FROM RESEARCH TO INDUSTRY

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ABINIT Hands-on 2017

A newcomer-oriented school to ab initio nanoscience simulations

January 30-February 3, 2017 - Bruyères-le-Châtel, France

TUNING ABINIT

SPEED-UP PRECISION CONVERGENCE

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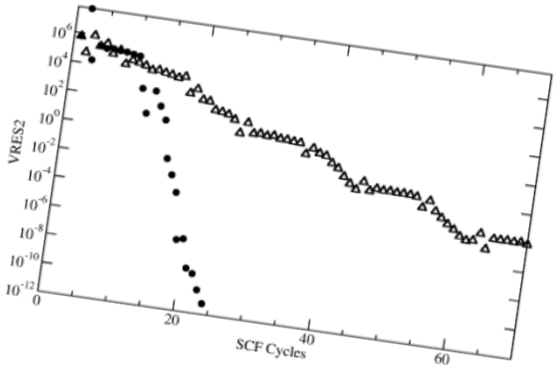



```
accuracy 2
autoparal 1

natom 36
ntypat 3
```

OUTLINE

ABINIT: precision vs speed

- Precision, accuracy, speed
- What can be tuned in a plane-wave DFT code?
- Automatic tuning

Speeding-up ABINIT

- Basics: discretization, size
- Advanced

Helping ABINIT to converge…

- Mixing of the density
- Optimization of the wave-funtctions
- Brillouin zone sampling

ABINIT
PRECISION VS SPEED

PRECISION VS SPEED?

- **Properties needing precision**
  - Fine comparisons of energies
  - Derivatives of the energy: forces, stresses, phonons, pressure…
  - Structural relaxation (forces)
  - Wave-functions in view of excited states/response function
  - Magnetism
  - Etc.
- **Properties needing speed**
  - Molecular Dynamics
  - High-throughput computing (mass calculations)

By default, ABINIT settings favor precision

PRECISION VS ACCURACY

- By tuning the input parameters, you can increase precision…
  - Get more significant digits
  - Increase the size of the basis
  - Do more iterations
  - …
- … not accuracy
  - Calculations (PAW) are supposed to match all-electron calculations, not experiment
  - Precision can be improved by:
    - changing the pseudopotential (change frozen-core)
    - adding more physics in the theory (e.g. *more sophisticated exchange/correlation, exact exchange, …)*
  - …

ACCURACY VS PRECISION

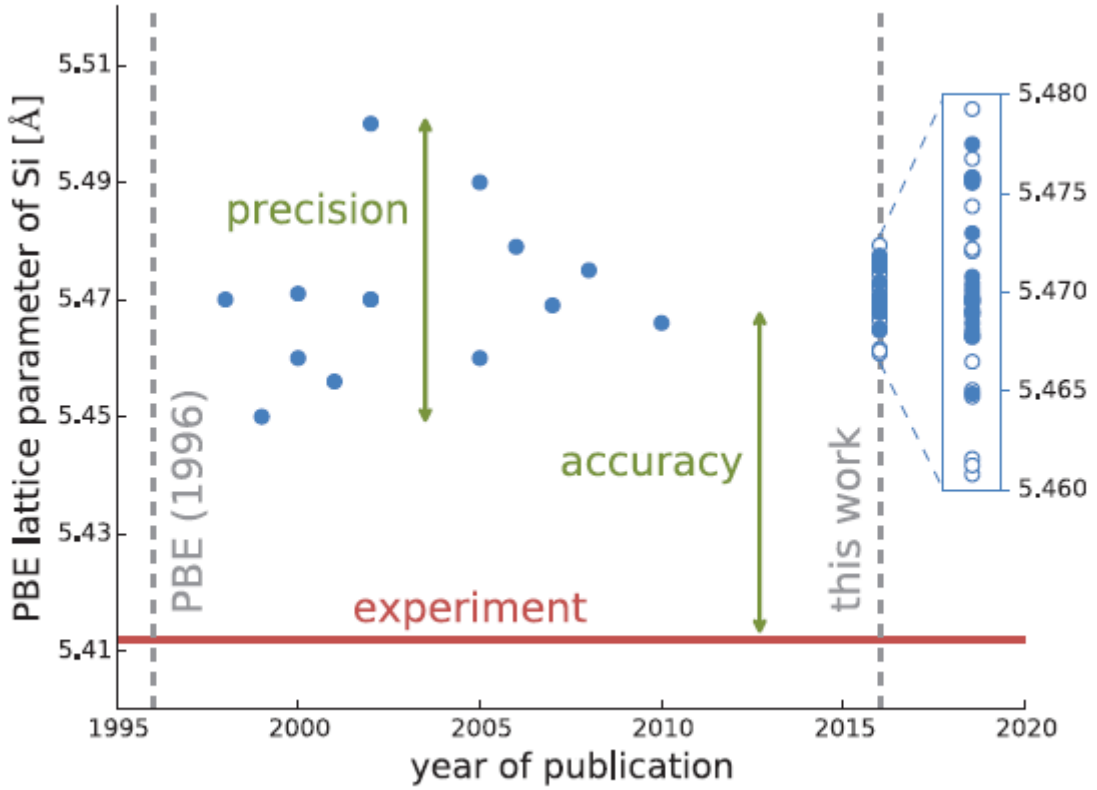


Fig. 1. Historical evolution of the predicted equilibrium lattice parameter for silicon.

Lejaeghere et al., Science 351 (2016)

PRECISION IN DFT CODES - DISCRETISATION

Electronic density formula

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

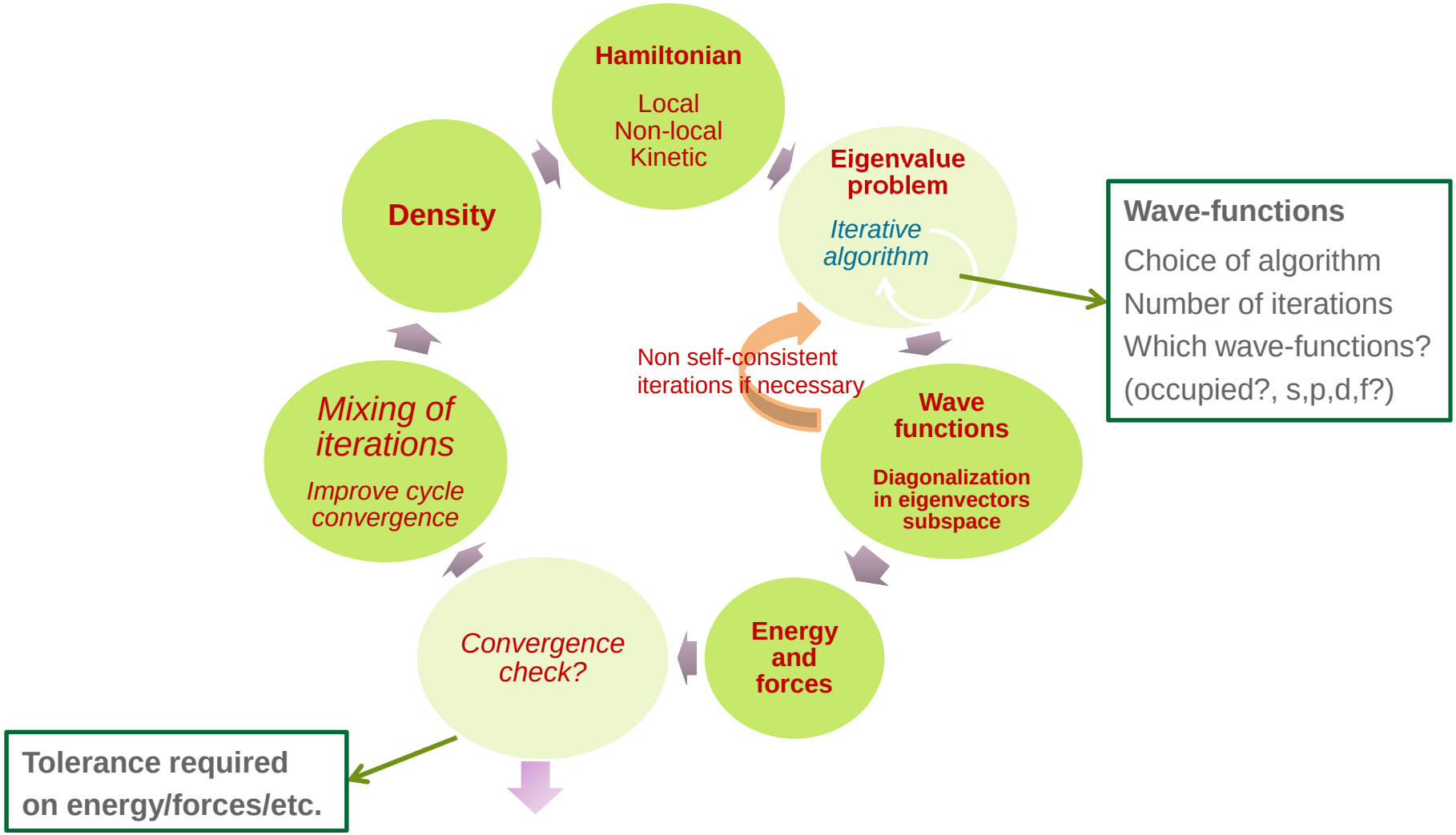
Discretization of reciprocal space
Number of k points
Electronic occupations f_{nk}

Size of the plane wave basis
Determined by the cut-off energy

Discretization of the real space
Number of grid points (FFT grid)

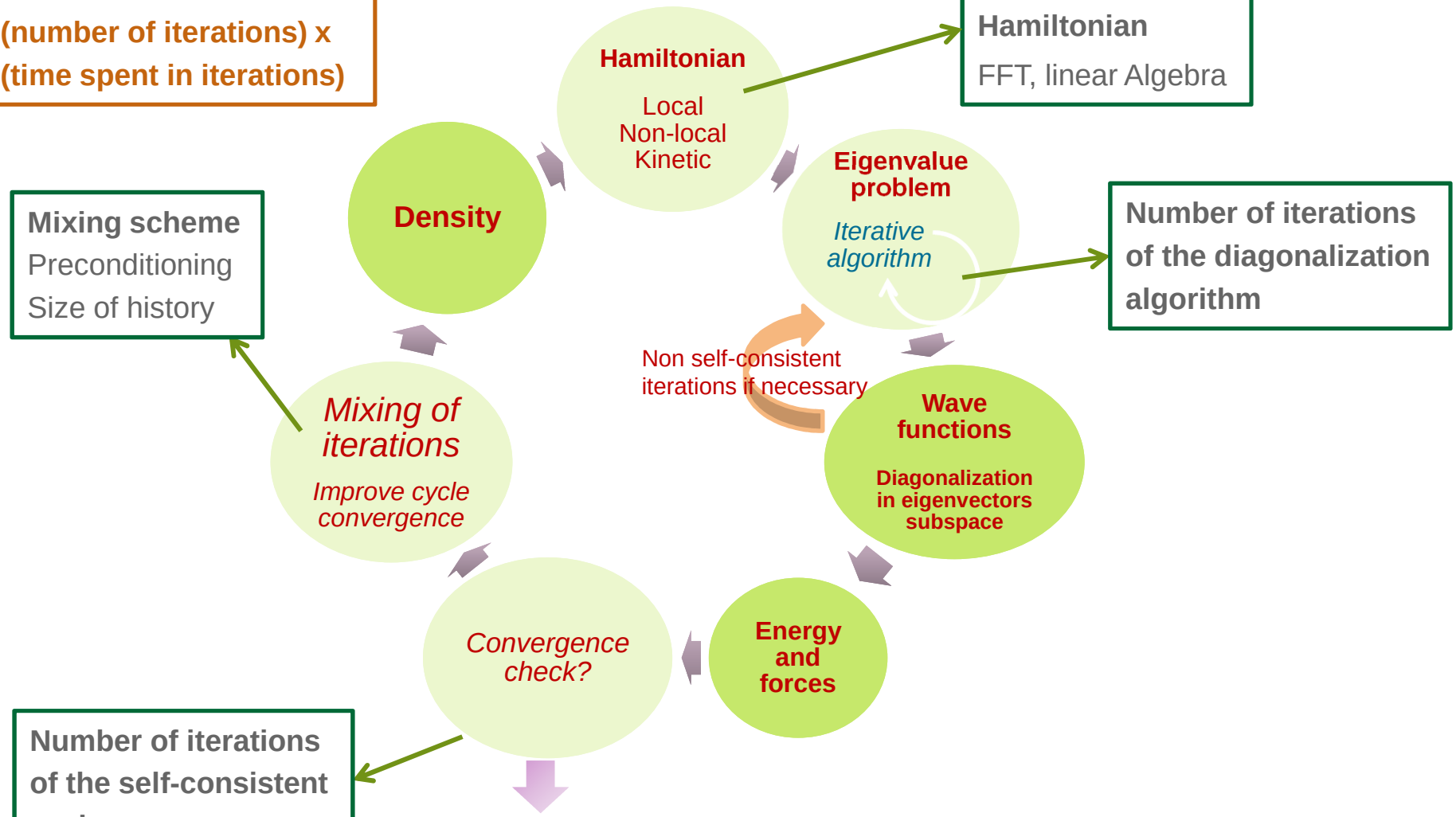
Discretization in numerical schemes, in fitting procedures, etc.

PRECISION IN DFT CODES - CONVERGENCE



PLANE WAVE DFT - WHERE DO WE SPEND TIME?

Time=
(number of iterations) x
(time spent in iterations)



PRECISION VS SPEED - WHAT CAN WE TUNE?

- **Improve speed, decrease precision…**
  - Decrease the cost of the Hamiltonian application
    - Less plane-waves
    - Smaller FFTs
  - Decrease the sampling of the reciprocal space
    - Less k-points
  - Decrease the number of required significant digits
    - Increase the tolerance(s)

…or the contrary

Warning!
Tolerance should always be chosen according to the property of interest

PRECISION VS SPEED - WHAT CAN WE TUNE?

- **Improve speed, without decreasing precision**
  - Use parallelism
  - Decrease the number of empty bands
  - Improve the efficiency of the SCF cycle
    - Improve efficiency of the mixing scheme
    - Decrease the number of iterations
  - Improve the efficiency of the iterative diagonalization
    - Fine tune the parameters of the algorithm

ABINIT TUNING – AUTOMATIC OR MANUAL?

- Automatic tuning - Pros
  - It’s convenient!
  - It’s a good starting point
  - Manual tuning is a challenging task
- Automatic tuning - Cons
  - It is not optimal for all systems
  - Some problem can be hidden

ABINIT – « ACCURACY » INPUT VARIABLE

accuracy

Mnemonics: ACCURACY

Characteristic:

Variable type: integer

Default is 0

Allows to tune the accuracy of a calculation by setting automatically the variables ecut, boxcutmin, fband, tolvrs, tolmxf, optforces, timopt, npulayit, nstep, prteig, prtden, and if usepaw=1, pawecutdg, [illegible]dg, pawxcdev, pawmixdg, pawovlp, pawnhatxc, according to the following table:

accuracy	1	2	3	4	5	6

accuracy=4
Default ABINIT behavior

- **accuracy = 1 : precision is low**
  Intended for use in Molecular Dynamics
- **accuracy = 6 : precision is high**
  Designed to prepare response function calculations

ABINIT – « ACCURACY » INPUT VARIABLE

Default values for plane wave cut-off enregy

- Default values for `ecut` variable can be read from the PAW pseudo potential file
- Only if `accuracy` and PAW are activated
- Only with the "JTH" atomic data table (www.abinit.org)
- 3 default precision values: *low, medium, high*
  Choice made according to `accuracy` input variable
- Values based on the comparison of the pure material Equation of States with all-electron results
- No guarantee for alloys, oxides…
- To activate it: **don't put `ecut` in the input file**

ABINIT – « ACCURACY » INPUT VARIABLE


```
<?xml version="1.0"?>
-<paw_dataset version="0.7">
<atom valence=« 3.00" core="10.00" Z=« 13.00" symbol=« Al"/>
<pw_ecut high="15.00" medium="12.00" low="10.00"/>
<xc_functional name="PBE" type="GGA"/>
<generator name="atompaw-4.0.0.12" type="scalar-relativistic"/>
```

ABINIT – « AUTOPARAL » INPUT VARIABLE

autoparal

Mnemonics: AUTOmatisation of the PARALlelism

Characteristic: DEVELOP

Variable type: integer

Default is 0

This input variable is used only when running ABINIT in parallel and for Ground-State calculations.

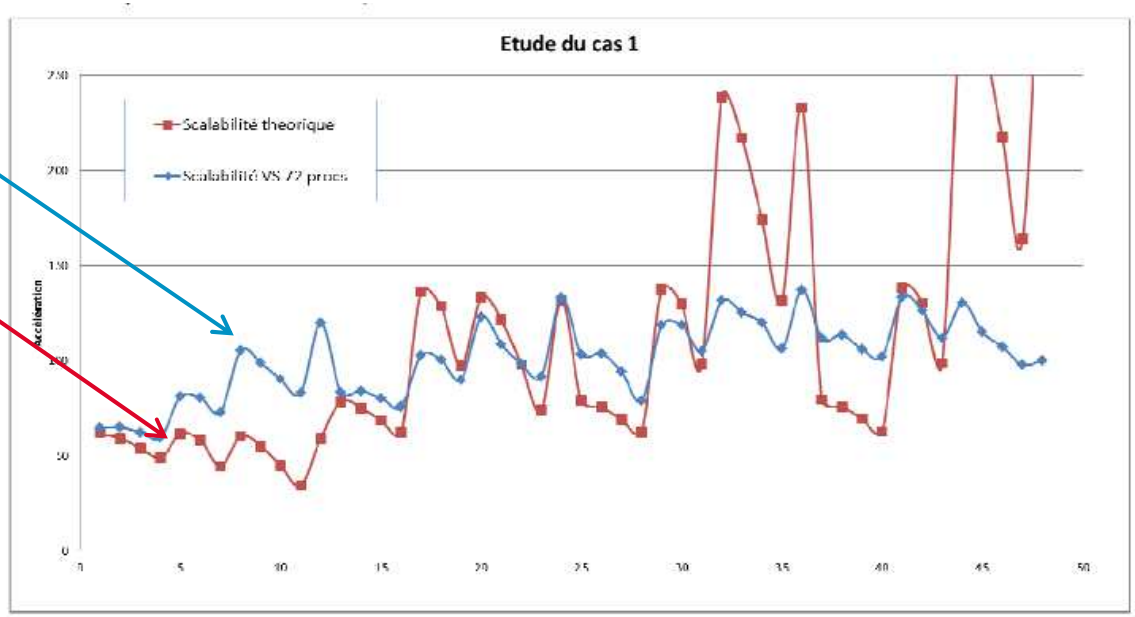
It controls the automatic determination of parameters related to parallel work distribution (if not imposed in input file). Given a total number of processors, ABINIT can find a suitable distribution that fill (when possible) all the different levels of parallelization. ABINIT can also determine

- **autoparal = 1 : automatic parallelization is on**
  ABINIT tries to determine the best distribution of processors on the different parallelization levels taking into account their respective efficient
- A simple heuristics is used

ABINIT – « AUTOPARAL » INPUT VARIABLE

REAL SPEEDUP

PREDICTED SPEEDUP



Overestimation
for FFT parallelism

SPEEDING-UP ABINIT

SPEEDING-UP ABINIT

- **Find the best compromise between**
  - the time required for one SCF iteration
  - the number of iterations

  - Increasing the precision required for one iteration usually decreases the number of iterations
    but takes longer per iteration!

See “Helping ABINIT to converge” section

SPEED-UP ABINIT – BASICS 1

Using parallelism

See lecture on parallelism – See `autoparal` *input variable*

- ABINIT takes fully advantage of the parallelism
- Can be activated even on scalar computers
  Modern “processors” are multicore
- *openMP* (multi-threading) will be very efficient with ABINIT v8.4

Deactivating useless file access

- If you run only Ground-State calculations, wave-function file is not required
- Molecular Dynamics can be restarted without density/wave-functions, etc.
- Some files are used by specific post-processes (ex.: GSR file)

ABINIT input variables

- **`prtwf`**: printing of wave-function (can be deactivated)
- **`prtden`**: printing of wave-function (can be deactivated most of the time)
- **`prtgsr`**: printing of GSR file (can be deactivated if abipy is not used)

SPEED-UP ABINIT – BASICS 2

Discretization

- Decrease the plane-wave basis size
- Decrease the sampling of the Brillouin zone
- Decrease the size of the real space/FFT grid

ecut: PW cut-off energy

ngkpt: k-points sampling

ngfft: size of FFT grid

Size of the system

- Decrease the number of electronic states
  (do not compute useless empty bands)
- Use a suitable pseudopotential
  (do not treat semi-core states when unnecessary)

nband: number of bands

Warnings!

- Always check convergence (don't use rule of thumb)
- Always check convergence with the studied property
- Some parameters depend on the chemical specie, some on the simulation cell

SPEED-UP ABINIT – CONVERGENCE CRITERIA

- **Always check the convergence with the studied properties!**
  - **Energy** – Use tolerance on the total energy (`toldfe`)
    Cohesive energy, barrier, phase stability, etc.
  - **Forces (1)** – Use tolerance on all forces (`toldff / tolrff`)
    Molecular Dynamics
  - **Forces (2)** – Use tolerance on the maximal force precision (`tolmxf`)
    Structural relaxation
  - **Wave-functions** – Use tolerance on the WF residual (`tolwfr`)
    Preparation of excited states runs or response function runs
  - **Other** – Use tolerance on the density/potential residual (`tolvrs`)
    A generalist criterion (good compromise)

    - ABINIT input variables
      - **`toldfe, toldff, tolrff, tolmxf, tolwfr, tolvrs`**:
        Tolerance criteria
        Except for `tolwfr`*, only one criterion can be used*

SPEED-UP ABINIT – ADVANCED 1

Decrease the number of SCF iterations – tuning the mixing

See "Helping ABINIT to converge" section

- Adapt the density/potential mixing to the simulation cell
  Metal, insulator, cristal, inhomogeneous material, collinear magnetism, spin-orbit coupling, etc…
- The numerical behavior of the density during the SCF cycle is highly system dependent
- Number of iterations can be strongly decreased with a tuning of the mixing scheme

ABINIT input variables

- **`diemix`**, **`diemac`**: parameters for density residual preconditioning
- **`iscf, npulayit`**: parameters for density mixing

SPEED-UP ABINIT – ADVANCED 2

Decreasing the size of the real space/FFT grid

$$\rho(\mathbf{r}) = \sum_i |\Psi_i(r)|^2$$

For an exact calculation, if the wave-function Ψ is expressed with all wave vectors up to $\mathbf{G}_{\mathbf{cut}}^2 \leq \mathbf{2E_{cut}}$, density should be expressed with wave-vectors up to $\mathbf{2G_{cut}}$.

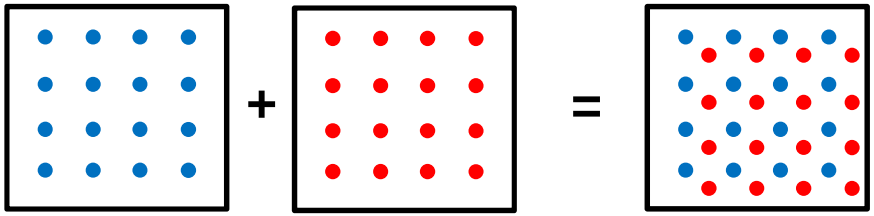
- N_{FFT} for density should be **2x** N_{FFT} for wave-function
- This ratio (`boxcutmin` input variable) can be decreased without a significant loss of precision.
- Always check!
- Not suitable if you prepare excited state or response function…
- **Very efficient on the execution time!**

ABINIT input variables

- **`boxcutmin`**: ratio between wave-function and density FFT grids

SPEED-UP ABINIT – ADVANCED 3

Use shifted k-points grids



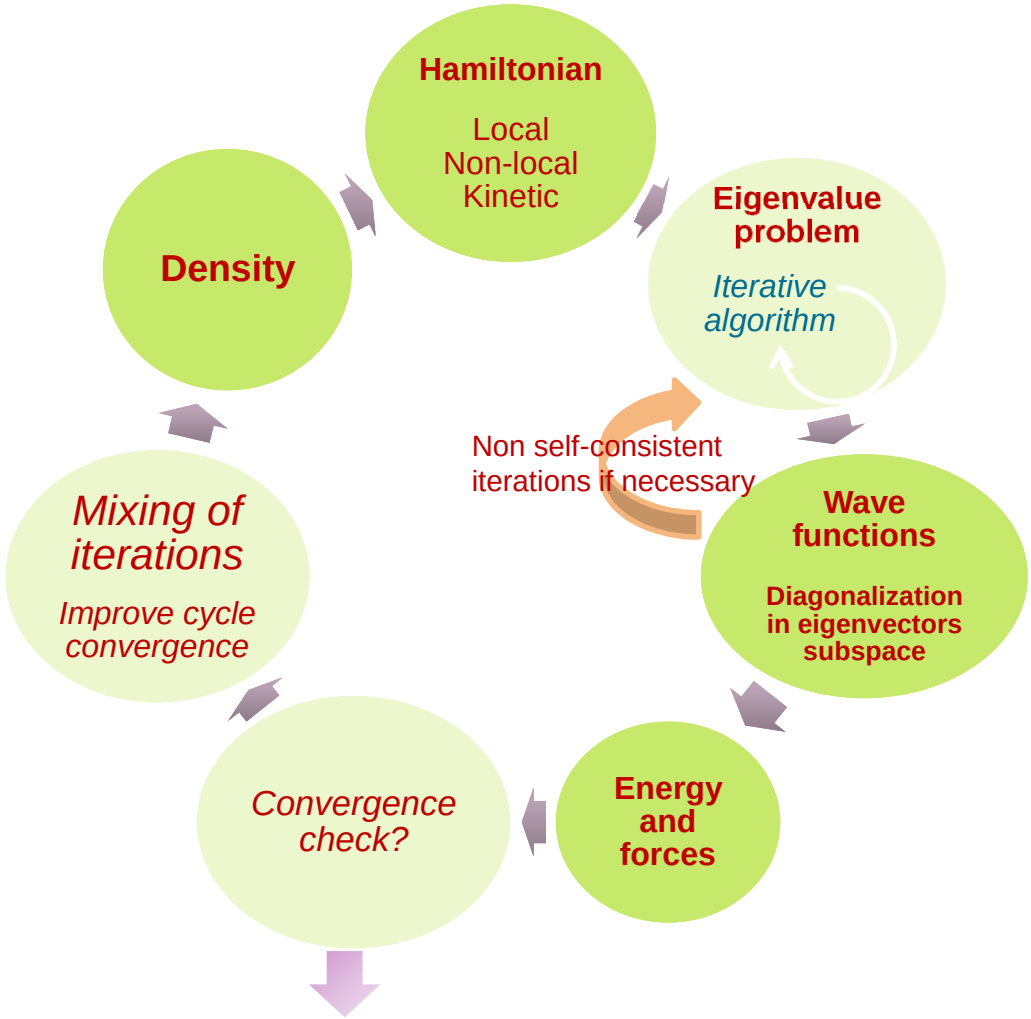
- There are optimal shifts for each Bravais lattice
- Much more efficient and less consuming than increasing the k-point density of one grid

ABINIT input variables

- **`shiftk, nshiftk`**: shifts to be applied to the k-points grid
  Default : one shift (½, ½, ½)

HELPING ABINIT TO CONVERGE

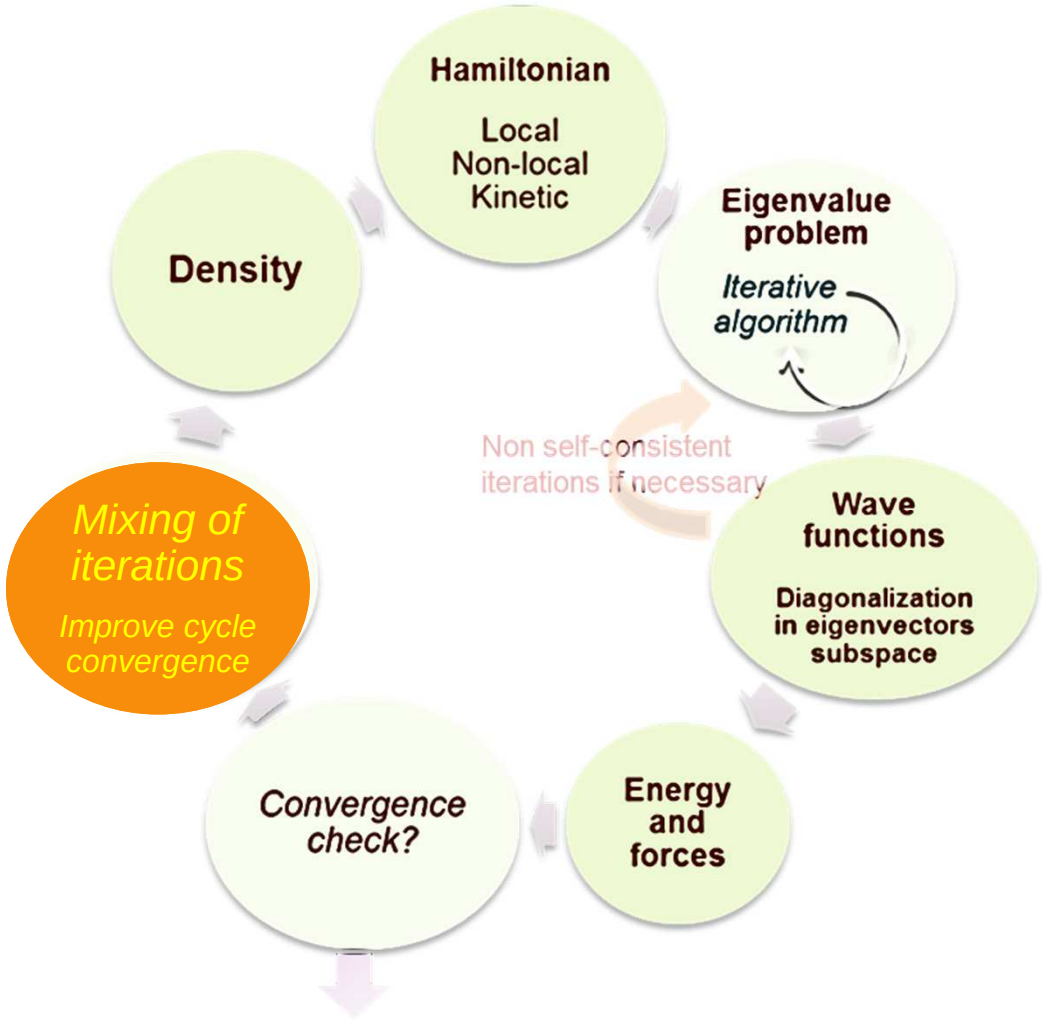
SELF-CONSISTENT CYCLE



SELF-CONSISTENT CYCLE - MIXING

Mixing the density with the densities of previous iterations

=> Damping of the oscillations



MIXING THE DENSITY

Mixing the new iteration and previous one

- Density residual : $\boldsymbol{\rho^{RES}(\mathbf{r}) = \rho^{OUT}(\mathbf{r}) - \rho^{IN}(\mathbf{r})}$
- If no mixing : $\boldsymbol{new\ \rho(\mathbf{r}) = \rho^{IN}(\mathbf{r}) + \rho^{RES}(\mathbf{r}) = \rho^{OUT}(\mathbf{r})}$

- **Preconditioning**

  Applying a transformation to $\boldsymbol{\rho^{RES}(\mathbf{r})}$ in order to damp instabilities

$$\boldsymbol{\rho^{RES}(\mathbf{r}) \leftarrow \mathbf{P}\rho^{RES}(\mathbf{r})}$$

- **Mixing**

  Mixing the new density and previous ones (favor small residuals)

$$\boldsymbol{new\ \rho_{i+1}(\mathbf{r}) = \rho_i^{IN}(\mathbf{r}) + \underset{j \leq i}{\mathbf{mix}}\left[\rho^{OUT}(\mathbf{r}), \mathbf{P}\rho^{RES}(\mathbf{r})\right]}$$

MIXING THE DENSITY – ABINIT INPUT VARIABLES

Preconditioning

Use inverse of a model dielectric matrix

$$\varepsilon = \frac{d\rho}{dV}$$

$$\mathrm{P(K)} = \varepsilon^{-1}(K) = \mathbf{diemix} \cdot \left(\frac{1}{\mathbf{diemac}} + \mathbf{dielng}^2 K^2 \right) / (1 + \mathbf{dielng}^2 K^2)$$

ABINIT input variables

- **`diemix`**: decrease to help convergence (but will slow it)
- **`diemac`**: huge for metals, 5-10 for insulators
- **`dielng`**: not really important (fine tuning)

MIXING THE DENSITY – ABINIT INPUT VARIABLES

Mixing

Can mix density or potential – Default algorithm : Pulay algorithm

Can modify the size of the history (but a large history is memory-consuming)

$$\textit{new}\ \rho_{i+1}(\mathbf{r}) = \rho_i^{IN}(\mathbf{r}) + \underset{j \le i}{\mathbf{mix}}\left[\rho^{OUT}(\mathbf{r}), \mathbf{P}\rho^{RES}(\mathbf{r})\right]$$

$$\textit{new}\ V_{i+1}(\mathbf{r}) = V_i^{IN}(\mathbf{r}) + \underset{j \le i}{\mathbf{mix}}\left[V^{OUT}(\mathbf{r}), \mathbf{P}V^{RES}(\mathbf{r})\right]$$

ABINIT input variables

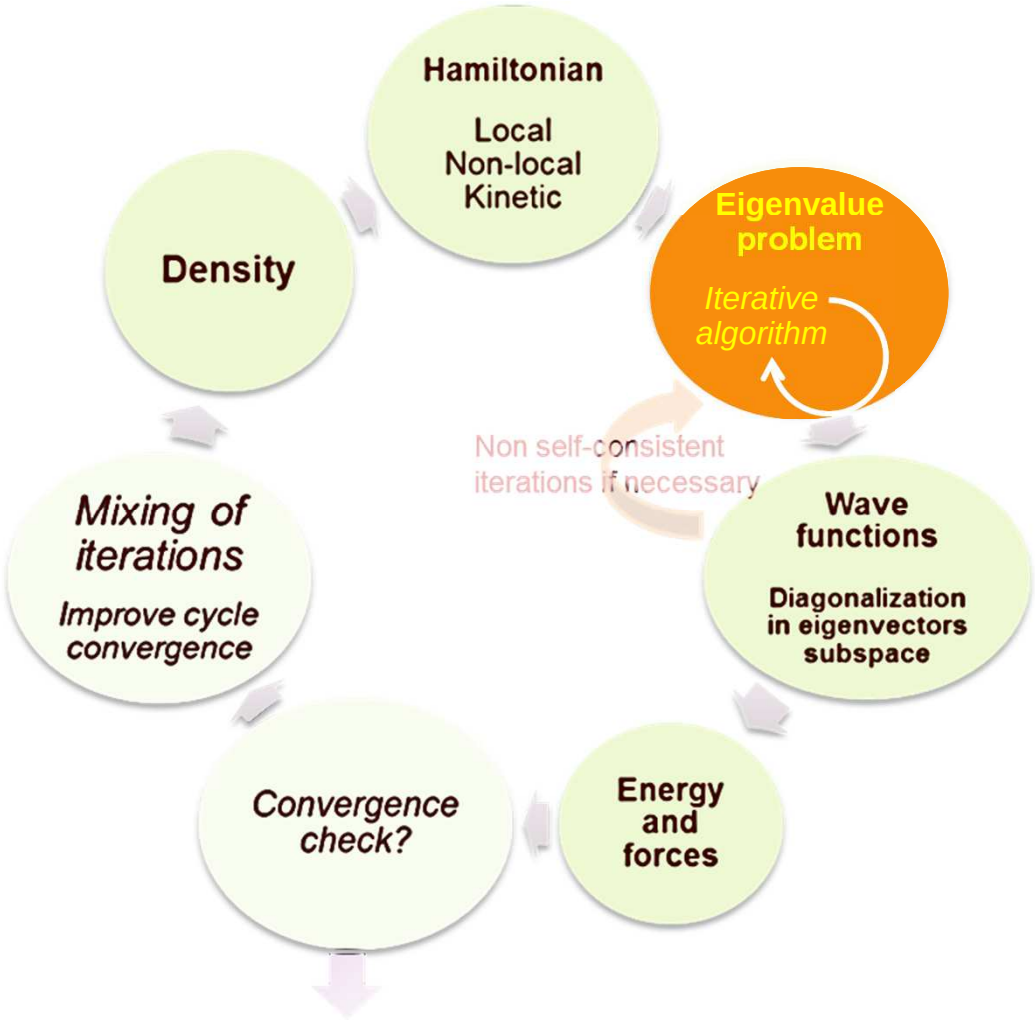
- **`iscf`**: **7** → mix the potential, **17** → mix the density
  Can change the behavior of the convergence
- **`npulayit`**: size of history of Pulay algorithm (default=7)
  Increasing the size can be very efficient (→ 30)

OPTIMIZATION OF WAVE-FUNCTIONS

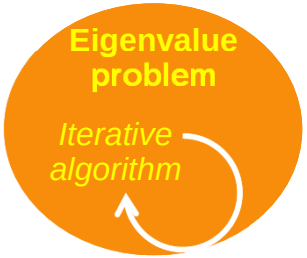
Better converge the wave-functions

=> Can reduce the Number of iterations

=> Each iteration takes more time



OPTIMIZATION OF WAVE-FUNCTIONS ALGORITHM AND PARAMETERS



- Convergence depends on:
  - System of interest
  - Iterative diagonalization(minimization) algorithm

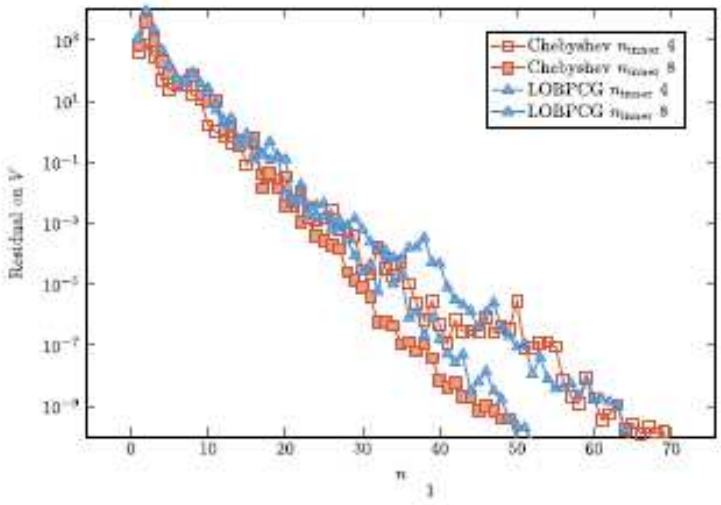


Fig. 6. Self-consistent convergence. The blocksize for LOBPCG was 128.

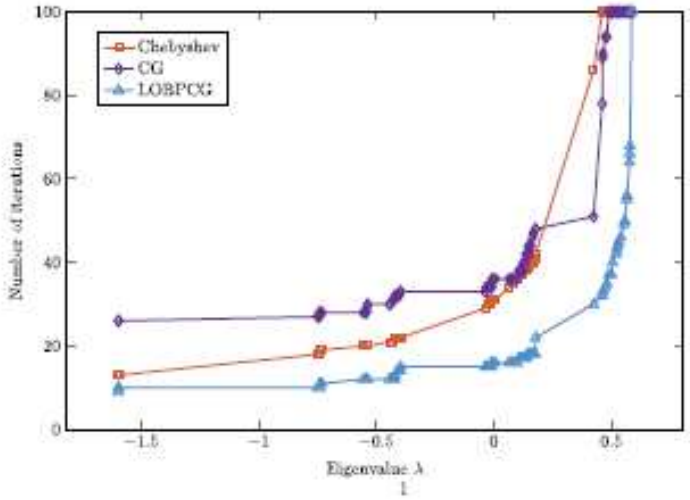
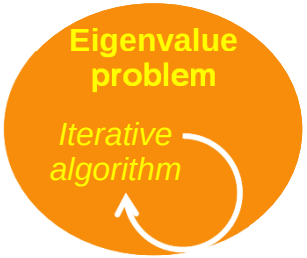


Fig. 4. Number of iterations to obtain a precision of 10^{-10}, $BaTiO_3$, 100 bands.

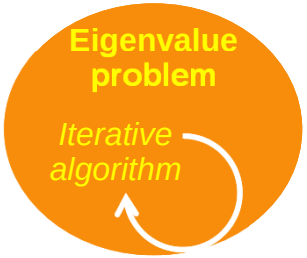
OPTIMIZATION OF WAVE-FUNCTIONS ALGORITHM AND PARAMETERS



- Choice of algorithm
  - **Conjugate Gradient**
    Default when no parallelization or k-points parallelization
  - **Block conjugate gradient** (LOBPCG)
    Default when Band-FFT parallelization
  - **Chebyshev Filtering**
    For a very large number of processors

- ABINIT input variables
  - **`wfoptalg`**: **0** → conjugate gradient
    14 → block conjugate gradient
    1 → Chebyshev filtering

OPTIMIZATION OF WAVE-FUNCTIONS ALGORITHM AND PARAMETERS

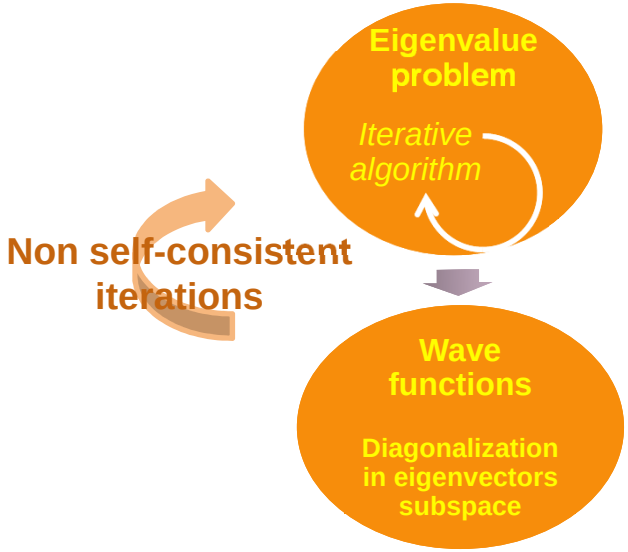


- Algorithm parameters
  - Required tolerance on wave-functions
  - Number of max. iterations
  - Block Conjugate Gradient: size of the blocks
    – One block (size N_{band}) converges better than N_{band} blocks (size 1)
    – But can takes longer

- ABINIT input variables
  - **`tolwfr`**: Tolerance of Wave-Function residual
    Decreasing it improve convergence but takes longer.
  - **`nline`**: number of iterations of the diagonalization algorithm
    Increasing it improves convergence but takes longer
  - **`bandpp`**: Bands Per Proc
    Increase it to increase the size of blocks

OPTIMIZATION OF WAVE-FUNCTIONS NON SELF-CONSISTENT ITERATIONS

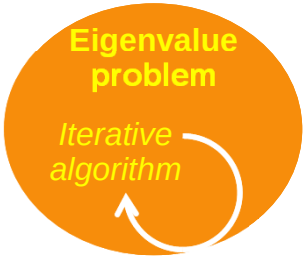
- Last chance if still no convergence…
  - Run the diagonalization algorithm several times, resetting it
  - **Increase the number of Non-Self-Consistent Iterations**

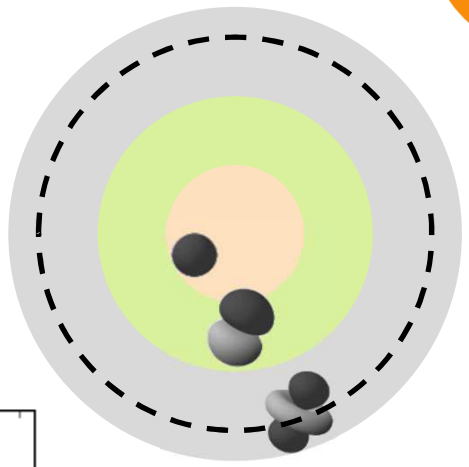


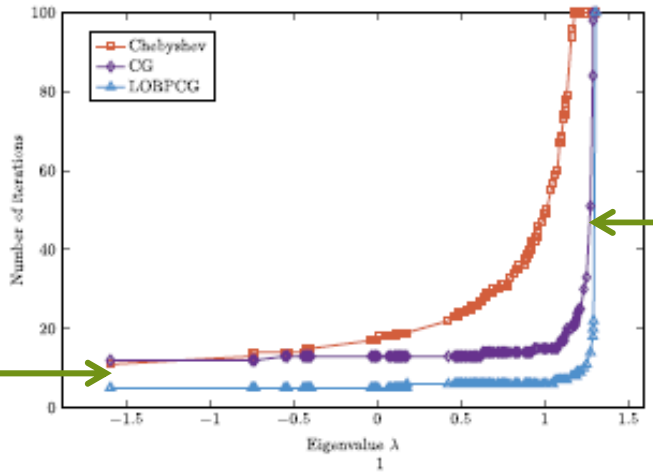
- ABINIT input variables
  - **nnsclo**: Number of Non Self-COnsistent iterations
    Default: 2 iterations for steps 1 and 2, then 1 iteration

OPTIMIZATION OF WAVE-FUNCTIONS EMPTY BANDS (METALS)

- Empty bands do not converge as fast as occupied ones
  - Depends on algorithm (CG, LOBPCG…)
  - Last bands can really not converge
  - Worst case: optimize partially an electron shell







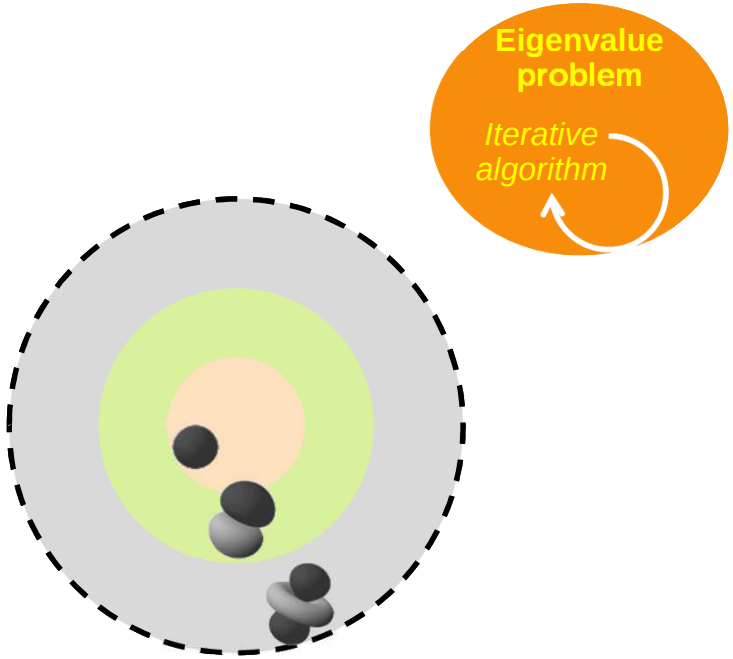
Occupied bands
Few iterations
to converge

Empty bands
Many iterations
to converge

Fig. 5. Number of iterations to get to obtain a precision of 10^{-10}, $BaTiO_3$, 200 bands.

OPTIMIZATION OF WAVE-FUNCTIONS EMPTY BANDS (METALS)

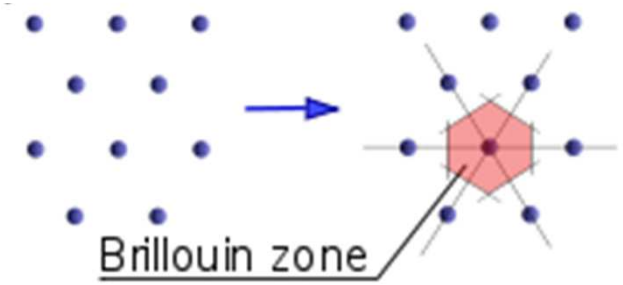
- Solution :
  - Change N_{band} in order to include all the states of the last shell



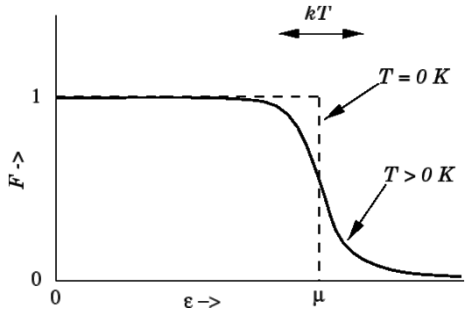
- ABINIT input variables
  - **nband**: Number of BANDs to optimize
    Warning (metals): check that last states are really empty!

METALS OR MAGNETISM – SAMPLING OF BRILLOUIN ZONE

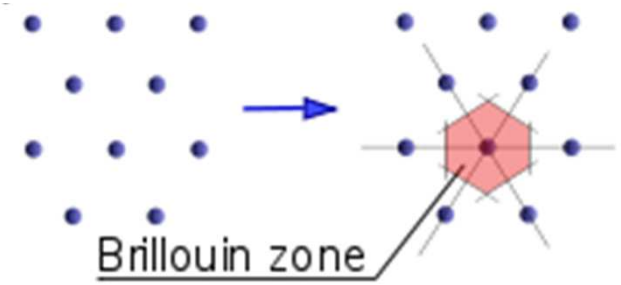
- Impact of sampling of Brillouin Zone:
  - Many properties are obtained from an integral over the Brillouin Zone
  - Magnetic moment is numerically sensitive



- Smearing method:
  - In metals, integral over Brillouin Zone are discontinuous at Fermi level
  - Replace step function by a smoother function:
    $\rightarrow$ use a artificial electronic temperature
  - Modification of the electronic occupations



METALS OR MAGNETISM – SAMPLING OF BRILLOUIN ZONE



- Impact of sampling of Brillouin Zone:
  - Many properties are obtained from an integral over the Brillouin Zone
  - Magnetic moment is numerically sensitive

- Solution:
  - **Find the right balance between smearing and sampling density**

- ABINIT input variables
  - **`nkpt/ngkpt/etc.`**: number of k-points
  - **`occopt`**: smearing scheme for occupations (3<=`occopt`<=7)
  - **`tsmear`**: smearing temperature

CONCLUSION

TUNING ABINIT – KEYS POINTS

- ABINIT default settings favor precision
- To run ABINIT faster, you can use the automatic method or the manual one
- To help ABINIT to converge it is necessary to have a minimal knowledge of the internal algorithms
  - Convergence cycles
  - Mixing algorithms
  - Discretization

Commissariat à l’énergie atomique et aux énergies alternatives

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