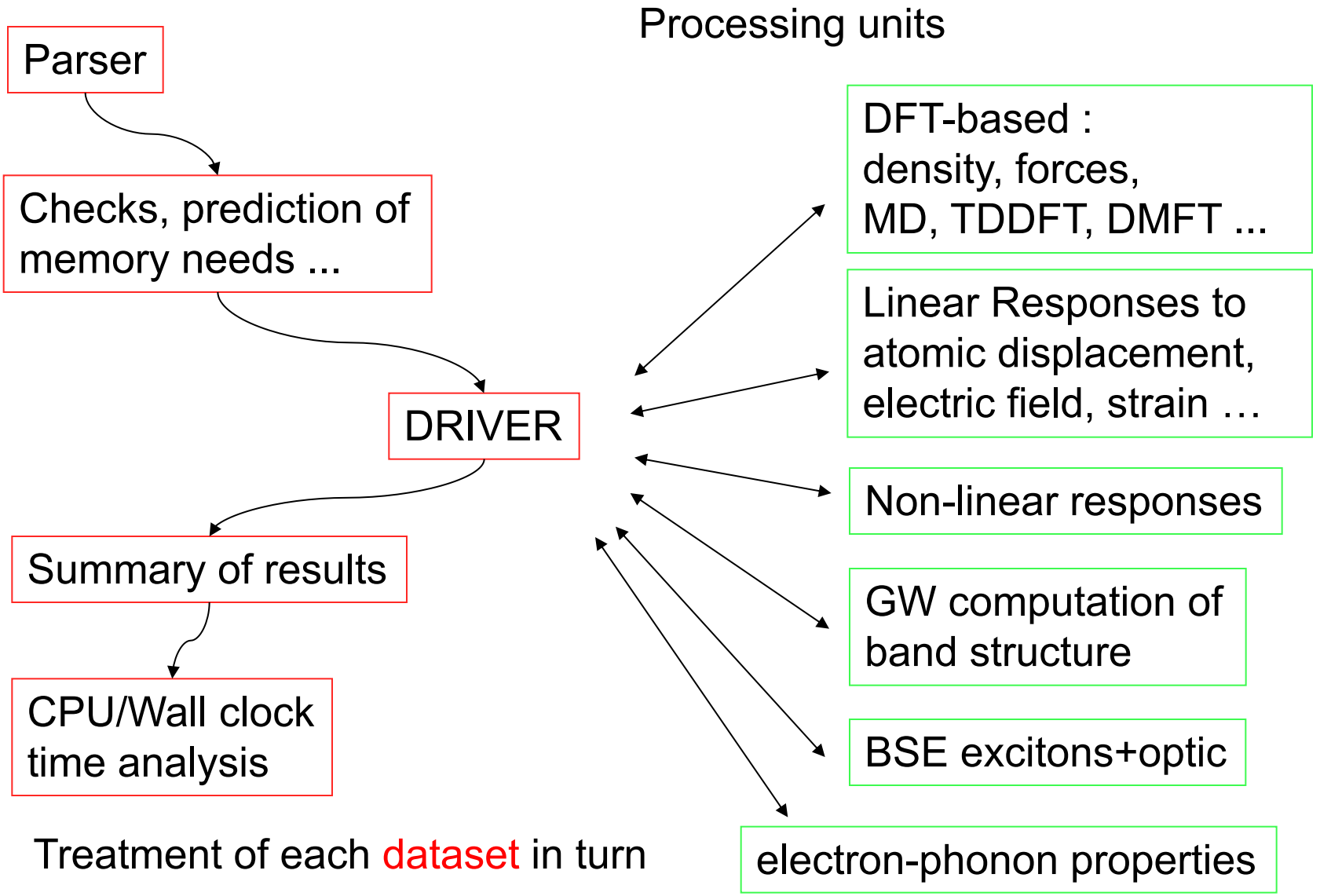
Text files : log, main output, energy derivatives (_DDB) ...

Binary F90 files : density (_DEN), potential (_POT), wavefunctions (_WFK), ...

netCDF files (similar to F90) : _DEN.nc, _POT.nc, _WFK.nc

Advantage of netCDF : portable, addressed by content, extensible, Python-friendly

ABINIT : the pipeline and the driver



A basic ‘input’ file : dihydrogen (I)

```
# H2 molecule in big cubic box
# Characters after  ’#’ or after ‘!’ are comments, will be ignored.
# Keywords followed by values. Order of keywords in file is not important.

# Definition of the unit cell
acell 10 10 10          # Keyword "acell" refers to lengths of primitive vectors (default in Bohr)
# Definition of the atom types
ntypat 1                # Only one type of atom
znucl 1                 # Keyword "znucl" refers to atomic number of possible type(s) of atoms.
pseudos "Pseudodojo_nc_sr_04_pw_standard_psp8/H.psp8"
        # Pseudopotential file name, for the only type of atom, hydrogen.
        # It comes from pseudodojo site http://www.pseudo-dojo.org/  (NC SR LDA standard),
        # and was generated using the LDA XC functional (PW=Perdew-Wang, ixc -1012).
        # By default, abinit uses same XC functional than the one of input pseudopotential(s)
# Definition of the atoms
natom 2                 # Two atoms
typat 1 1               # Both are of type 1, that is, Hydrogen
xcart                   # Keyword  " xcart" indicates that location of the atoms
                        # will follow, one triplet of numbers for each atom
  -0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 1, in Bohr
   0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 2, in Bohr
```

A basic input file : dihydrogen (II)

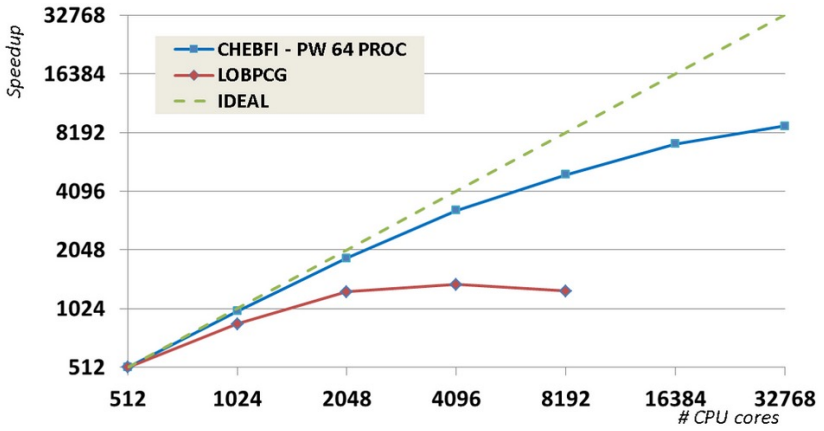
```
# Definition of planewave basis set
ecut 10.0          # Maximal plane-wave kinetic energy cut-off, in Hartree

# Definition of k-point grid
kptopt 0           # Enter 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 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
                   # differs by less than toldfe (default in Hartree)
diemac 2.0         # Although this is not mandatory, it is worth to precondition the
                   # SCF cycle. A model dielectric function, used as standard
                   # preconditioner, is described in "dielng" input variable section.
                   # Here, we follow prescriptions for molecules in a big box
## After modifying the following section, one might need to ...
#%%<BEGIN TEST_INFO>
```

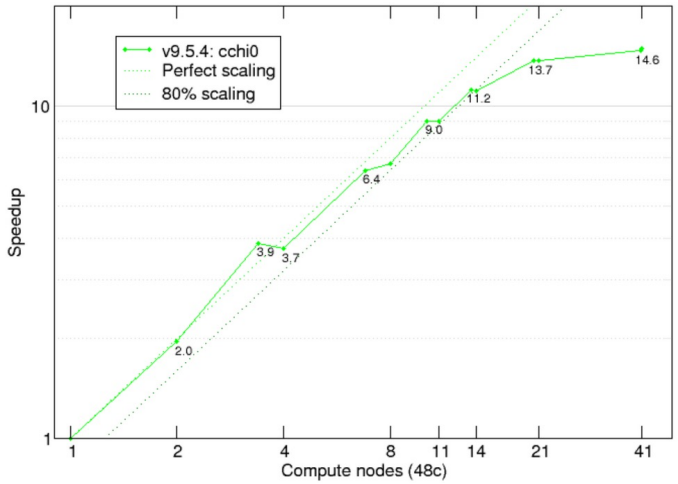
Metadata … to be ignored in the tutorial !

HPC with ABINIT

CPU : MPI + OpenMP parallelism

Ground state DFT calculations
(1) Wavevectors in the BZ + spins + spinors
(2) Band / plane wave
DFPT calculations
(1) Wavevectors in the BZ + spins + spinors
(2) Bands
GW calculations : (old) quartic algorithm
Unoccupied bands
GW calculations : low-scaling algorithm
SEE LATER IN THIS SCHOOL !



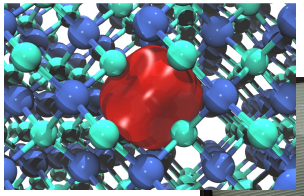


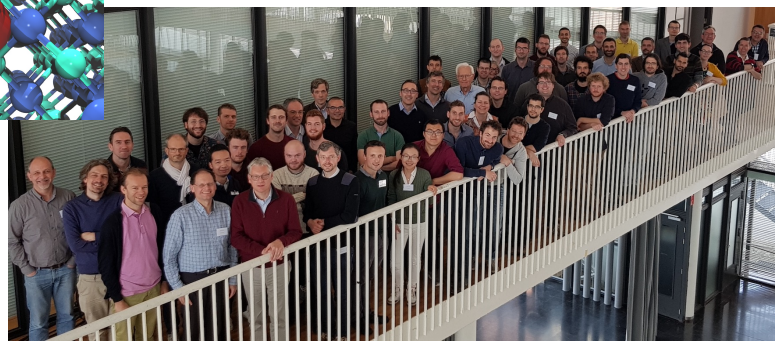
GPU (+CPU)

Ground state DFT calculations
Old (CUDA based – 10 years ago, still working)
New (CUDA/OpenMP, also OpenACC+KOKOS)

Automatic parallelization:
`autoparal 1`

Wrap-up

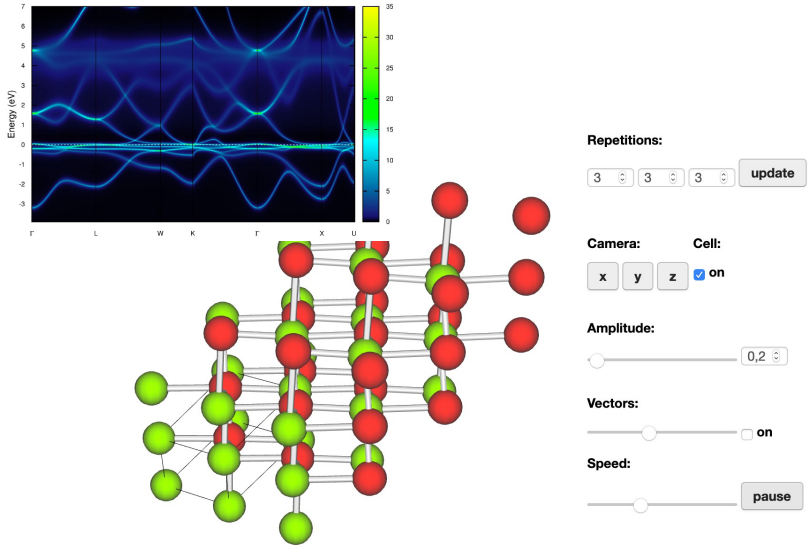




+ ABINIT : open source, many capabilities, well documented, well tested, strong on phonon and electron-phonon properties

+ CPU / GPU

+ DFT / GW / DMFT



Technicalities :
- Plane waves
- Wavevector sampling
- Pseudopotentials

Running ABINIT