

# Density Functional Theory in the *abinit* code

**Gian-Marco Rignanes**

International summer school on  
New trends in computational approaches for many-body systems

Sherbrooke, Québec, Canada

May 28 to June 8, 2012



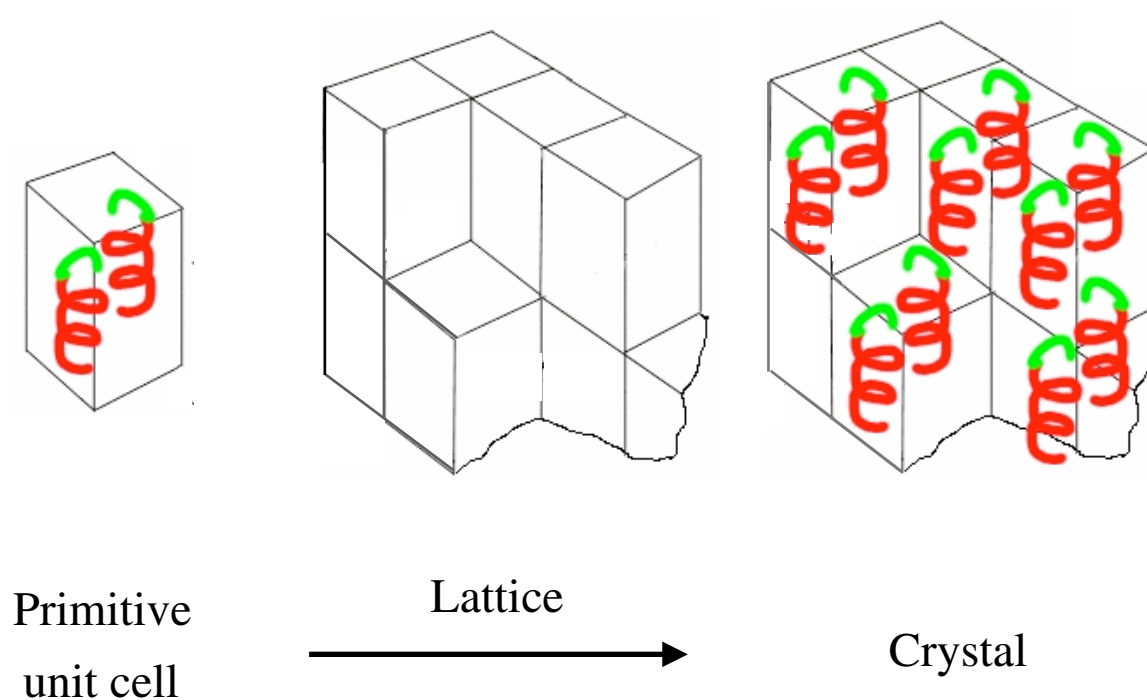
# What is ABINIT?

- ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a plane-wave basis-set [...].
- ABINIT also includes options to optimize the geometry according to the DFT forces and stresses [...].
- Excited states can be computed within the Many-Body Perturbation Theory (the *GW* approximation and the Bethe-Salpeter equation) [...].
- ABINIT is a project that favors development and collaboration.

**Describing the structure  
of the system to be investigated**

# The primitive cell

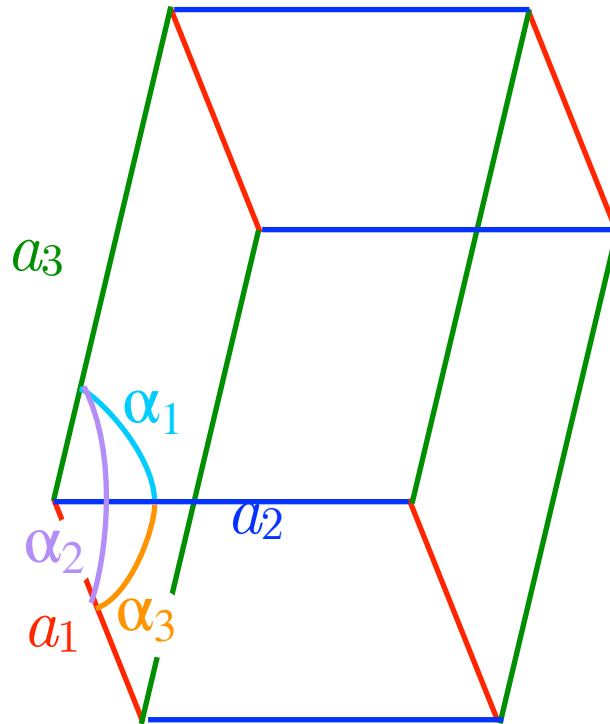
- A crystal is a solid in which the constituent atoms, molecules, or ions are packed in a regularly ordered, repeating pattern (called the primitive cell) extending in all three spatial dimensions.



# The lattice

- The lattice is defined by its primitive vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$  which are independent and such that each point of the lattice can be written as:

$$\mathbf{R} = l \mathbf{a}_1 + m \mathbf{a}_2 + n \mathbf{a}_3 \text{ avec } l, m, n \in \mathbb{Z}$$



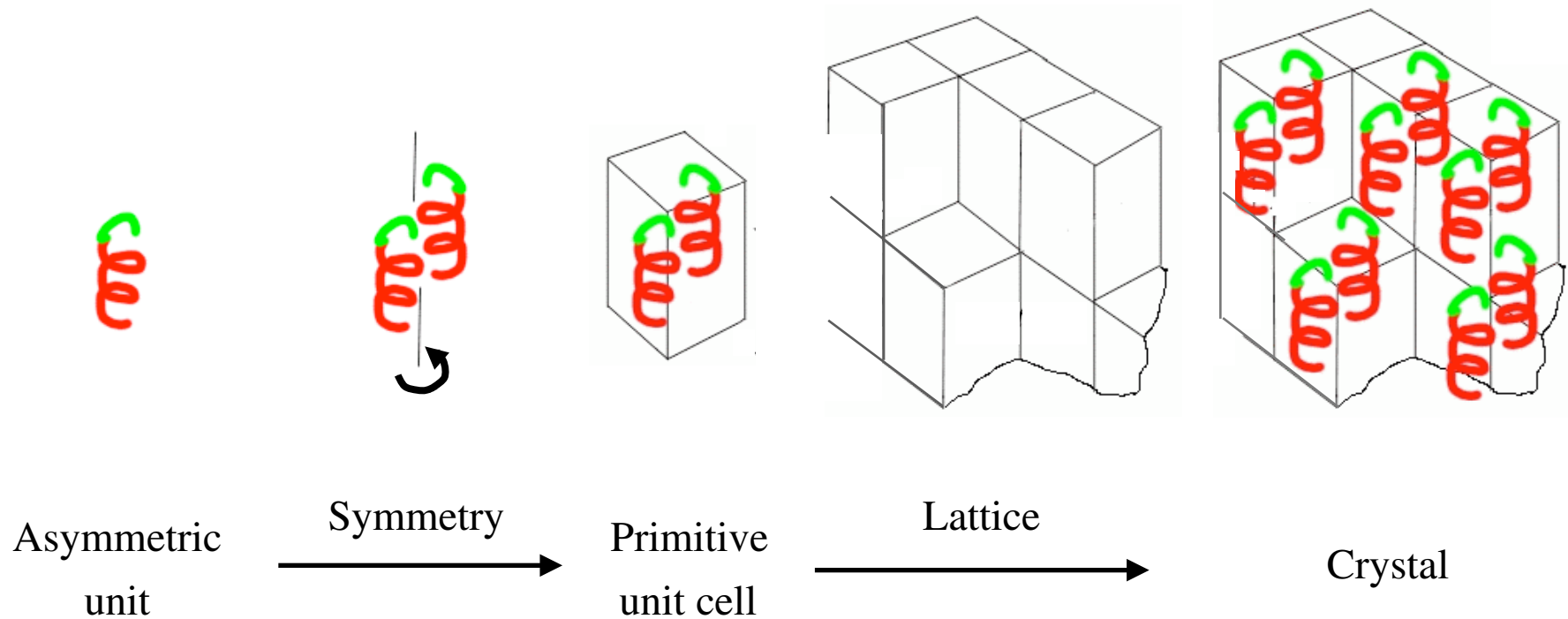
Primitive volume

$$\begin{aligned}\Omega &= \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \\ &= \mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1) \\ &= \mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)\end{aligned}$$

- Examples: triclinic ( $a_1 \neq a_2 \neq a_3$  and  $\alpha_1 \neq \alpha_2 \neq \alpha_3$ )  
cubic ( $a_1 = a_2 = a_3$  and  $\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$ )

# The asymmetric unit

- The asymmetric unit is the smallest part of the cell from which it is possible to built completely the primitive cell applying the symmetry operations of the system (space group).

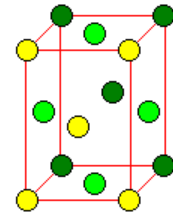


# The primitive vectors in ABINIT

- $a_i(j) \rightarrow rprimd(j,i) = scalecart(j) \times rprim(j,i) \times acell(i)$

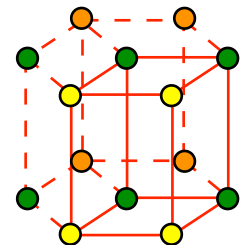
scalecart	9.5000000000E+00	9.8000000000E+00	1.0000000000E+01
rprim	0.0000000000E+00	5.0000000000E-01	5.0000000000E-01
	5.0000000000E-01	0.0000000000E+00	5.0000000000E-01
	5.0000000000E-01	5.0000000000E-01	0.0000000000E+00

face-centered  
orthorhombic



acell	9.5000000000E+00	9.5000000000E+00	1.0000000000E+01
rprim	0.8660254038E+00	5.0000000000E-01	0.0000000000E+00
	-0.8660254038E+00	5.0000000000E-01	0.0000000000E+00
	0.0000000000E+00	0.0000000000E+00	1.0000000000E+00

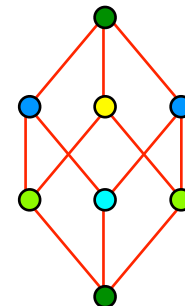
hexagonal



- $a_i \rightarrow acell(i) / \alpha_i \rightarrow angdeg(i)$

acell	9.5000000000E+00	9.5000000000E+00	1.0000000000E+01
angdeg	120	90	90

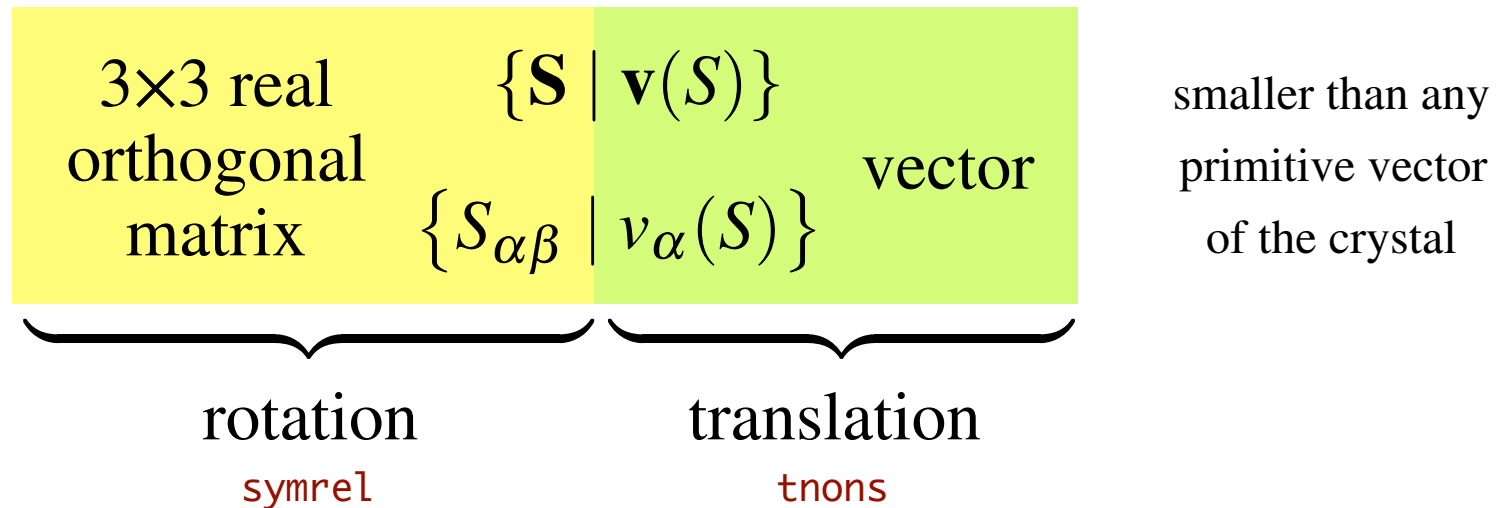
trigonal



acell	9.0000000000E+00	9.0000000000E+00	9.0000000000E+00
angdeg	48	48	48

# The symmetries in ABINIT

- We adopt the **Seitz notation** for the symmetry operations of the crystal:



- Applied to the equilibrium position vector of atom  $\kappa$  relative to the origin of the cell  $\tau_{\kappa}$ , this symmetry transforms it as:

$$\{\mathbf{S} \mid \mathbf{v}(S)\} \tau_{\kappa} = \mathbf{S} \tau_{\kappa} + \mathbf{v}(S) = \tau_{\kappa'} + \mathbf{R}^a$$

$$\{S_{\alpha\beta} \mid v_{\alpha}(S)\} \tau_{\kappa\alpha} = S_{\alpha\beta} \tau_{\kappa\alpha} + v_{\alpha}(S) = \tau_{\kappa'\alpha} + R_{\alpha}^a$$

where  $\mathbf{R}^a$  is a translation vector of the crystal.



# The atomic positions in ABINIT

- number of atoms → `natom`
- reduced coordinates → `xred`
- cartesian coordinates → `xcart` (in Bohr) / `xangst` (in Å)
- type of atoms → `typat`
- space group → `spgroup` + `natred`
- number of symmetries → `nsym`
- symmetry operations → `symrel` + `tions`

# Example 1: c-ZrO<sub>2</sub>

- with WPASSIGN on the Bilbao Crystallographic Server:

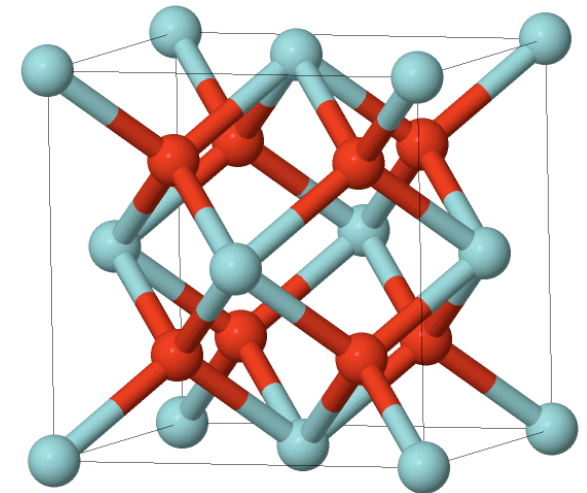
Bilbao Crystallographic Server → Assignment of Wyckoff Positions

## Assignment of Wyckoff Positions

### Atoms Data:

AT.	WP	SS	Representative	Atomic orbit
Zr1	4a (0,0,0)	m-3m	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000) (0.000000,0.500000,0.500000) (0.500000,0.000000,0.500000) (0.500000,0.500000,0.000000)
O2	8c (1/4,1/4,1/4)	-43m	(0.250000,0.250000,0.250000)	(0.250000,0.250000,0.250000) (0.750000,0.750000,0.250000) (0.750000,0.250000,0.750000) (0.250000,0.750000,0.750000) (0.250000,0.250000,0.750000) (0.750000,0.750000,0.750000) (0.250000,0.750000,0.250000) (0.750000,0.250000,0.250000)

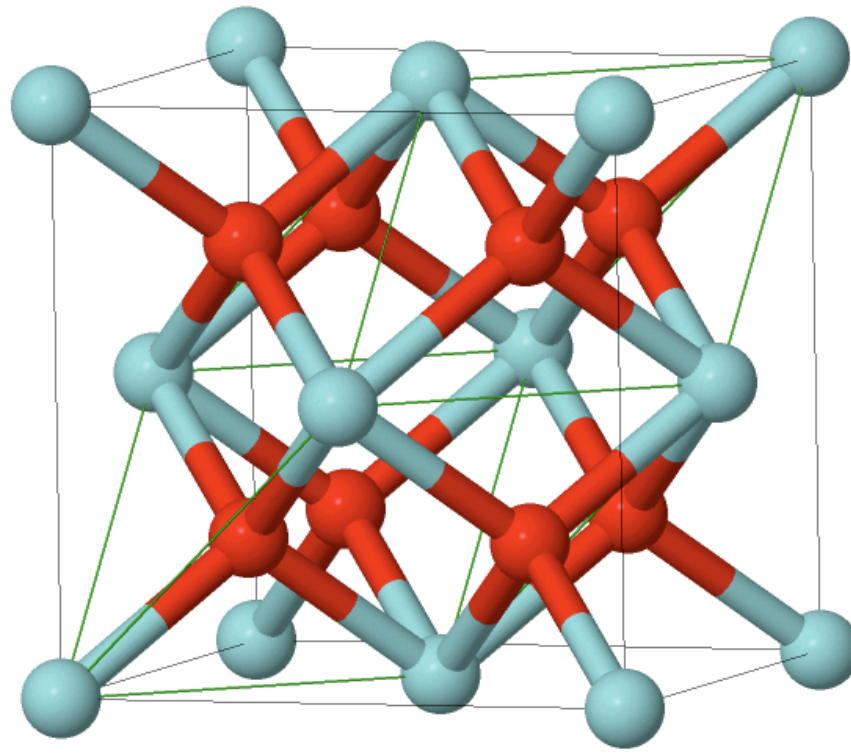
Fm-3m  
a=5.010Å  
b=5.010Å  
c=5.010Å  
α=90.0°  
β=90.0°  
γ=90.0°



# Example 1: c-ZrO<sub>2</sub>

- with ABINIT (input file):

```
natom          3
acell          5.0100000000E+00  5.0100000000E+00  5.0100000000E+00  ANGST
rprim          0.0000000000E+00  5.0000000000E-01  5.0000000000E-01
              5.0000000000E-01  0.0000000000E+00  5.0000000000E-01
              5.0000000000E-01  5.0000000000E-01  0.0000000000E+00
typat          1  2  2
xred           0.0000000000E+00  0.0000000000E+00  0.0000000000E+00
              2.5000000000E-01  2.5000000000E-01  2.5000000000E-01
              -2.5000000000E-01 -2.5000000000E-01 -2.5000000000E-01
```



# Example 1: c-ZrO<sub>2</sub>

- with ABINIT (output file):

Symmetries : space group Fm -3 m (#225); Bravais cF (face-center cubic)

spgroup 225

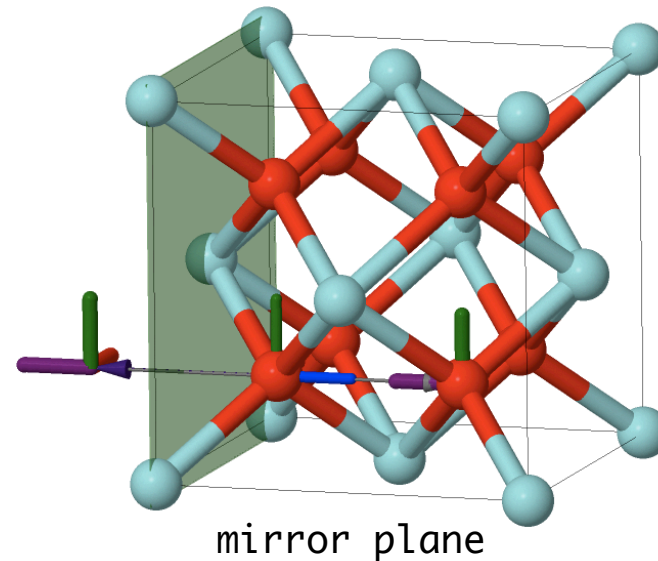
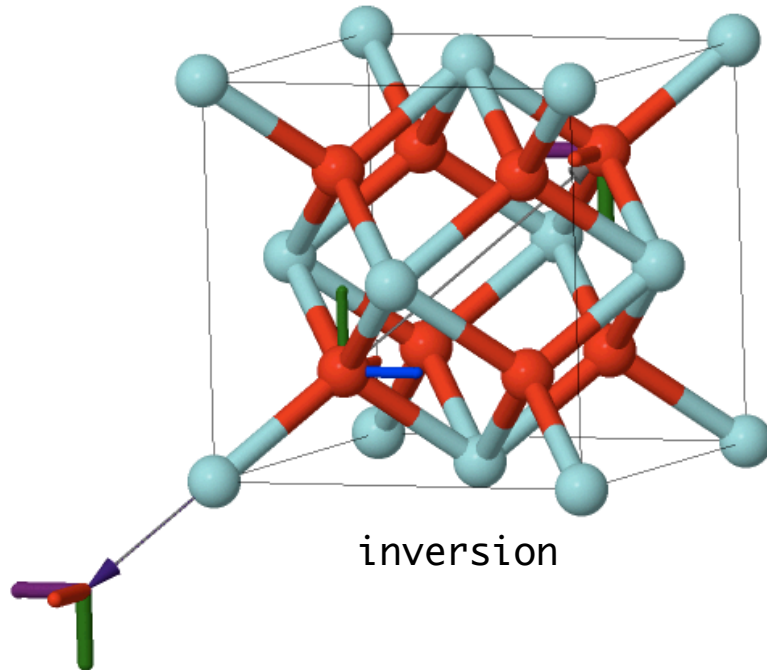
symrel	1	0	0	0	1	0	0	0	1	-1	0	0	0	-1	0	0	0	-1
	0	-1	1	0	-1	0	1	-1	0	0	1	-1	0	-1	1	0	0	0

...

...

0	0	-1	1	0	-1	0	1	-1
-1	1	0	-1	0	1	-1	0	0

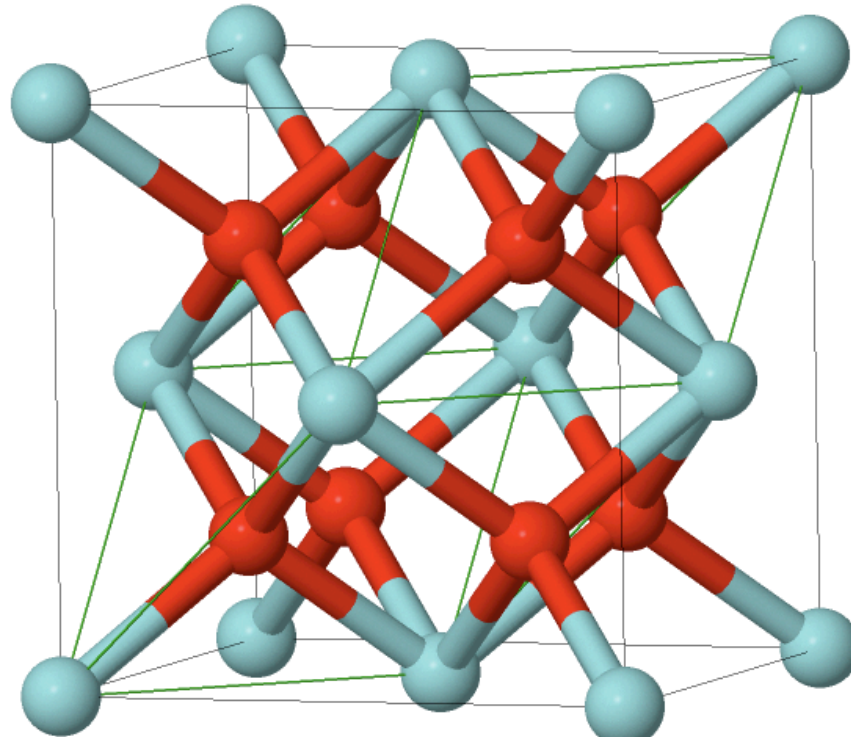
0	0	1	-1	0	1	0	-1	1
1	-1	0	1	0	-1	1	0	0



# Example 1: c-ZrO<sub>2</sub>

- with ABINIT (input file):

```
natom          3
acell  5.0100000000E+00  5.0100000000E+00  5.0100000000E+00  ANGST
rprim   0.0000000000E+00  5.0000000000E-01  5.0000000000E-01
        5.0000000000E-01  0.0000000000E+00  5.0000000000E-01
        5.0000000000E-01  5.0000000000E-01  0.0000000000E+00
typat    1  2  2
spgroup   225
natred    2
xred     0.0000000000E+00  0.0000000000E+00  0.0000000000E+00
        2.5000000000E-01  2.5000000000E-01  2.5000000000E-01
```



# Example 2: Si

- with WPASSIGN on the Bilbao Crystallographic Server:

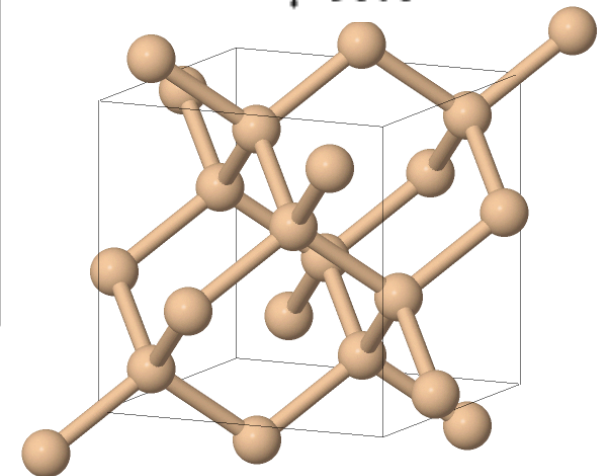
Bilbao Crystallographic Server → Assignment of Wyckoff Positions

## Assignment of Wyckoff Positions

### Atoms Data:

AT.	WP	SS	Representative	Atomic orbit
Si1	8a (1/8,1/8,1/8)	-43m	(0.125000,0.125000,0.125000)	(0.125000,0.125000,0.125000) (0.625000,0.125000,0.625000) (0.125000,0.625000,0.625000) (0.625000,0.625000,0.125000) (0.875000,0.375000,0.375000) (0.875000,0.875000,0.875000) (0.375000,0.375000,0.875000) (0.375000,0.875000,0.375000)

F d 3 m  
 a=5.431Å  
 b=5.431Å  
 c=5.431Å  
 $\alpha=90.0^\circ$   
 $\beta=90.0^\circ$   
 $\gamma=90.0^\circ$



```

natom          2
acell    5.4310000000E+00  5.4310000000E+00  5.4310000000E+00  ANGST
rprim      0.0000000000E+00  5.0000000000E-01  5.0000000000E-01
           5.0000000000E-01  0.0000000000E+00  5.0000000000E-01
           5.0000000000E-01  5.0000000000E-01  0.0000000000E+00
typat       1  1
xred        1.2500000000E-01  1.2500000000E-01  1.2500000000E-01
           8.7500000000E-01  8.7500000000E-01  8.7500000000E-01
  
```

# Example 2: Si

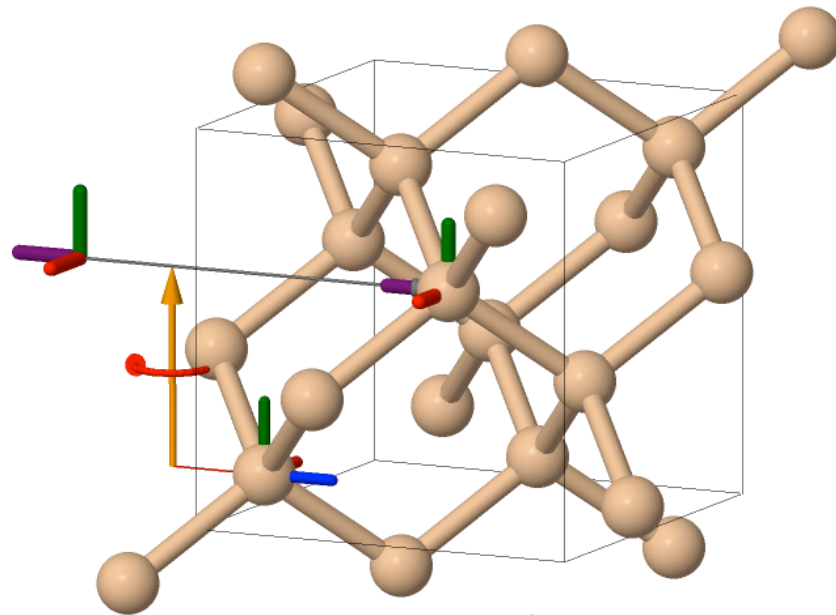
- with ABINIT (input file):

Symmetries : space group Fd -3 m (#227); Bravais cF (face-center cubic)

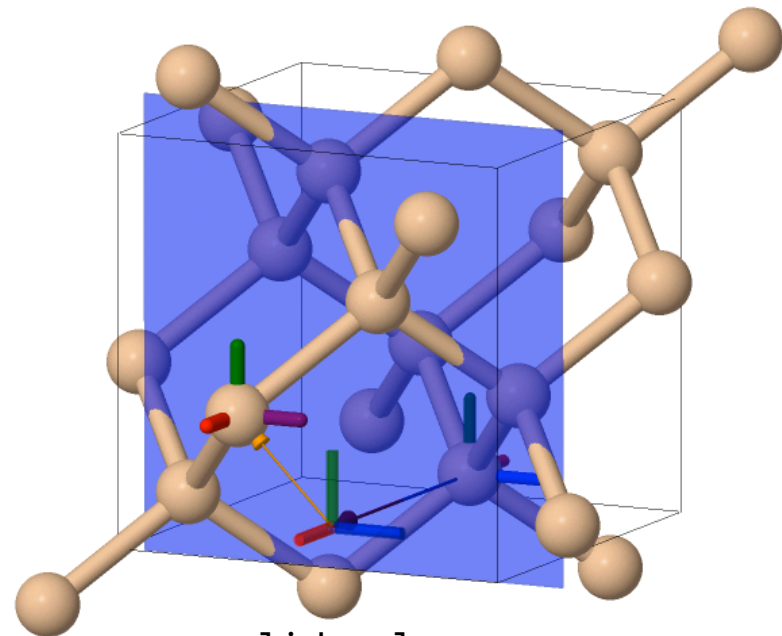
spgroup 227

symrel	1	0	0	0	1	0	0	0	1	-1	0	0	0	-1	0	0	0	-1
	0	-1	1	0	-1	0	1	-1	0	0	1	-1	0	1	0	-1	1	0
...										...								

tions	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	0.5000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.5000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
...										...								



screw axis



glide plane

# The plane-wave basis set



# Treatment of periodic systems

- For periodic systems (with the lattice vectors  $\mathbf{R}$ ), Bloch theorem's states:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \quad \text{with} \quad u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$$

- If we define the reciprocal lattice (with the lattice vectors  $\mathbf{G}$ ), such that:

$$e^{i\mathbf{G}\cdot\mathbf{R}} = 1$$

the periodic part of the Bloch's function can be written:

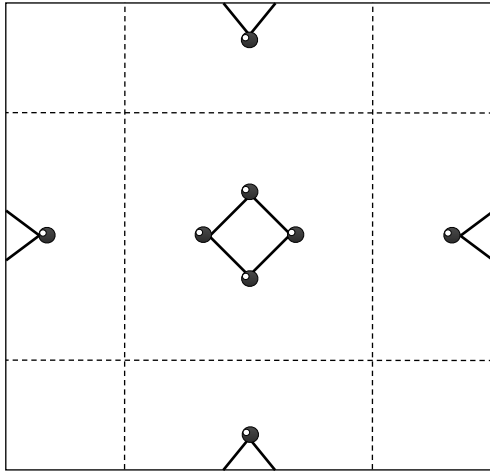
$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} u_{n\mathbf{k}}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}$$

where the coefficients  $u_{n\mathbf{k}}(\mathbf{G})$  are obtained by a Fourier transform:

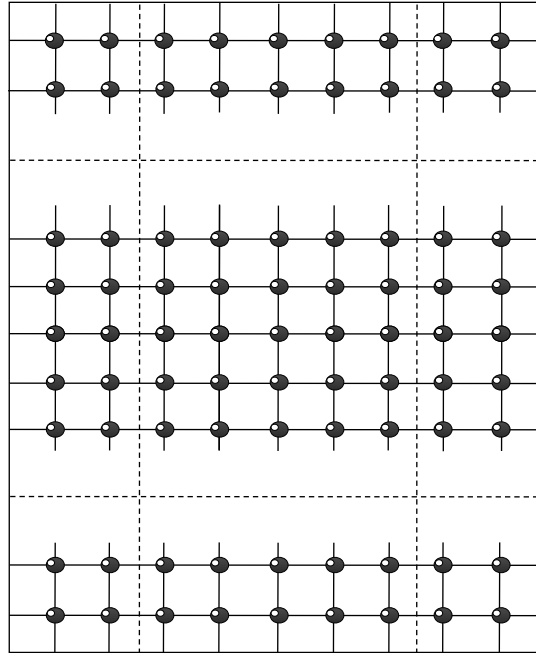
$$u_{n\mathbf{k}}(\mathbf{G}) = \frac{1}{\Omega} \int_{\Omega} u_{n\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} \quad \text{and} \quad \psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} u_{n\mathbf{k}}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

# The supercell technique for non-periodic systems

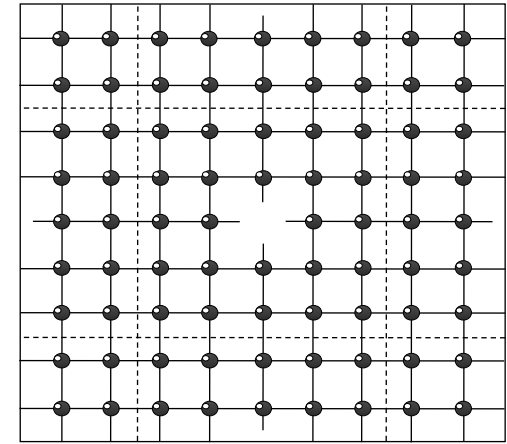
Molecule



Surface



Point defect in a bulk solid



The supercell must be sufficiently big : convergence study

# Kinetic energy cut-off

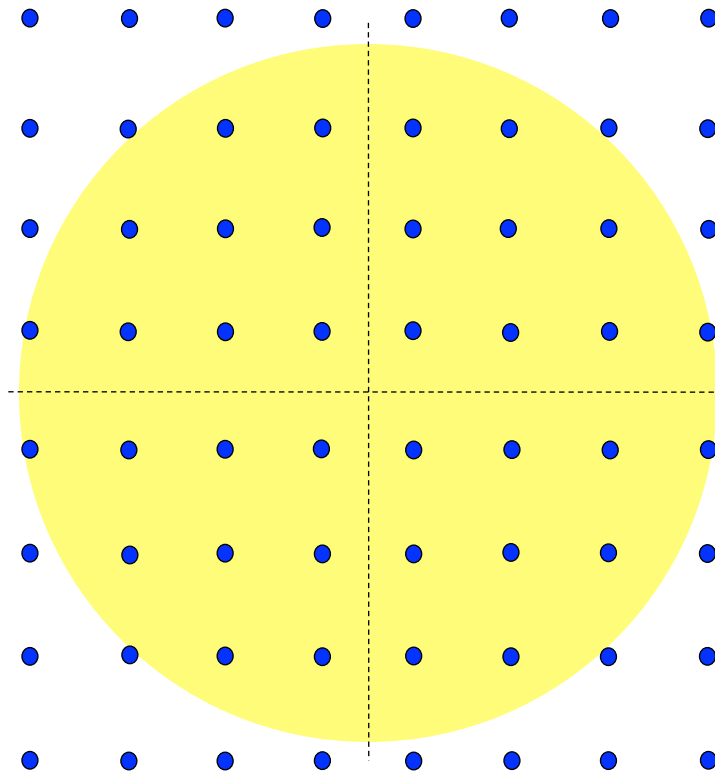
- The coefficients  $u_{n\mathbf{k}}(\mathbf{G})$  for the lowest-energy eigenfunctions decrease exponentially with the kinetic energy  $(\mathbf{k}+\mathbf{G})^2/2$ .
- The plane-waves to be considered in the sum are selected using a kinetic energy cut-off  $E_{cut}$  (which defines the plane-wave sphere):

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

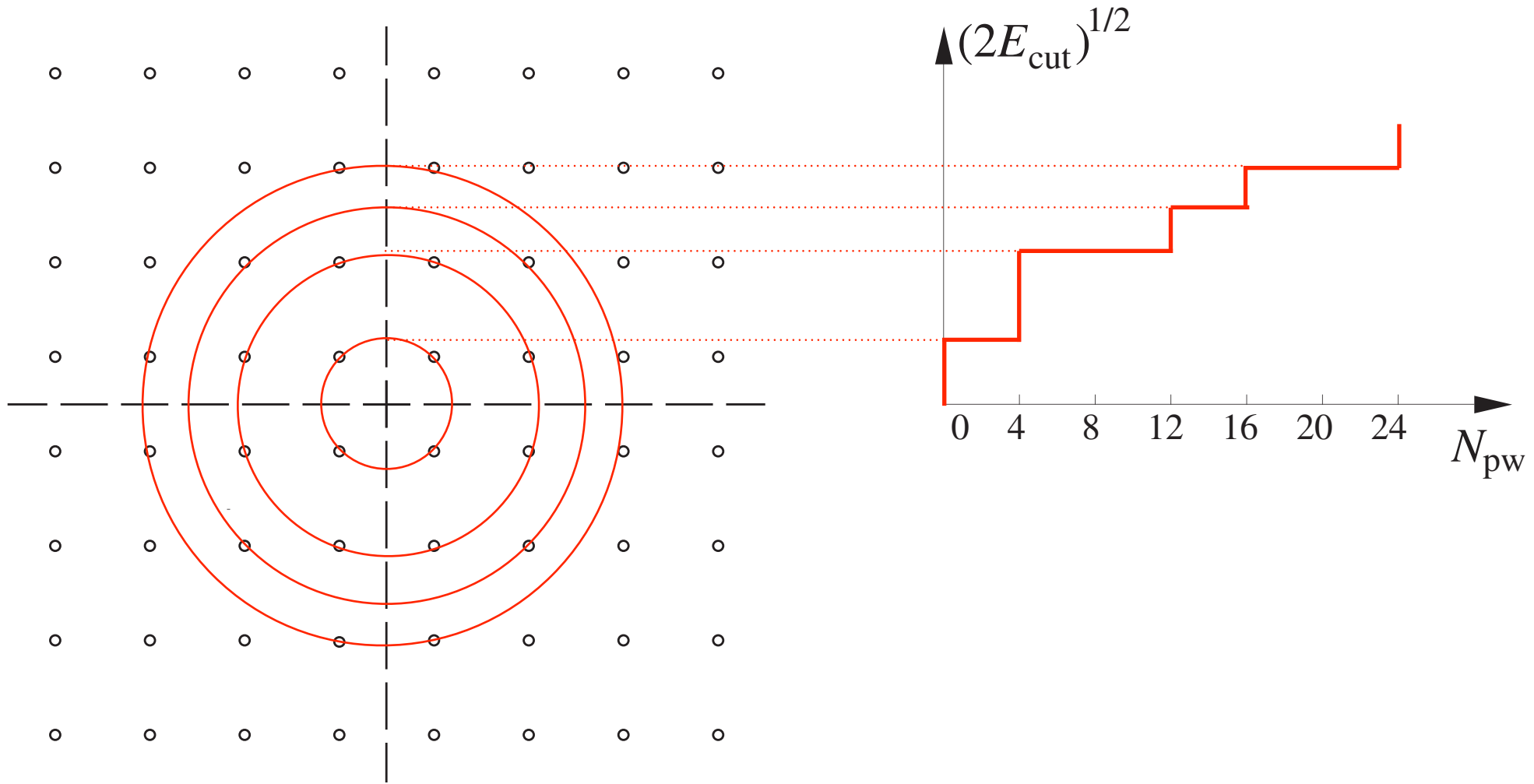
↑

$$-\frac{1}{2} \nabla^2 e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

ecut

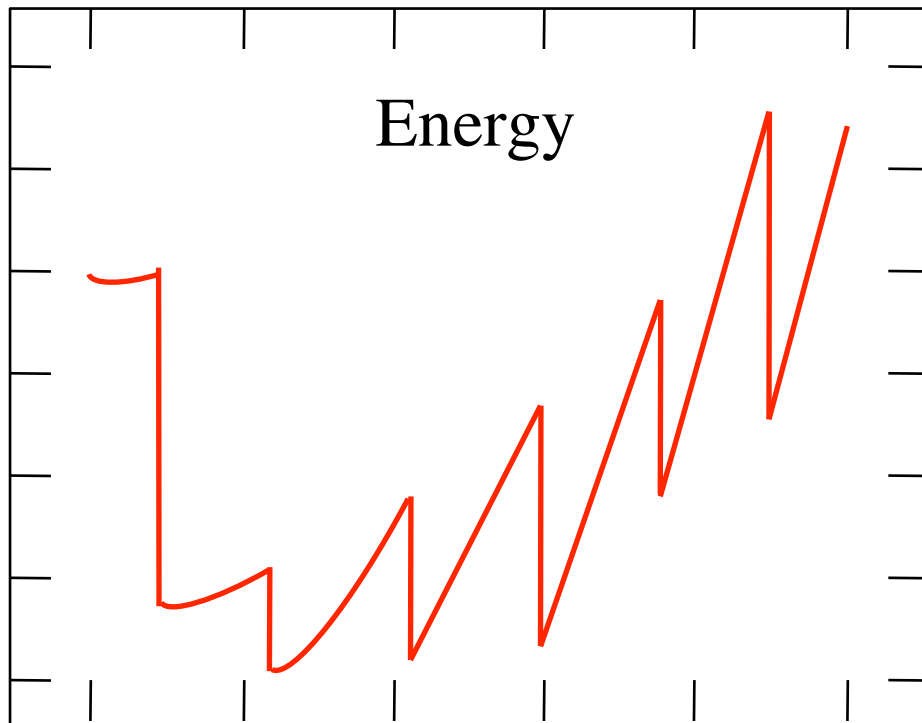


**The number of plane-waves is not a continuous function of the cut-off energy...**

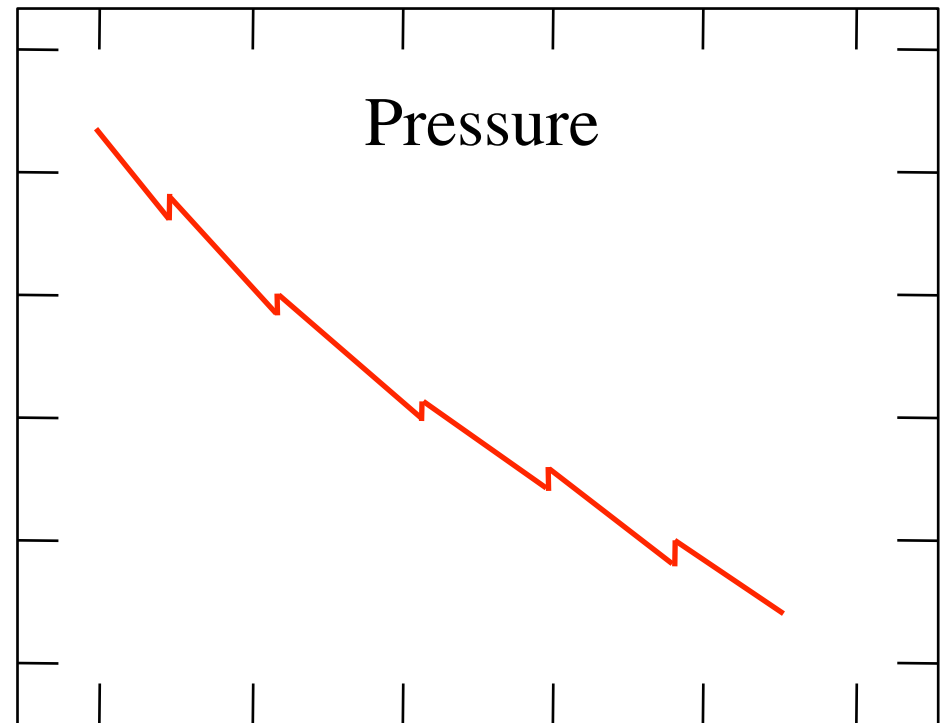


**... nor it is as a function of the lattice parameter**

# There are discontinuities in the pressure and energy curves



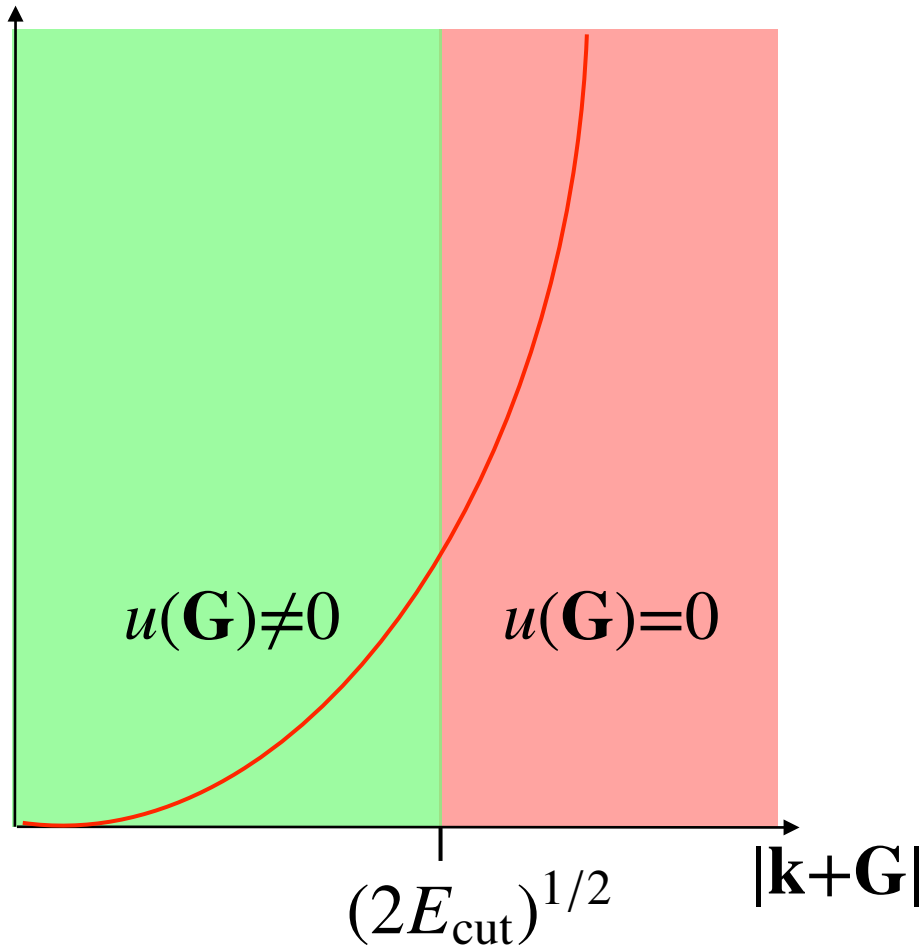
Lattice parameter



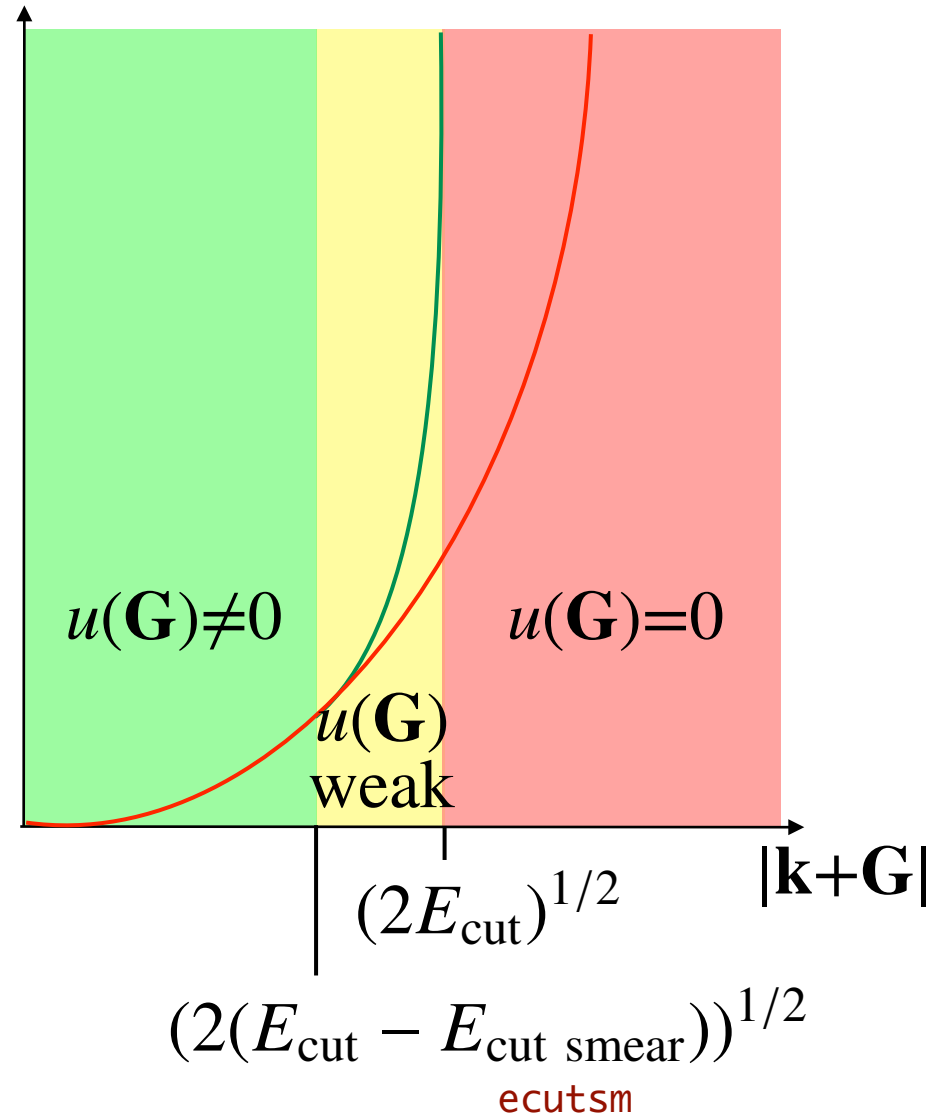
Lattice parameter

# Removal of the discontinuities

Kinetic energy



Kinetic energy



# Plane-waves are a natural and simple basis...

- The Fourier transform theory teaches us that:
  - details in real space are described if their characteristic length is larger than the inverse of the largest wave-vector norm (roughly speaking)
  - the quality of a plane wave basis set can be systematically increased by increasing the cut-off energy
- Problem : huge number of PWs is required to describe localized features (core orbitals, oscillations of other orbitals close to the nucleus)
- Pseudopotentials (or, in general, « pseudization ») are needed to eliminate the undesirable small wavelength features

# Pseudopotentials



# Core and valence electrons (I)

- Idea: Exploit the fact that core electrons occupy orbitals that are the « same » in the atomic environment or in the bonding environment
- Separation between core and valence orbitals for the density:

$$\begin{aligned}n(\mathbf{r}) &= \sum_i^N \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) \\ &= \sum_{i \in \text{core}}^{N_{\text{core}}} \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) + \sum_{i \in \text{val}}^{N_{\text{val}}} \psi_i^*(\mathbf{r})\psi_i(\mathbf{r})\end{aligned}$$

- « Frozen core » approximation: for  $i \in \text{core}$  :  $\psi_i(\mathbf{r}) = \psi_i^{\text{atom}}(\mathbf{r})$   
This approximation obviously influences the accuracy of the calculation !

# Small / large core

- It depends on the target accuracy of the calculation !
- 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:

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

- Gd atom: small core with  $n=1,2,3$  shells, might include  $4s$ ,  $4p$ , and  $4d$  in the core,  $4f$  partially filled

# Core and valence electrons (II)

- Separation between core and valence orbitals for the energy:

$$E_{\text{KS}}[\{\psi_i\}] = \sum_i \langle \psi_i | -\frac{1}{2} \nabla^2 | \psi_i \rangle + \int V_{\text{ext}}(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \frac{n(\mathbf{r}_1) n(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 + E_{\text{xc}}[n]$$

$$\begin{aligned} E_{\text{KS}}[\{\psi_i\}] &= \sum_{i \in \text{core}}^{N_{\text{core}}} \langle \psi_i | -\frac{1}{2} \nabla^2 | \psi_i \rangle + \int V_{\text{ext}}(\mathbf{r}) n_{\text{core}}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \frac{n_{\text{core}}(\mathbf{r}_1) n_{\text{core}}(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 \\ &+ \sum_{i \in \text{val}}^{N_{\text{val}}} \langle \psi_i | -\frac{1}{2} \nabla^2 | \psi_i \rangle + \int V_{\text{ext}}(\mathbf{r}) n_{\text{val}}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \frac{n_{\text{val}}(\mathbf{r}_1) n_{\text{val}}(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 \\ &+ \int \frac{n_{\text{val}}(\mathbf{r}_1) n_{\text{core}}(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 + E_{\text{xc}}[n_{\text{core}} + n_{\text{val}}] \end{aligned}$$

- One needs an expression for the energy of the valence electrons ...

# Valence electrons in a screened potential

- The potential of the nuclei  $\kappa$  is screened by the core electrons:

$$V_{\text{ion},\kappa}(\mathbf{r}) = -\frac{Z_{\kappa}}{|\mathbf{r} - \mathbf{R}_{\kappa}|} + \int \frac{n_{\text{core},\kappa}(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|} d\mathbf{r}_1$$

$$V_{\text{ion},\kappa}(\mathbf{r}) = -\frac{Z_{\text{val},\kappa}}{|\mathbf{r} - \mathbf{R}_{\kappa}|} + \left( -\frac{Z_{\text{core},\kappa}}{|\mathbf{r} - \mathbf{R}_{\kappa}|} + \int \frac{n_{\text{core},\kappa}(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|} d\mathbf{r}_1 \right)$$

- The total energy becomes

$$E = \left( E_{\text{val}} + \sum_{\kappa} E_{\text{core},\kappa} \right) + \frac{1}{2} \sum_{\substack{(\kappa,\kappa') \\ \kappa \neq \kappa'}} \frac{Z_{\text{val},\kappa} Z_{\text{val},\kappa'}}{|\mathbf{R}_{\kappa} - \mathbf{R}_{\kappa'}|}$$

with  $E_{\text{val,KS}}[\{\psi_i\}] = \sum_{i \in \text{val}} \langle \psi_i | -\frac{1}{2} \nabla^2 | \psi_i \rangle + \int \left( \sum_{\kappa} V_{\text{ion},\kappa}(\mathbf{r}) \right) n_{\text{val}}(\mathbf{r}) d\mathbf{r}$

$$+ \frac{1}{2} \int \frac{n_{\text{val}}(\mathbf{r}_1) n_{\text{val}}(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 + E_{\text{xc}}[n_{\text{core}} + n_{\text{val}}]$$

Non-linear XC core correction

# Removing core electrons (I)

- The valence orbitals must still be orthogonal to core orbitals  
⇒ oscillations, slope at the nucleus, ...
- Pseudopotentials try to remove completely the core orbitals from the simulation by removing the strong changes within a « cut-off radius »

( $r < r_{\text{cut}}$ ):

$$\left(-\frac{1}{2}\nabla^2 + V\right) |\psi_i\rangle = \epsilon_i |\psi_i\rangle$$

$$\left(-\frac{1}{2}\nabla^2 + V_{\text{ps}}\right) |\psi_i^{\text{ps}}\rangle = \epsilon_i^{\text{ps}} |\psi_i^{\text{ps}}\rangle$$

with  $V_{\text{ps}}(\mathbf{r})$  smooth for  $r < r_{\text{cut}}$  and  $V_{\text{ps}}(\mathbf{r}) = V_{\text{ion}}(\mathbf{r})$  for  $r \geq r_{\text{cut}}$

$\psi_i^{\text{ps}}(\mathbf{r})$  smooth for  $r < r_{\text{cut}}$  and  $\psi_i^{\text{ps}}(\mathbf{r}) = \psi_i(\mathbf{r})$  for  $r \geq r_{\text{cut}}$

$$\frac{d\psi_i^{\text{ps}}(\mathbf{r})}{d\mathbf{r}} = \frac{d\psi_i(\mathbf{r})}{d\mathbf{r}} \text{ for } r = r_{\text{cut}} \text{ and } \epsilon_i^{\text{ps}} = \epsilon_i$$

# Removing core electrons (II)

- Various conditions can be imposed: e.g. norm conservation

[D.R. Hamann, M. Schlüter, and C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979)]

$$\int_{r < r_{\text{cut}}} |\psi_i^{\text{ps}}(\mathbf{r})|^2 d\mathbf{r} = \int_{r < r_{\text{cut}}} |\psi_i(\mathbf{r})|^2 d\mathbf{r}$$

- The general form of pseudopotential acts on the wavefunctions as follows:

$$\langle \mathbf{r} | V_{\text{ps}} | \psi \rangle = \int v_{\text{ps}}(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}'$$

kernel

with  $v_{ps}(\mathbf{r}, \mathbf{r}') = v_{\text{loc}}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') + v_{\text{NL}}(\mathbf{r}, \mathbf{r}')$

and  $v_{\text{NL}}(\mathbf{r}, \mathbf{r}') = \sum_{l,m} Y_{l,m}^*(\theta, \phi) v_{\text{NL},l}(r, r') Y_{l,m}(\theta', \phi')$

# Forms of pseudopotentials

- The most widely used pseudopotentials belong to two different classes:

- the semi-local pseudopotentials for which:

$$v_{\text{NL},l}(r, r') = v_{\text{SL},l}(r)\delta(r - r')$$

[G.B. Bachelet, D.R. Hamann, and M. Schlüter, Phys. Rev. B **26**, 4199 (1982)]

- the separable pseudopotentials for which:

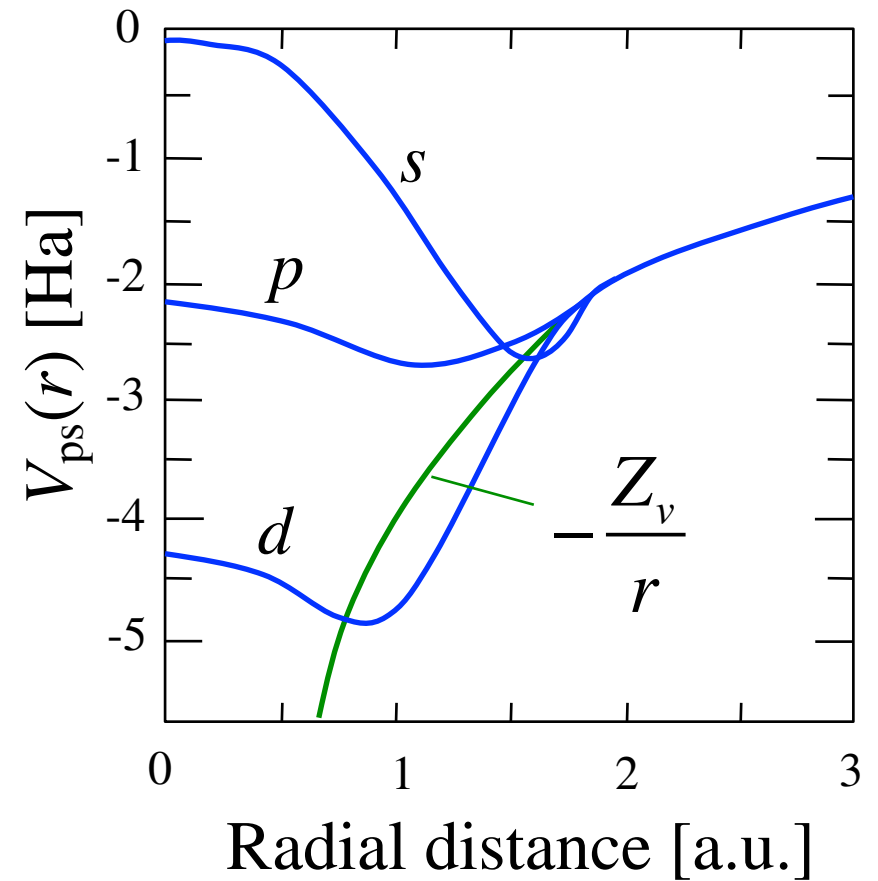
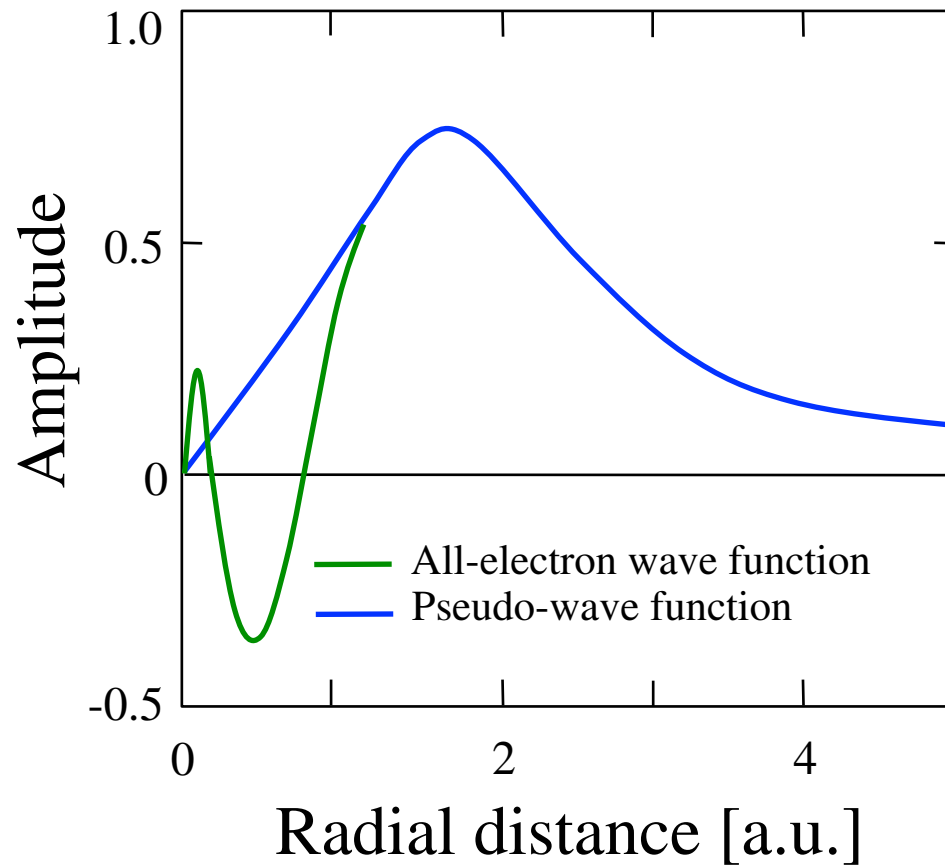
$$v_{\text{NL},l}(r, r') = \xi_l^*(r) f_l \xi_l(r')$$

[L. Kleinman and D.M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982)]

- Semi-local pseudopotentials are easily visualized, but separable ones are definitely more powerful for numerical techniques.
- A technique was introduced to transform semi-local pseudopotentials into a separable form (caution: ghost states may appear).

# Example of pseudopotential

## 3s Radial wave function of Si





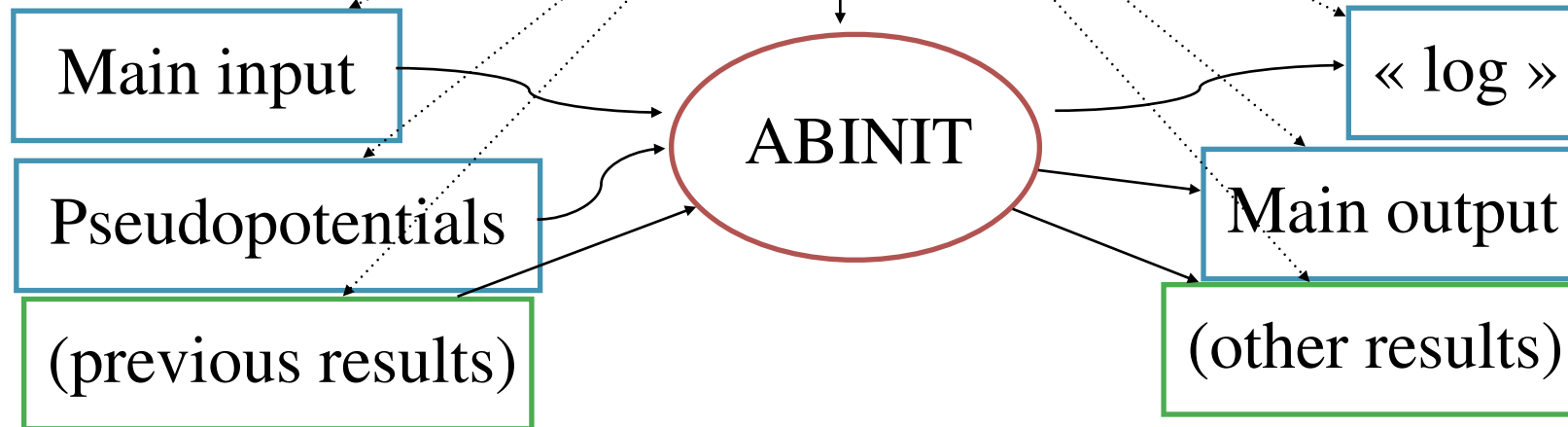
# External files in a ABINIT run

prompt:> abinit < t1x.files >& log

Example of "Filenames" file:

Filenames

```
../t11.in  
t1x.out  
t1xi  
t1xo  
t1x  
../../../../Pspgth
```



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

# **The ABINIT software project**

# What is ABINIT ?

- It is a software that allows one to perform **first-principles calculations** in the framework of:
  - **Density-Functional Theory (DFT)** → **ground-state**  
[P. Hohenberg & W. Kohn, Phys. Rev. **136**, B864 (1964);  
W. Kohn & L.J. Sham, Phys. Rev. **140**, A1133 (1965)]
  - **Many-Body Perturbation Theory (MBPT)** → **excited-states**  
[L. Hedin, Phys. Rev. **139**, A796 (1965);  
G. Onida, L. Reining, & A. Rubio, Rev. Mod. Phys. **74**, 601 (2002)]
  - **Density-Functional Perturbation Theory (DFPT)** → **response**  
[S. Baroni *et al.*, Rev. Mod. Phys. **73**, 515 (2001);  
X. Gonze, Phys. Rev. B **55**, 10337 (1997);  
X. Gonze and C. Lee, Phys. Rev. B **55**, 10355 (1997)]

# ABINIT v6 capabilities (I)

- **Basis sets**
  - planewaves
  - projector augmented waves (PAW)
  - wavelets (BIGDFT effort)
- **Representation of atoms:**
  - many pseudopotential types
  - different PAW generators
- **Exchange-correlation functionals for DFT:**
  - LDA } use LibXC
  - GGA }
  - LDA+U (or GGA+U)
  - + some advanced functionals (RPA)

# ABINIT v6 capabilities (II)

- **Beyond DFT**

- TDDFT: linear response (Casida) for finite systems excitation energies
- *GW* for accurate electronic quasiparticles
  - ★ 4 plasmon pole models, analytic continuation, or contour integration
  - ★ non-self-consistent ( $G^0W^0$ ), partly self-consistent ( $GW^0$  or  $G^0W$ ), quasiparticle self-consistent (QS*GW*), and vertex correction (*GW* $\Gamma$ )
  - ★ susceptibility matrix by sum over states (Adler-Wiser)
  - ★ extrapolar and effective-energy technique to reduce the number of unoccupied states
- Bethe-Salpeter for accurate optical properties calculations

# ABINIT v6 capabilities (III)

- **Density-Functional Perturbation Theory :**
  - Responses to atomic displacements, to static homogeneous electric field, and to strain perturbations
  - Second-order derivatives of the energy, giving direct access to :  
dynamical matrices at any  $\mathbf{q}$ , 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

# ABINIT v6 capabilities (IV)

- Insulators/metals - smearings : Fermi, Gaussian, Gauss-Hermite ...
- Collinear spin / non-collinear spin / spin-orbit coupling
- Forces, stresses, automatic optimization of atomic positions and unit cell parameters (Broyden and Molecular dynamics with damping)
- Molecular dynamics (Verlet or Numerov), Nosé thermostat, Langevin dynamics
- Electric field gradients
- Symmetry analyzer (database of the 230 spatial groups and the 1191 Shubnikov magnetic groups)

# A bit of history...

- It all started in 1997...

**Idea:** softwares for first-principles simulations become more and more sophisticated (not easy to develop and maintain).

**Solution:** worldwide collaboration of specialized, complementary groups

**Model:** Linux software development : ‘free software’ (GPL License)

- As of today (2011)

- the software consists of more than 400 kLines of F90
- there have been 80 contributors to ABINITv6
- there are more than 1300 people on the users mailing list



# The developers...

● **UCLouvain (Belgium) :**

X. Gonze, J.-M. Beuken, A. Jacques, G.-M. Rignanese, S. Leroux, M. Giantomassi,  
F. Da Pieve, A. Lherbier, M. Oliveira

● **CEA-Bruyeres (France) :**

M. Torrent, F. Jollet, G. Zérah, B. Amadon, G. Jomard, M. Mancini,  
F. Bottin, S. Mazevet, M. Delaveau, T. Rangel

● **University of Liège (Belgium) :**

M. Verstraete, Ph. Ghosez, J.-Y. Raty, P. Hermet

● **Chinese Academy of Science (China) :**

A. Zhou, L. Fang, L. He

● **CEA-Grenoble (France) :**

T. Deutsch, P. Boulanger, D. Caliste

● **University of Montréal (Canada) :**

M. Côté, S. Blackburn, J. Laflamme, G. Antonius

● **Ecole Polytechnique (France) :**

L. Reining, A. Berger

● **University of Milano (Italy) :**

G. Onida, D. Sangalli

● **CEA-Gif-sur-Yvette (France) :**

F. Bruneval

● **Rutgers University (USA) :**

D. Hamann

● **University of San Sebastian (Spain) :**

Y. Pouillon

● **University of Basel (Switzerland) :**

S. Goedecker

● **ESRF Grenoble (France) :**

L. Genovese

● **Dalhousie University (Canada) :**

J. Zwanziger

● **University of Caen (France) :**

P.-M. Anglade

● **University of Amman (Jordanian) :**

R. Shaltaf

● **ENS Lyon (France) :**

R. Caracas

● **CNRS-Grenoble (France) :**

V. Olevano

● **Corning Inc. (USA) :**

D.C. Allan

● **Mitsubishi Chemical Corp. (Japan) :**

M. Mikami

● **University of York (UK):**

R. Godby



**5th ABINIT Developer Workshop  
Han-sur-Lesse (Belgium), April 2011**

# The developers...



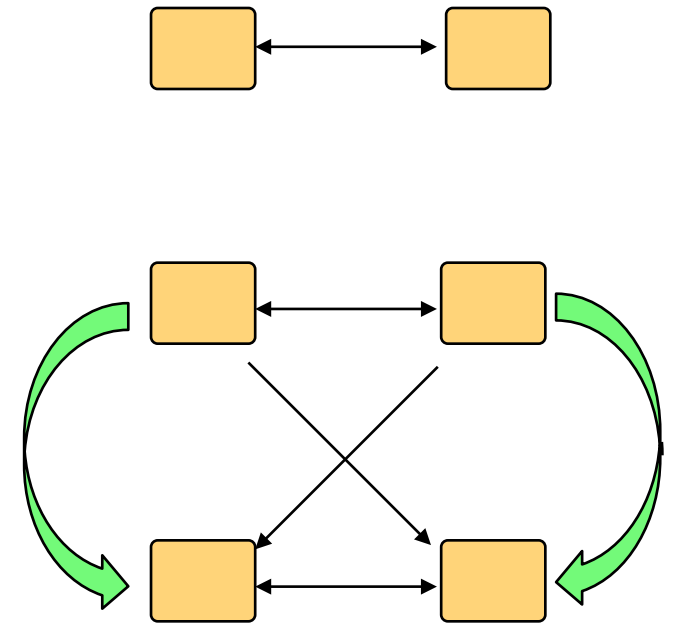
**5th ABINIT Developer Workshop  
Han-sur-Lesse (Belgium), April 2011**

# The essence of software programming

- “a scaling-up of a software entity is not merely a repetition of the same elements in larger size; it is necessarily an increase in the number of different elements. In most cases, the elements interact with each other in some nonlinear fashion, and the complexity of the whole increases much more than linearly”

[F. Brooks, *The mythical man-month. Essays on software engineering*, 1995 20th Anniversary edition]

- Brooks argued that essence is a substantial part of the development time, that it is inherently complex and ... incompressible !  
(the bearing of a child takes nine months, no matter how many women are assigned)



# Software reuse

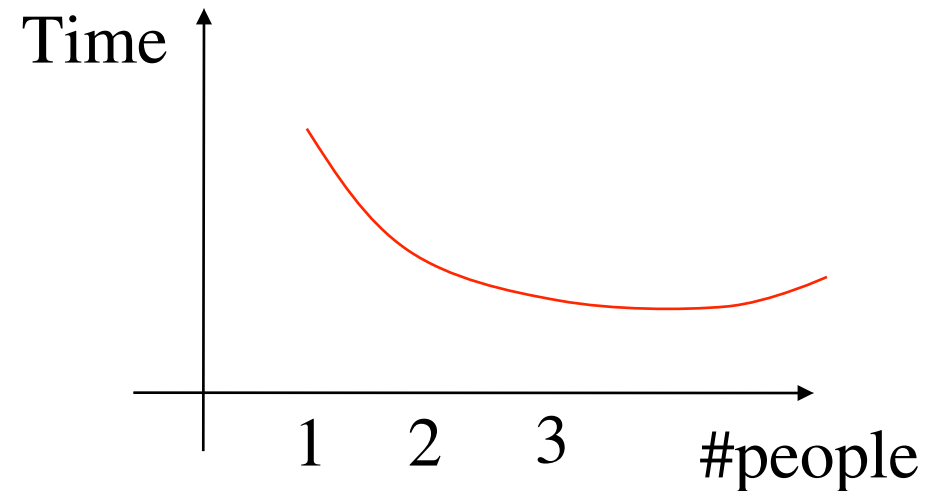
- How to address the “essence” bottleneck ?  
Use already existing software ! Software re-use.
  - Conceptual work already done
  - Debugged, tested, I/O set-up !
  - Add “integrated product” to the system (need adequate license)
  - Can be completely external
  - Can be internal re-use : need modularity !
  - Grow, not build software : incremental development.  
Also psychological: one has something that works.
- Building software takes some incompressible human time, even if we eliminate the accidental difficulties, and attack the essential difficulties in an efficient way.

# Maintenance

- Program maintenance :
  - not like for a car: no cleaning, lubricating, repair of deterioration
  - the needed changes repair design “defects”
  - these appear because of new functionalities to be implemented
  - other modifications are due to change of environment  
(hardware, compilers)
- Moreover, fixing a defect has a substantial (20%-50%) chance of introducing another ! Importance of automatic testing.
- The only constancy is change itself. So, plan the system for change...  
And have tools for version maintenance ...

# Group effort

- How to make a group have a better productivity ?
    - first, each person need training
    - then, software construction is a system effort
- ⇒ communication efforts can dominate the decrease in individual task time brought by partitioning.



- Need asynchronous work to build integrated products.
- Doing top-level work before delivery pays off :
  - less communication needed (complaints, fixes ...);
  - but training to do top-level work takes time !

# Distributed development

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

*More than 600 automatic tests have been set up, and new ones are added for securing each new feature.*

- Different groups use different platforms ... and how to reuse software

*The build system relies on the “autotools” (itself software reuse).*

*The build system has been designed for the easy inclusion of libraries (or “plug-ins”)*

# Distributed development

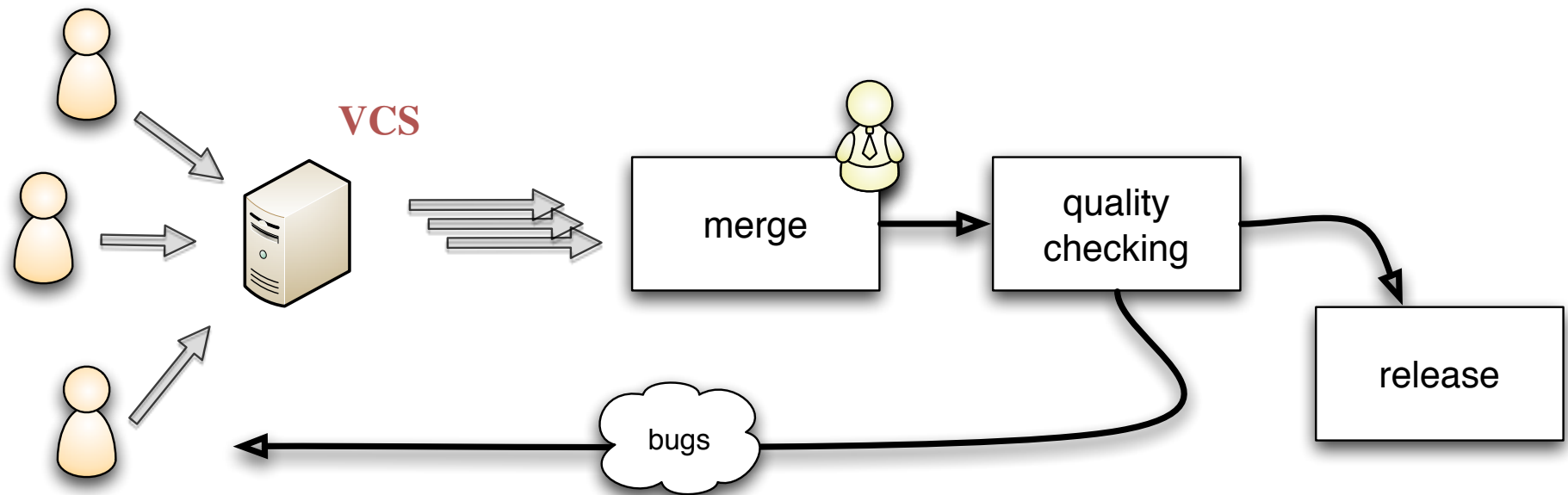
- Different groups might have different coding style ...  
*The F90 routines follow explicitly stated coding rules (ABINIT style), with a special format that allows processing by ROBODOC, and different utilities (in perl and python) that allow global management of sources.*
- How to synchronize the development effort ?  
*Use of a central repository, worldwide accessible, using the GNU Arch model, as implemented in the software BAZAAR.*
- Implementation of the “self-testing” and ”self-documentation” software concepts, as well as use of recent software engineering management tools.



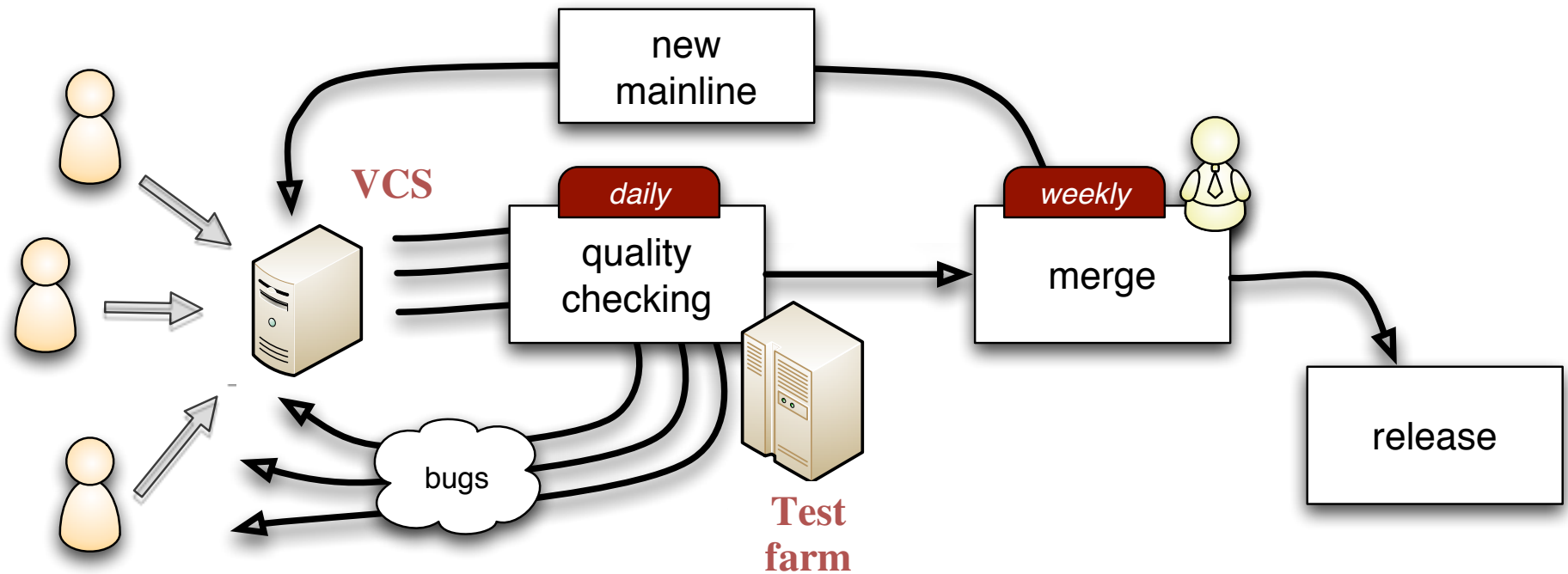
# Version control : BAZAAR (aka bZR)

- In 2007 we (finally) reached a first-class version control system (VCS) with bZR ...
  - Very easy to use and install
  - Each developer has one or more branches, that are easily merged with other branches (powerful merge algorithm ; of course, there might be conflicts to be resolved at merge time ...)
  - Worldwide access of the repository  
(everybody can see everybody's work)
  - Distributed version control system : easy to work with no access to the net, then synchronize with the repository when the net is accessed.
  - Renaming files (or directories) does not break history

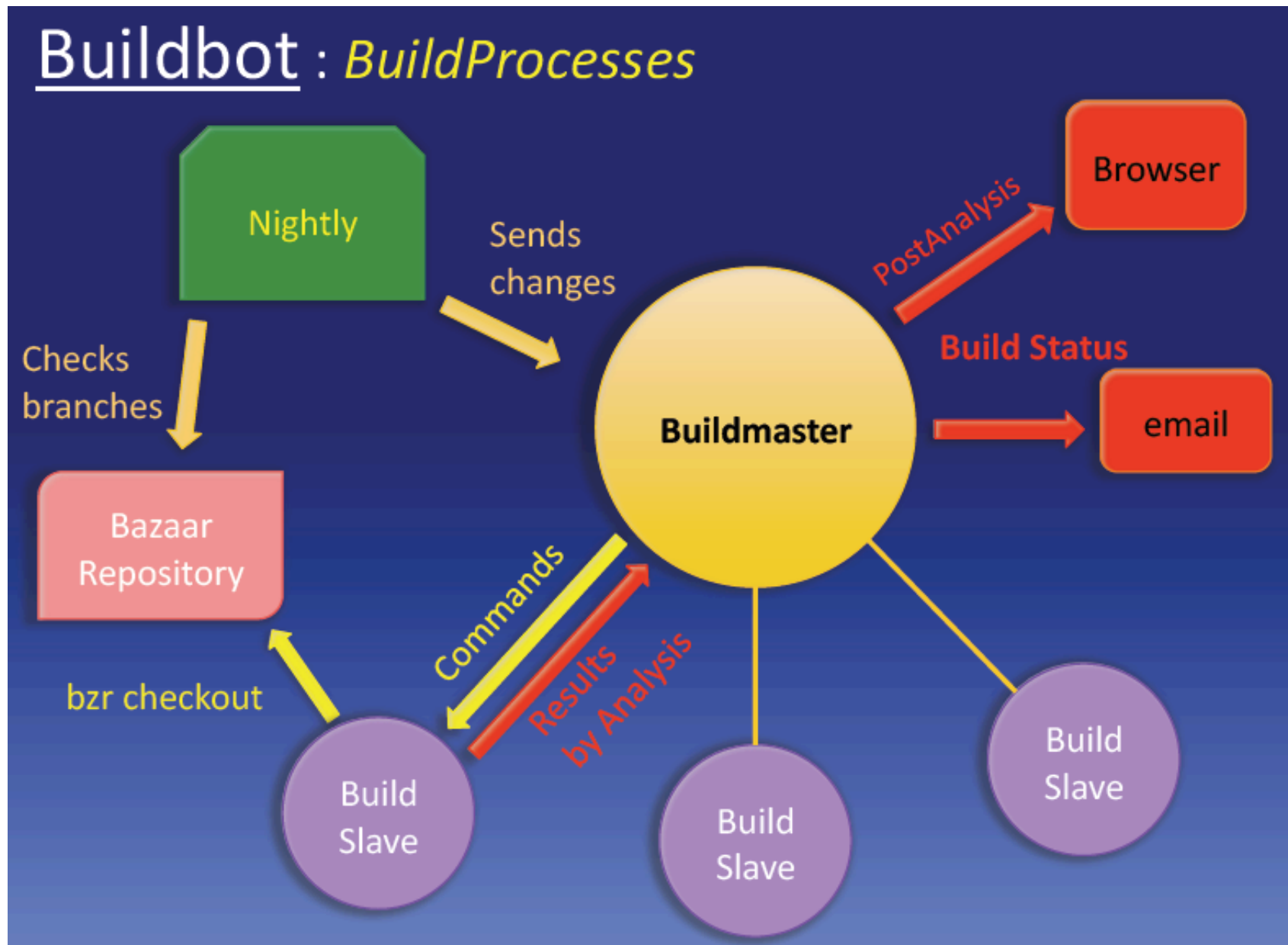
# Traditional development workflow



# An alternative.. the continuous integration



# ETSF Test farm, under control of buildbot



# ETSF test farm hardware inventory

Slave	Brand	CPU	Processor	RAM	OS	bots
testf	Bull R423-E2	Intel Xeon	2x Quad	12 GB	CentOS 5.3	2
chum	Sun X4200M2	AMD Opteron	2x Dual	32 GB	CentOS 5.3	1
green-bb	Dell PowerEdge	Intel Xeon	2x Quad	16 GB	SLinux 5.3	2
bigmac	Apple Mac Pro	Intel Xeon	2x Quad	6 GB	OSX 10.5	2
chpit	HP rx4640	Intel Itanium2	4	8 GB	Debian 5.0.1	1
fock	IBM OP 720	IBM Power5	2x Dual	32 GB	Suse 9.3	1
max	Apple XServe	IBM PowerPC G5	18x Dual	18x 4 GB	OSX 10.4	1
buda	SuperMicro	Intel Xeon	2x Quad	12 GB	CentOS 5.4	1
ibm6	IBM OP 520	IBM Power6	2x Dual	8 GB	AIX 6.1	1





# Automatic analysis of tests

bruneval\_6.11.1-public/r765

=====

Tests SEQ start at 01:15 and done after 2120s

test built\_in OK

=====

Serie	#tests	#succes	#passed	#failed	#missing
atompaw	1	0	1	0	0
bigdft	13	13	0	0	0
etsf_io	10	10	0	0	0
fast	27	27	0	0	0
gwdp	31	21	9	1	0
libxc	13	13	0	0	0
tutoplugs	4	0	4	0	0
tutorespfn	46	37	9	0	0
tutorial	53	44	9	0	0
unitary	4	4	0	0	0
v1	96	96	0	0	0
v2	95	86	9	0	0
v3	93	86	7	0	0
v4	94	79	15	0	0
v5	99	83	16	0	0
v6	89	76	13	0	0
wannier90	3	0	3	0	0
paral	66	51	14	1	0

=====

Paral Tests DONE ( time elapsed: 834s )

=====

Powered by Analysis V2.6.12

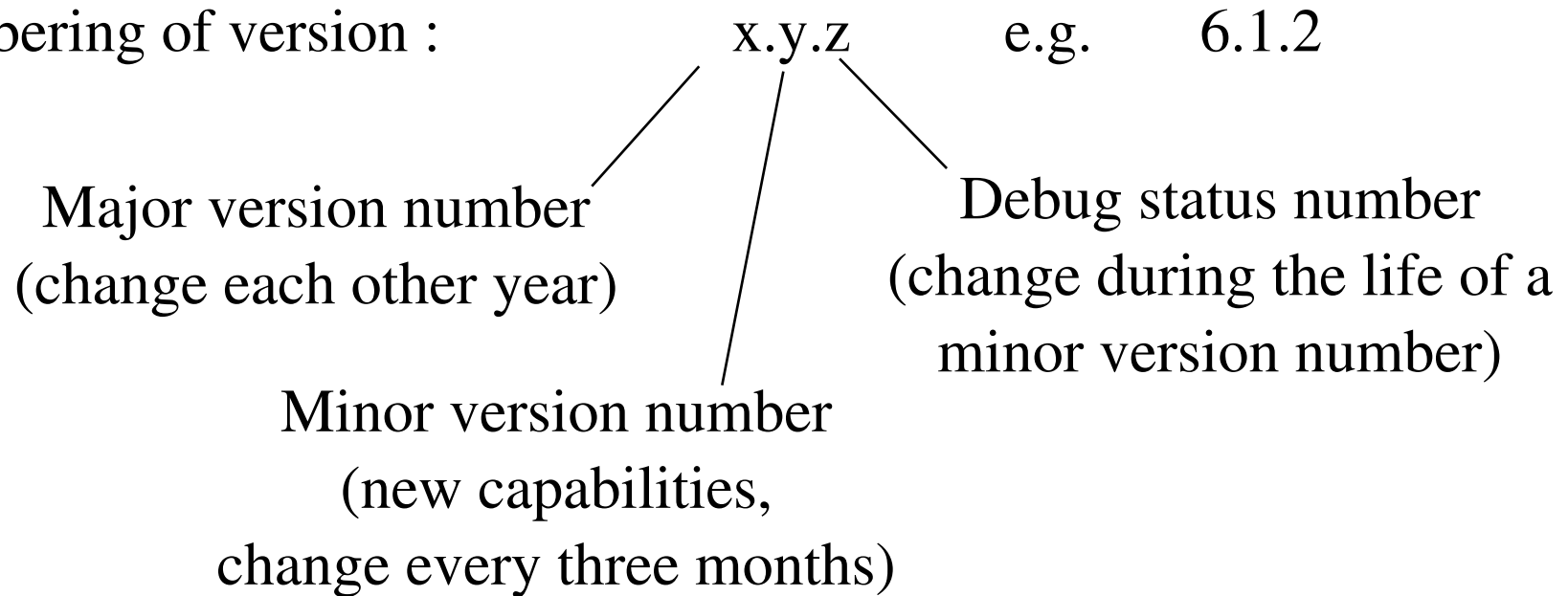
Date : 11/04/11

=====

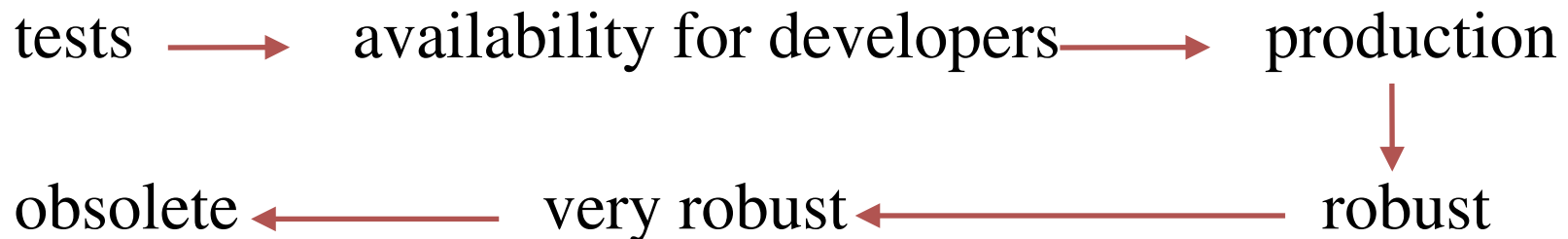


# Sources and binaries

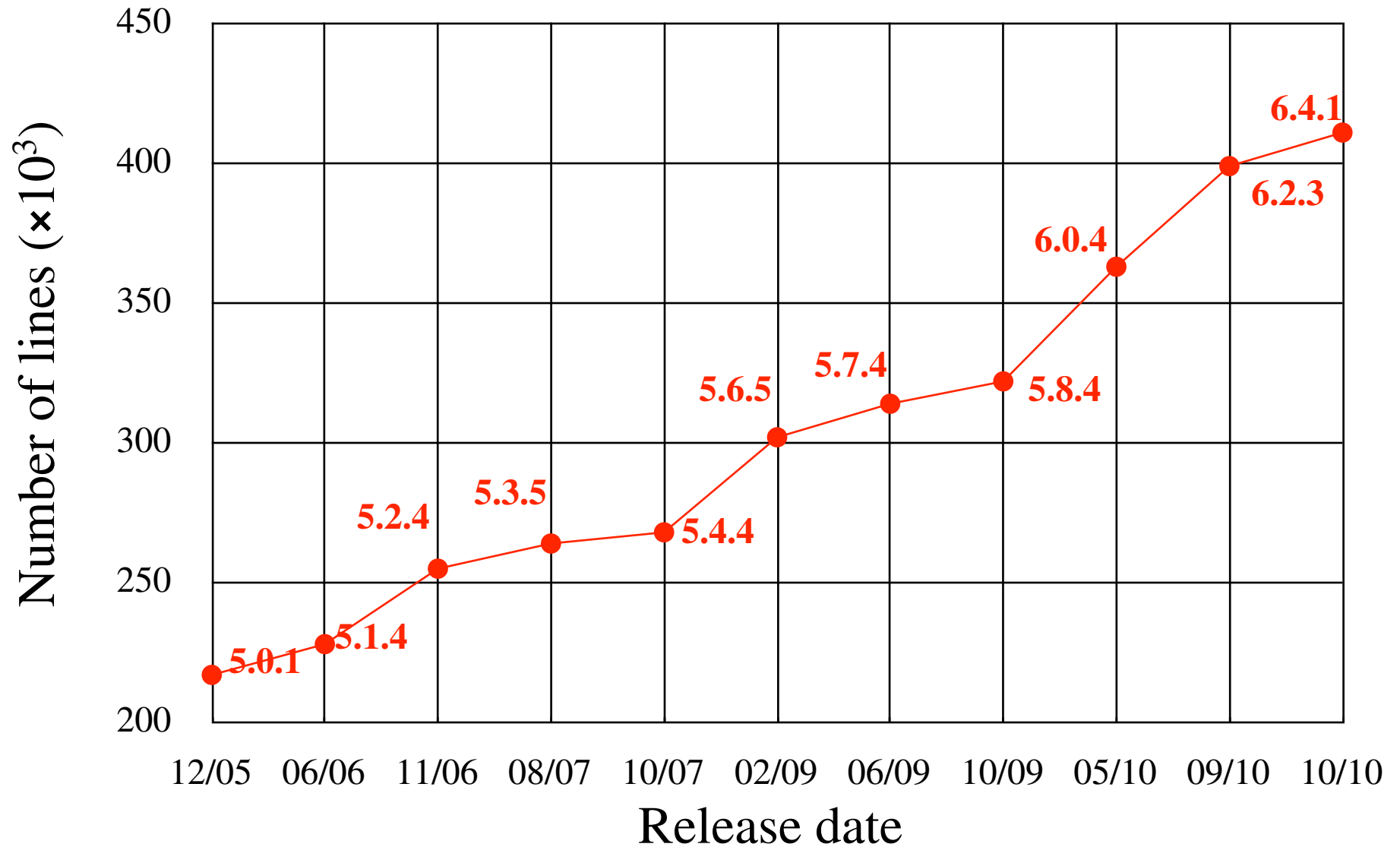
- Numbering of version :



- Usually, there are three « active » minor versions at all time.
- Life of a minor version (usually one year) :



# Time evolution from 2005 to 2010



# Functional structure of ABINIT

