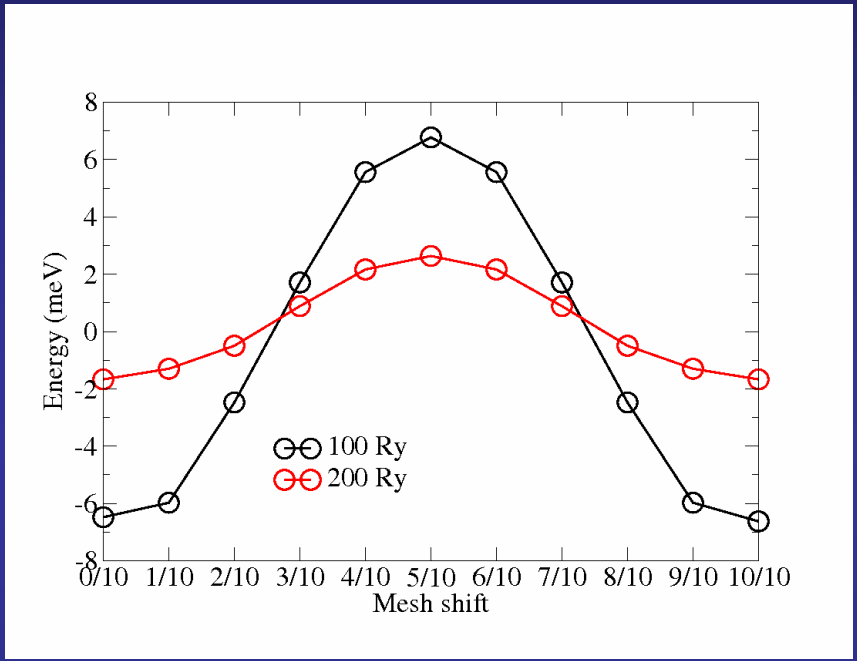
The eggbox effect: converging the mesh cutoff

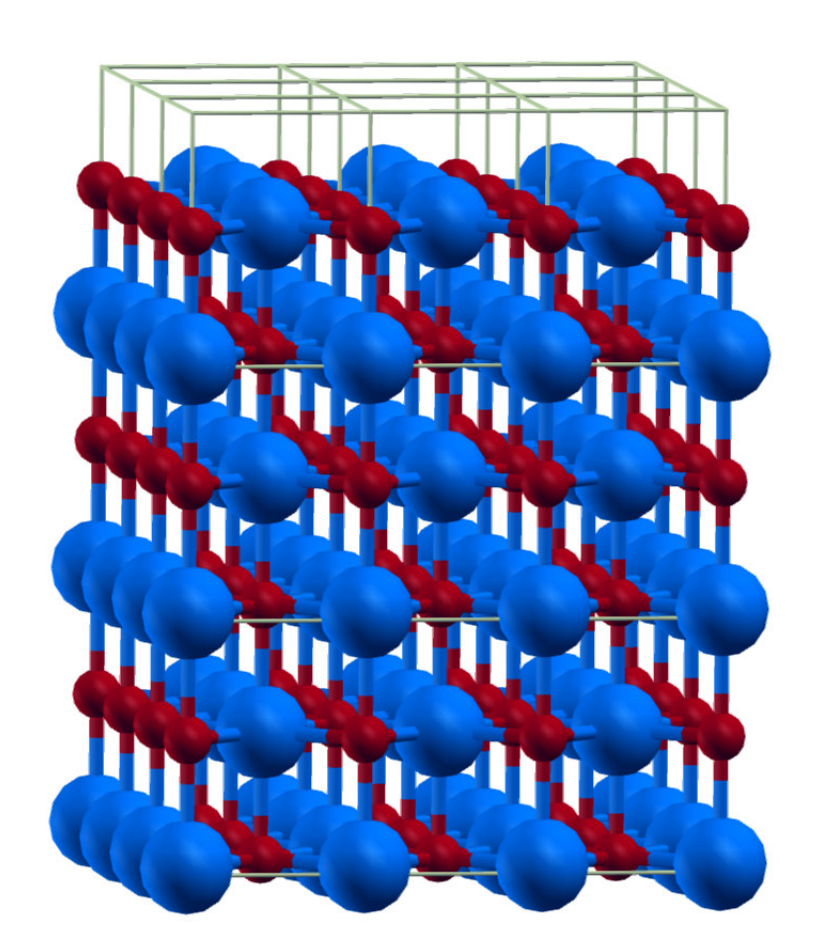


Objectives

- study the convergence of the energy and the forces with respect to the real space grid.

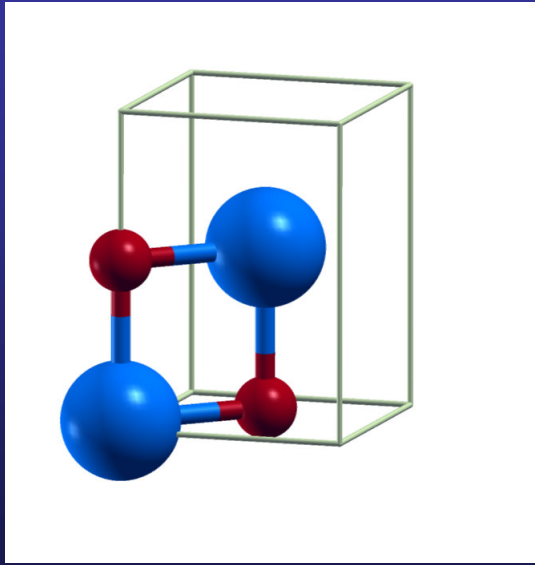
System where the tests will be performed: bulk MgO (rocksalt structure)

Instead of using the unit cell (FCC + 2 atoms of basis), the exercise will be more transparent if we use a conventional unit cell with orthogonal lattice vectors



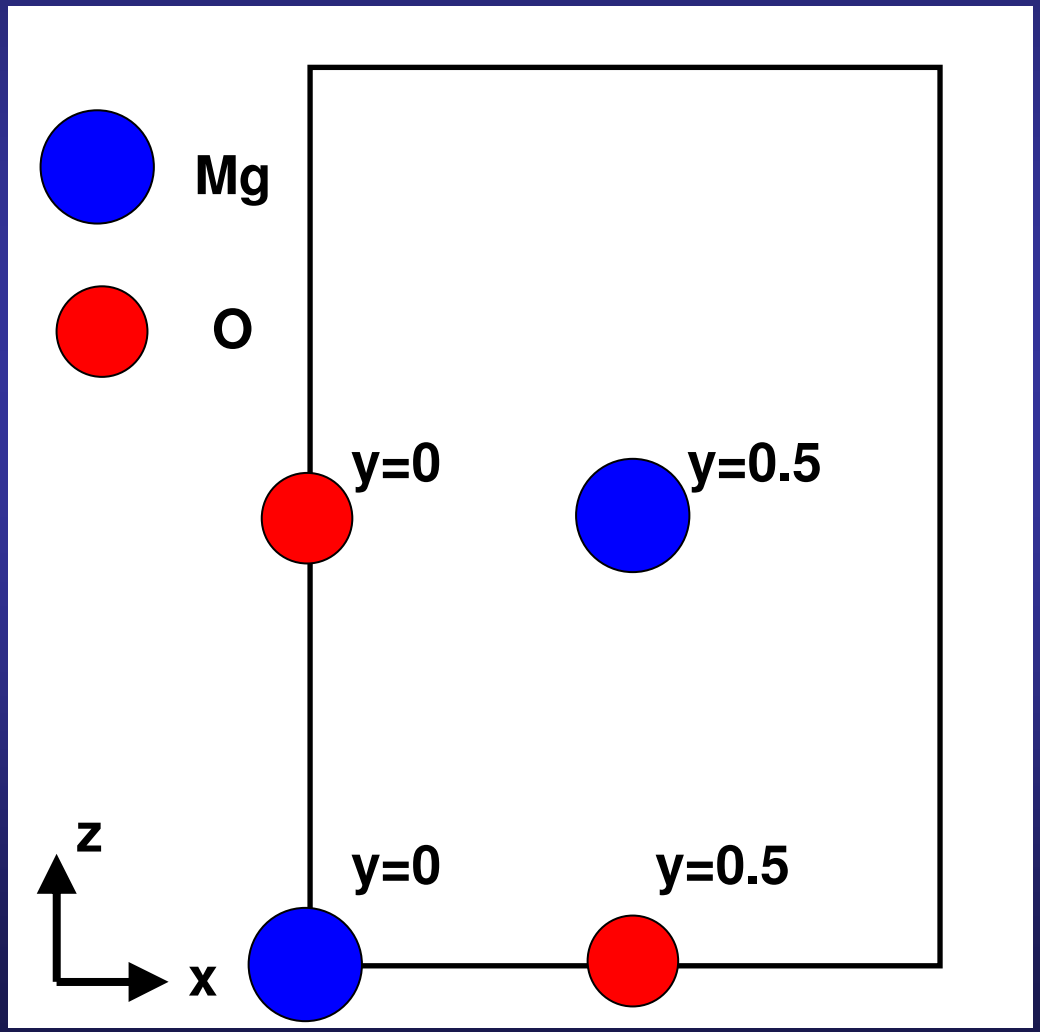
Simulation cell:

- Tetragonal
- 4 atoms/cell



Some of the integrals are computed in a three dimensional grid in real space

Let us project the atomic position in the (x,z) plane



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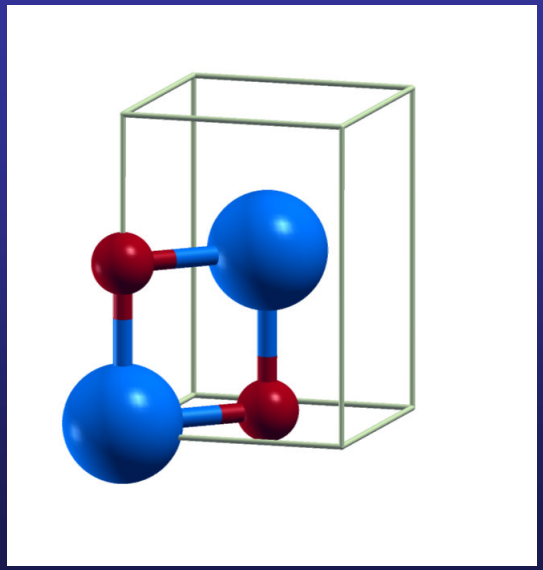
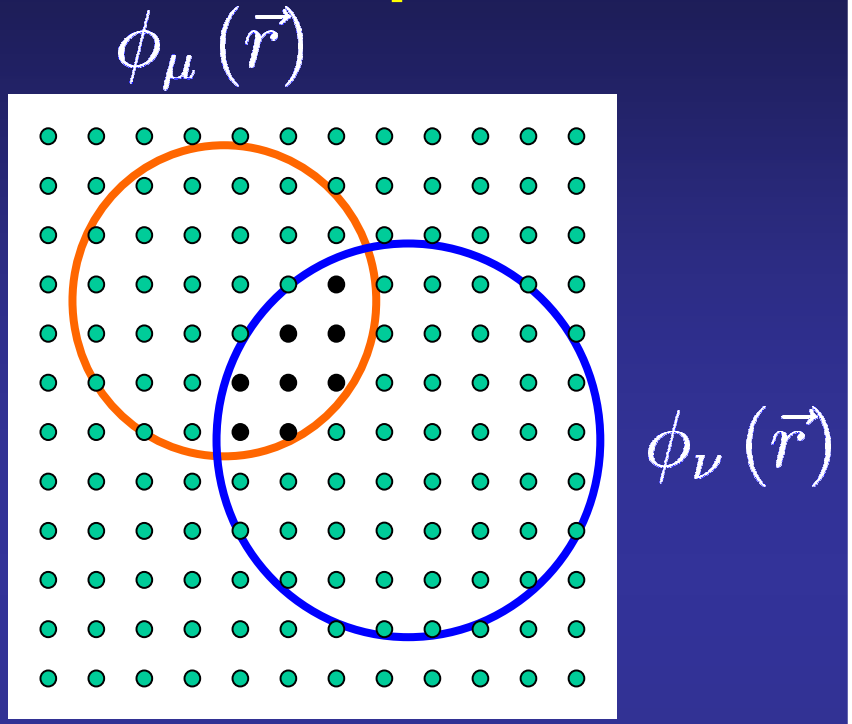
- 4 atoms/cell



Three dimensional grid to compute Hartree, exchange correlation and neutral atom potentials

$$\rho(\vec{r}) = \sum_{\mu\nu} \rho_{\mu\nu} \phi_\nu^*(\vec{r}) \phi_\mu(\vec{r})$$



Find all the atomic orbitals that do not vanish at a given grid point

(in practice, interpolate the radial part from numerical tables)

EVERYTHING O(N)

Once the density is known, we compute the charge density and the potentials

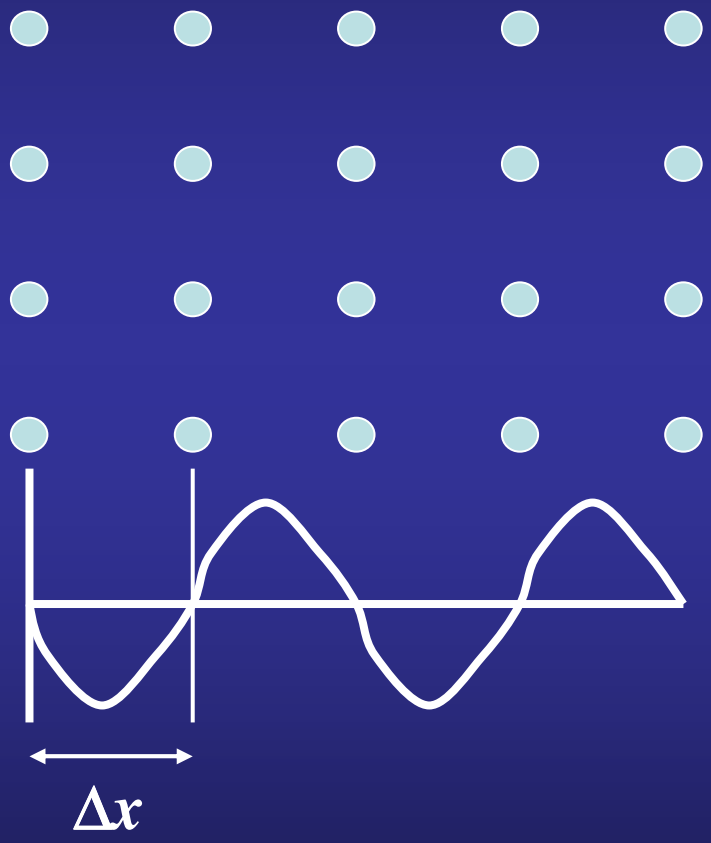
$$\rho(\vec{r}) \rightarrow V^{xc}(\vec{r})$$

$$\delta\rho(\vec{r}) = \rho(\vec{r}) - \rho_{atoms}(\vec{r})$$

$$\delta\rho(\vec{r}) \xrightarrow{FFT} \delta V^H(\vec{r})$$

Fineness of the grid controlled by a single parameter, the "MeshCutoff"

E_{cut} : maximum kinetic energy of the plane waves that can be represented in the grid without aliasing



$$E_{cut} = \frac{1}{2}\left(\frac{\pi}{\Delta x}\right)^2$$

where Δx is the grid interval

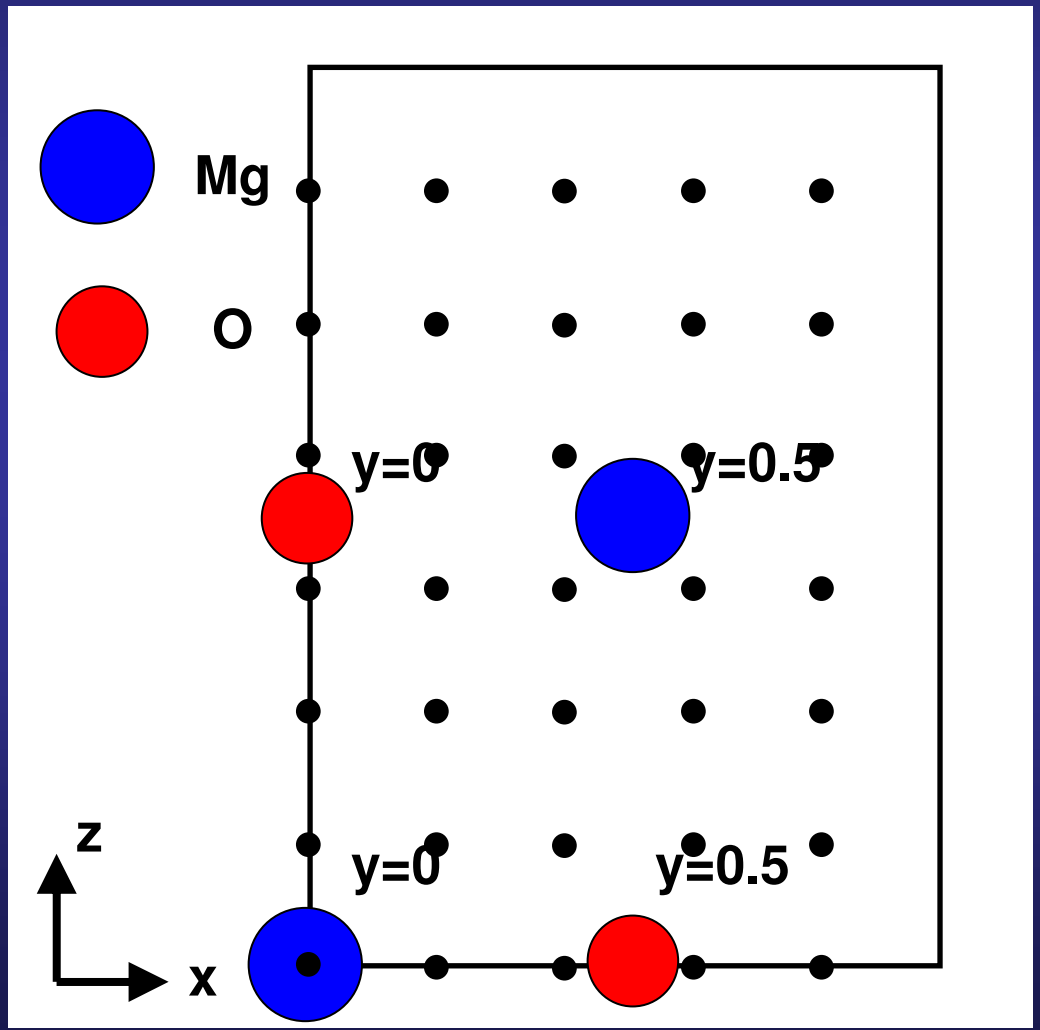
In the grid, we represent the density $\Rightarrow$ grid cutoff not directly comparable with the plane wave cutoff to represent wave functions

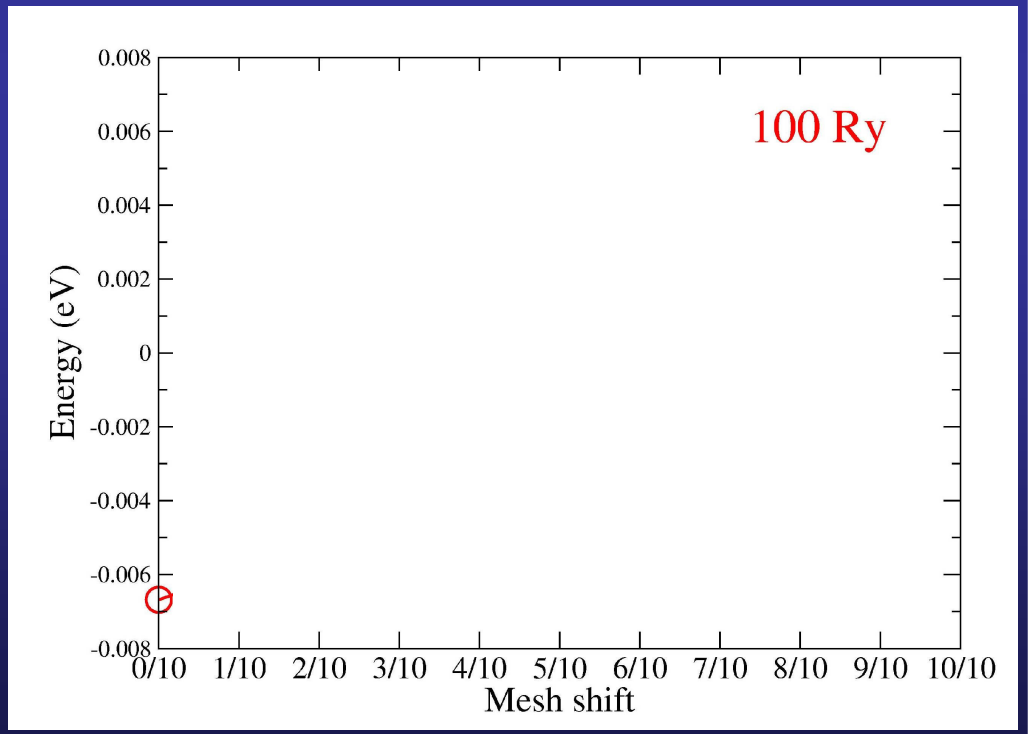
(Strictly speaking, the density requires a value four times larger)

Fineness of the grid controlled by a single parameter, the “MeshCutoff”

MeshCutOff = 100 Ry

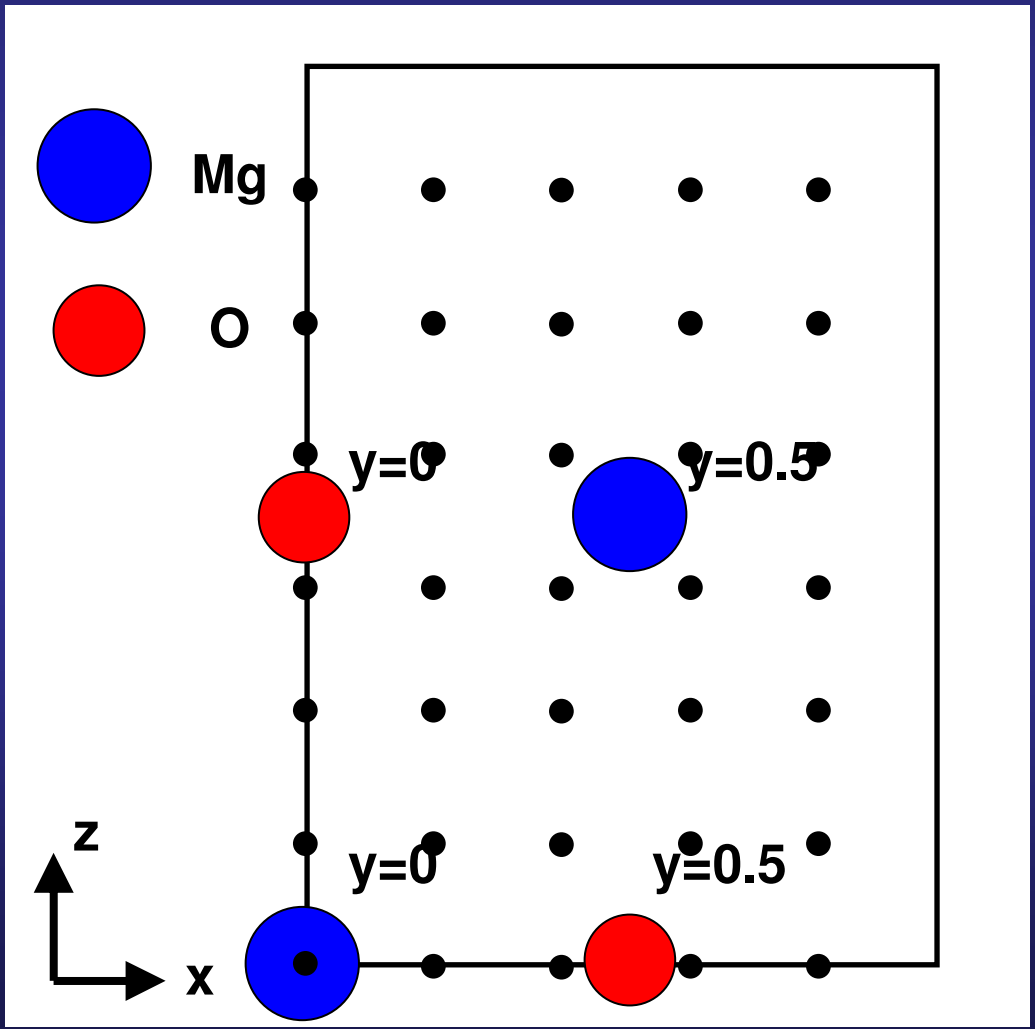
Grid of 18 x 18 x 30 points along the three lattice vectors





All the quantities should be invariant under translation as a whole, but the grid breaks translation symmetry.

The grid integrals make the energy dependent on the position of the atoms relative to the grid

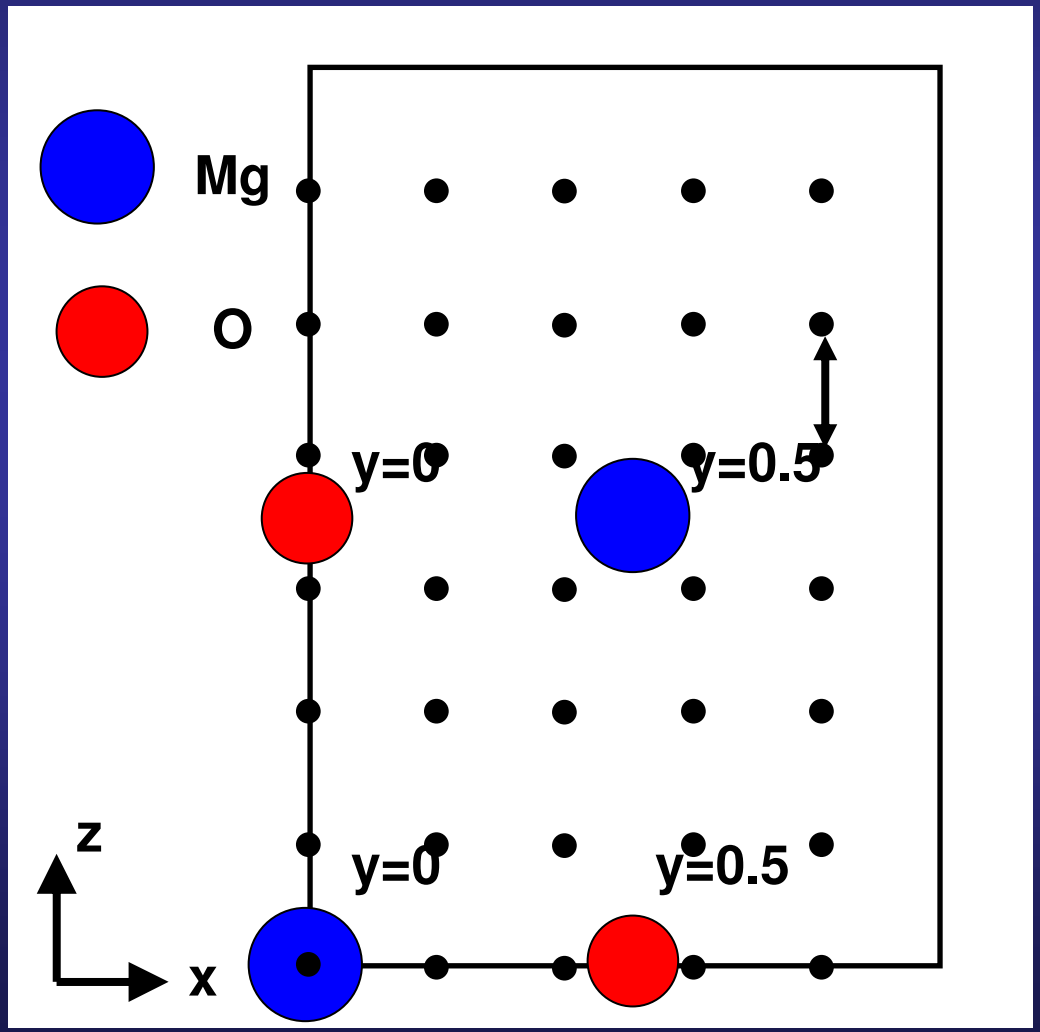


Relative position can be controlled by the input variable:

%block AtomicCoordinatesOrigin

The origin is given in the same units as the atomic coordinates.

The grid integrals make the energy dependent on the position of the atoms relative to the grid



MeshCutOff = 100 Ry

Grid of 18 x 18 x 30 points along the three lattice vectors

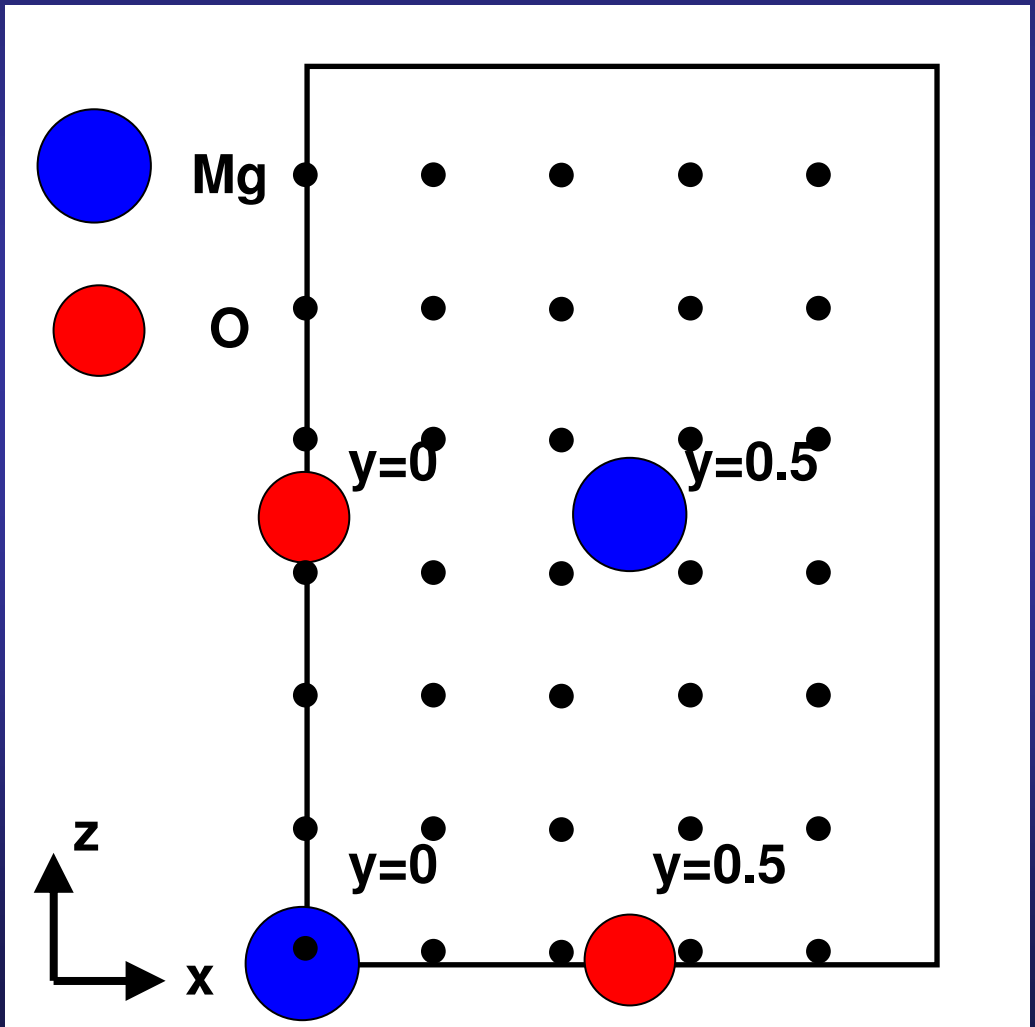
Distance between consecutive points in the grid along z (in reduced coordinates):

1/30

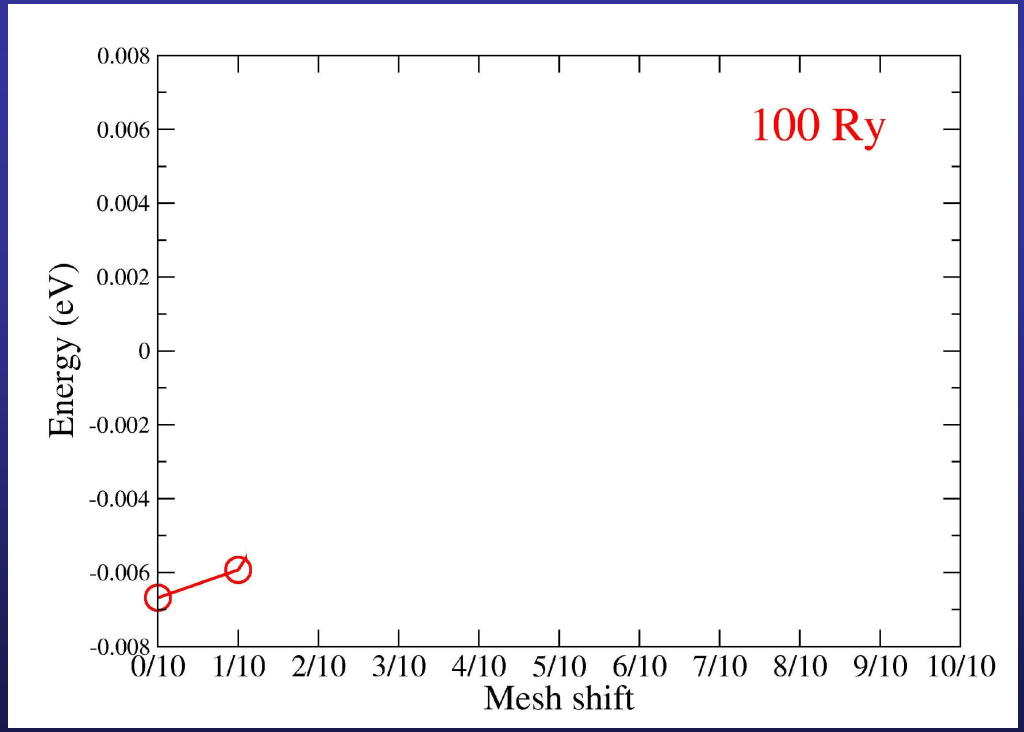
Let us compute the change in the energy and the forces when we displace rigidly all the atoms in the unit cell from one point of the grid to the next one (let us assume, in this case, in 10 steps)

```
%block AtomicCoordinatesOrigin
   0.0   0.0   (1/30)/10
%endblock AtomicCoordinatesOrigin
```

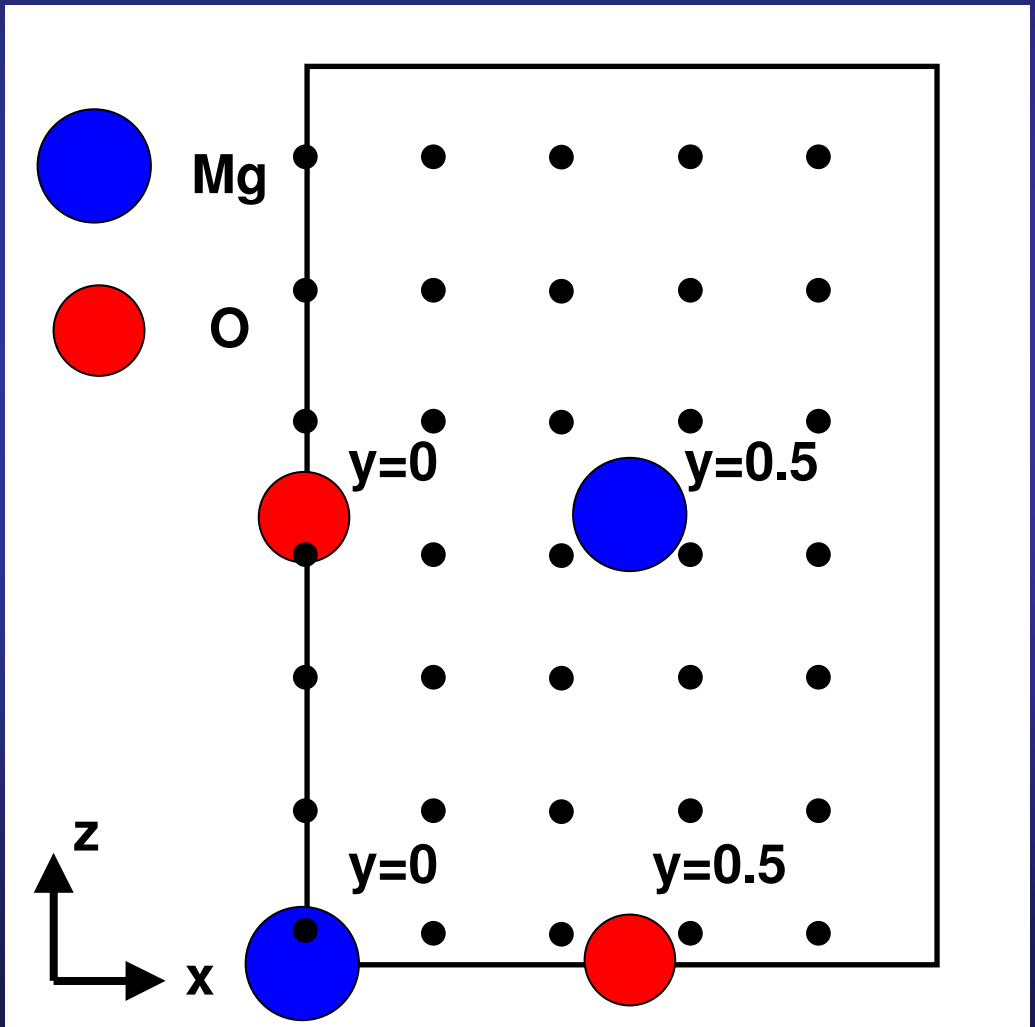
The grid integrals make the energy dependent on the position of the atoms relative to the grid



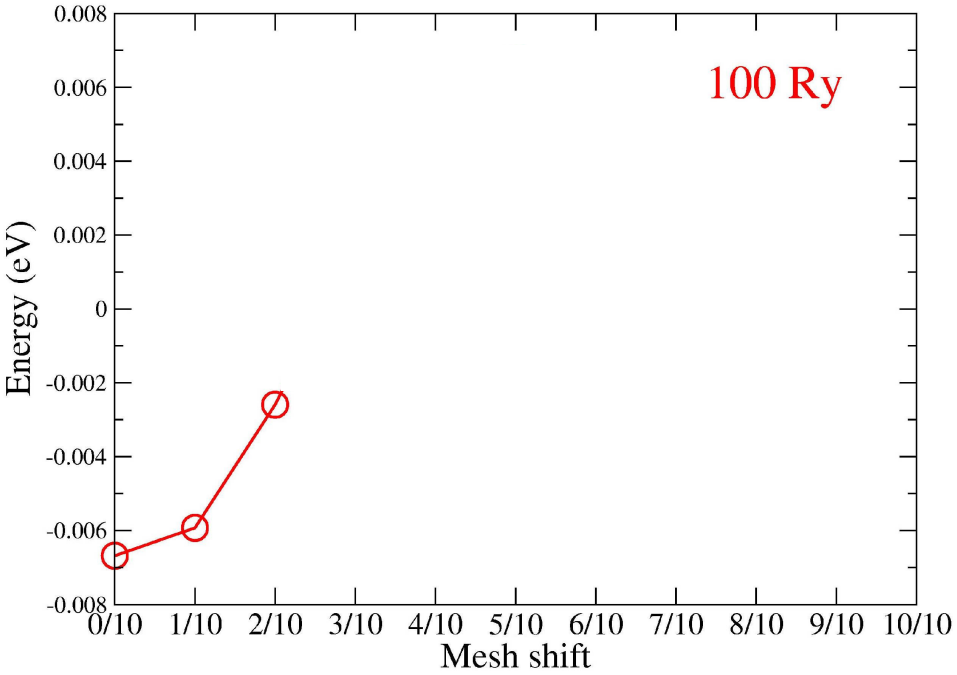

```
%block AtomicCoordinatesOrigin
  0.0   0.0   1/30/10
%endblock AtomicCoordinatesOrigin
```



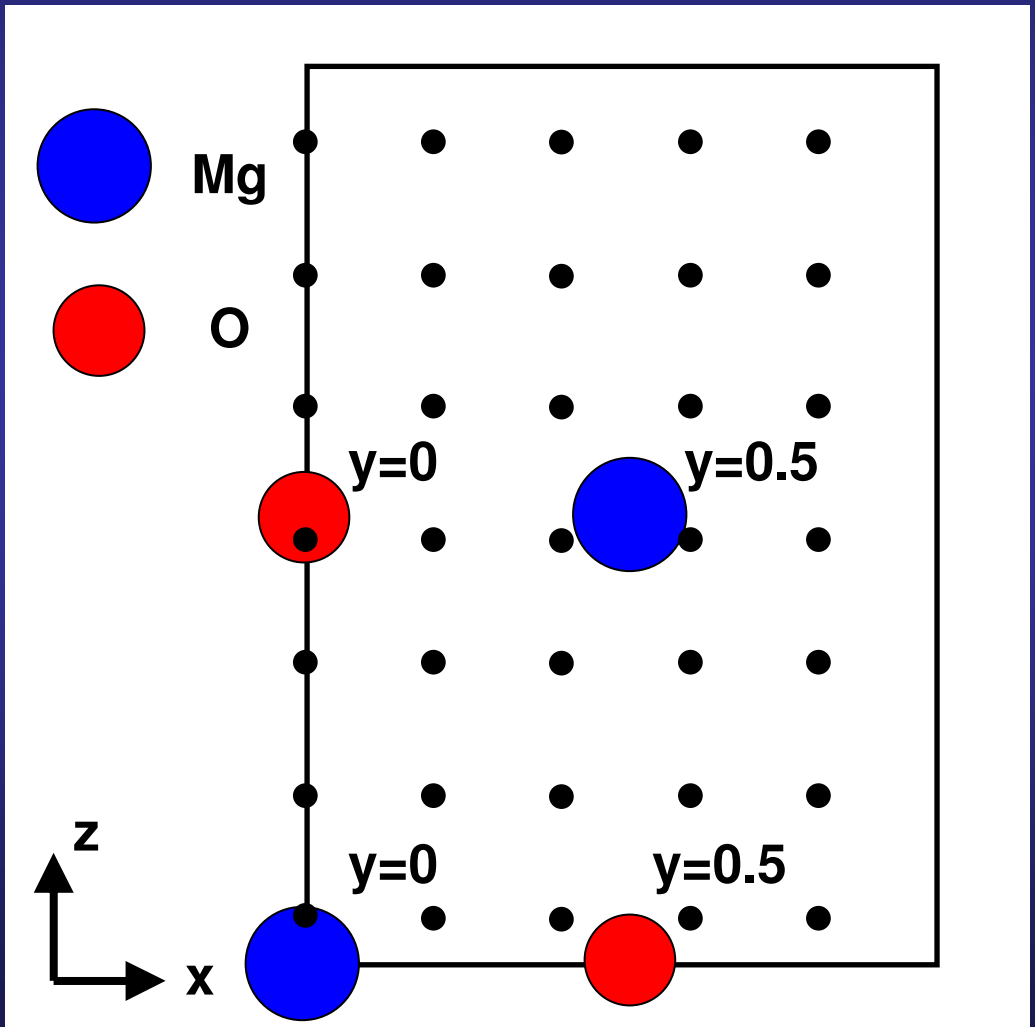
The grid integrals make the energy dependent on the position of the atoms relative to the grid



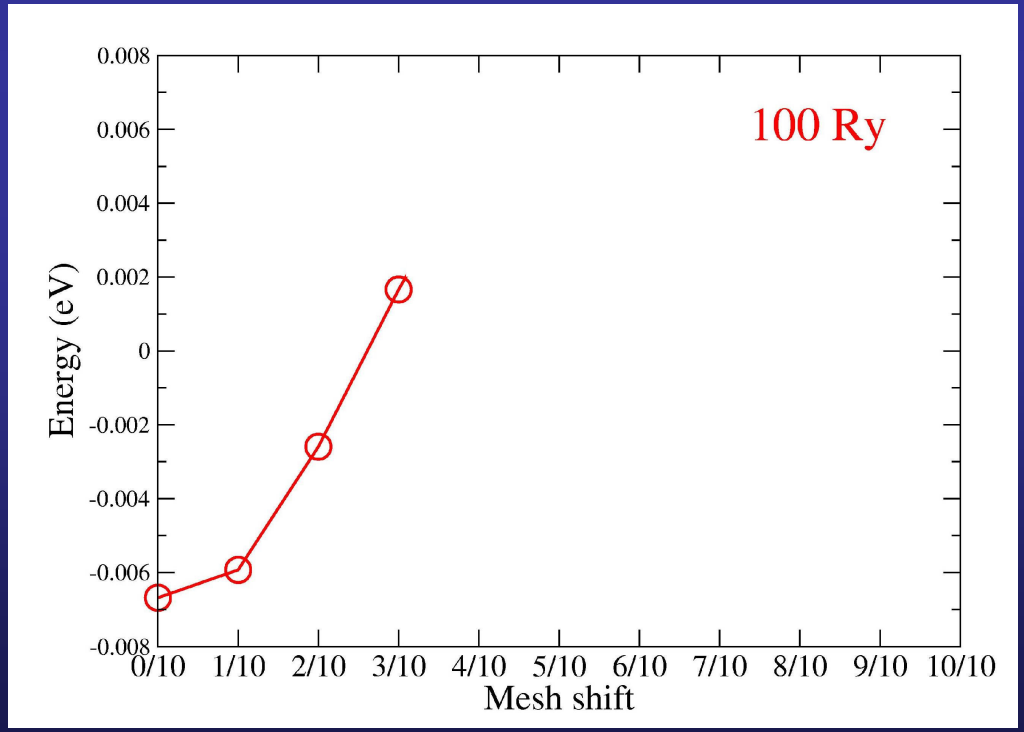

```
%block AtomicCoordinatesOrigin
  0.0   0.0   2/30/10
%endblock AtomicCoordinatesOrigin
```



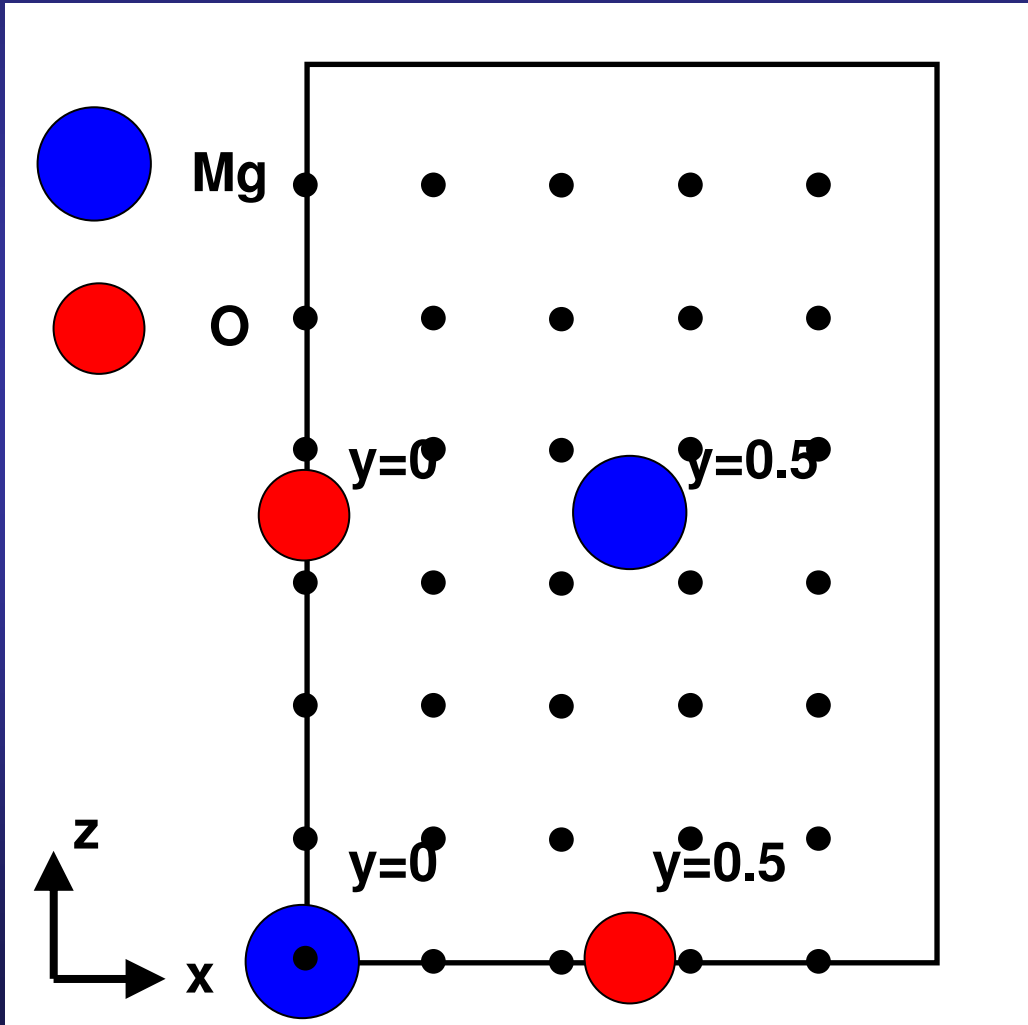
The grid integrals make the energy dependent on the position of the atoms relative to the grid



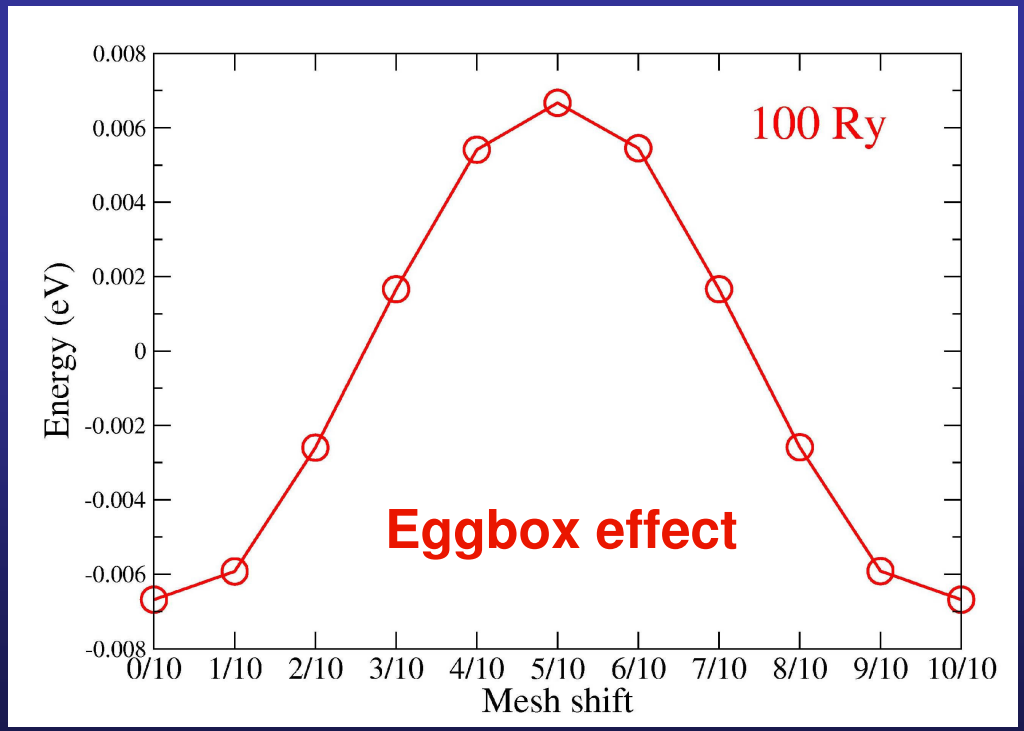

```
%block AtomicCoordinatesOrigin
  0.0   0.0   3/30/10
%endblock AtomicCoordinatesOrigin
```



The grid integrals make the energy dependent on the position of the atoms relative to the grid




```
%block AtomicCoordinatesOrigin
  0.0   0.0   10/30/10
%endblock AtomicCoordinatesOrigin
```



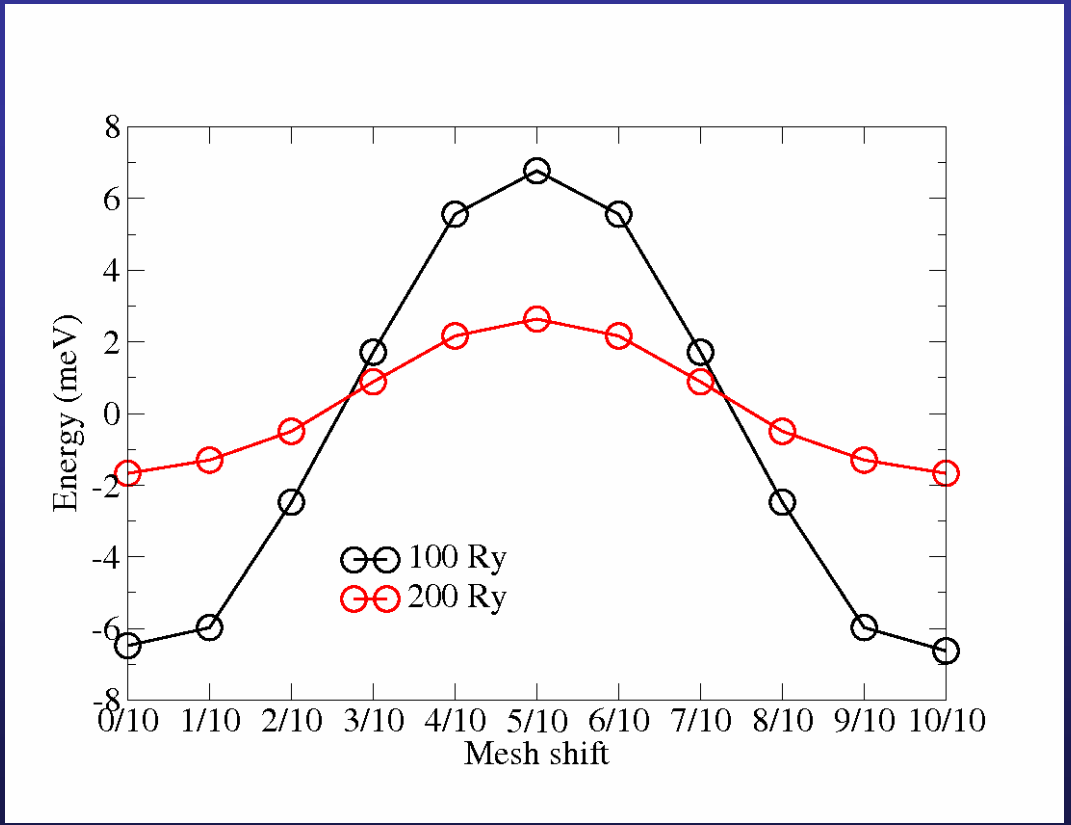
The war against the eggbox…
Solution 1: Increase the MeshCutoff

MeshCutOff = 100 Ry

Grid 18 x 18 x 30

MeshCutOff = 200 Ry

Grid 30 x 30 x 36



Extra cost in:

CPU time

Memory

The war against the eggbox…
Solution 2: the Grid-cell sampling

Achieve SCF for a given MeshCutoff and relative positions of the atoms with respect the grid points.

Freeze in the Density Matrix.

Translate the whole system rigidly by a set of points in a finer mesh.

Recalculate energy, forces, and stresses in the shifted configuration, using the Density Matrix frozen before (that is, the shifted calculations are non self-consistent).

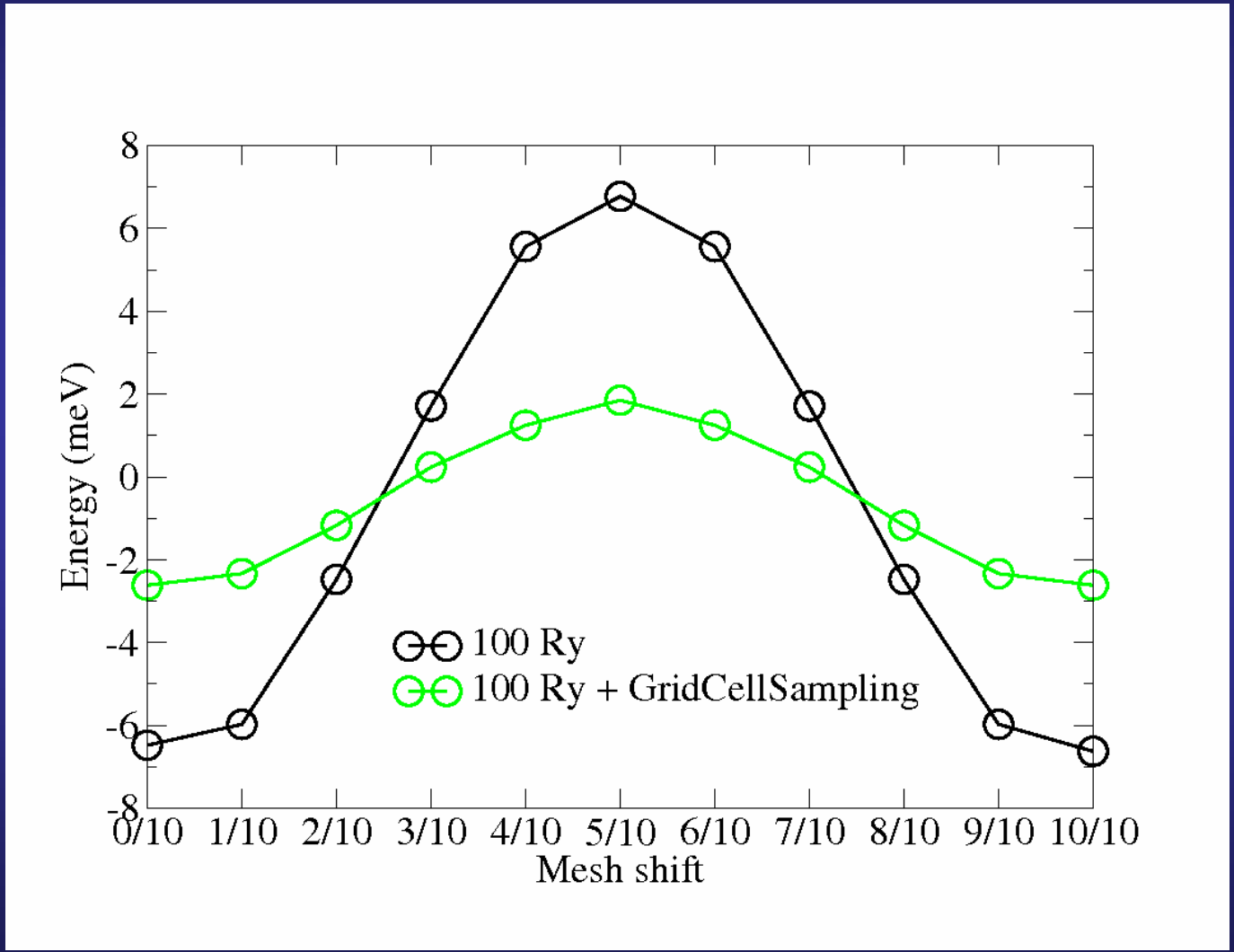
Take the average of the energies, forces, and stresses between all the sampled points.

No extra cost in memory.

It is done only at the end of the SCF iteration, for fixed DM. Only moderate cost in CPU time.

The war against the eggbox…
Solution 2: the Grid-cell sampling

```
%block GridCellSampling
  0.5  0.0  0.0
  0.0  0.5  0.0
  0.0  0.0  0.5
%endblock GridCellSampling
```



The war against the eggbox…
Solution 3: filtering the radial functions

PHYSICAL REVIEW B **73**, 115122 (2006)

Filtering a distribution simultaneously in real and Fourier space

Eduardo Anglada and José M. Soler

Optimal Fourier filtering of a function that is strictly confined within a sphere

José M. Soler and Eduardo Anglada

Computer Physics Communications 180, 1134 (2009)

The war against the eggbox…
Solution 3: filtering the radial functions

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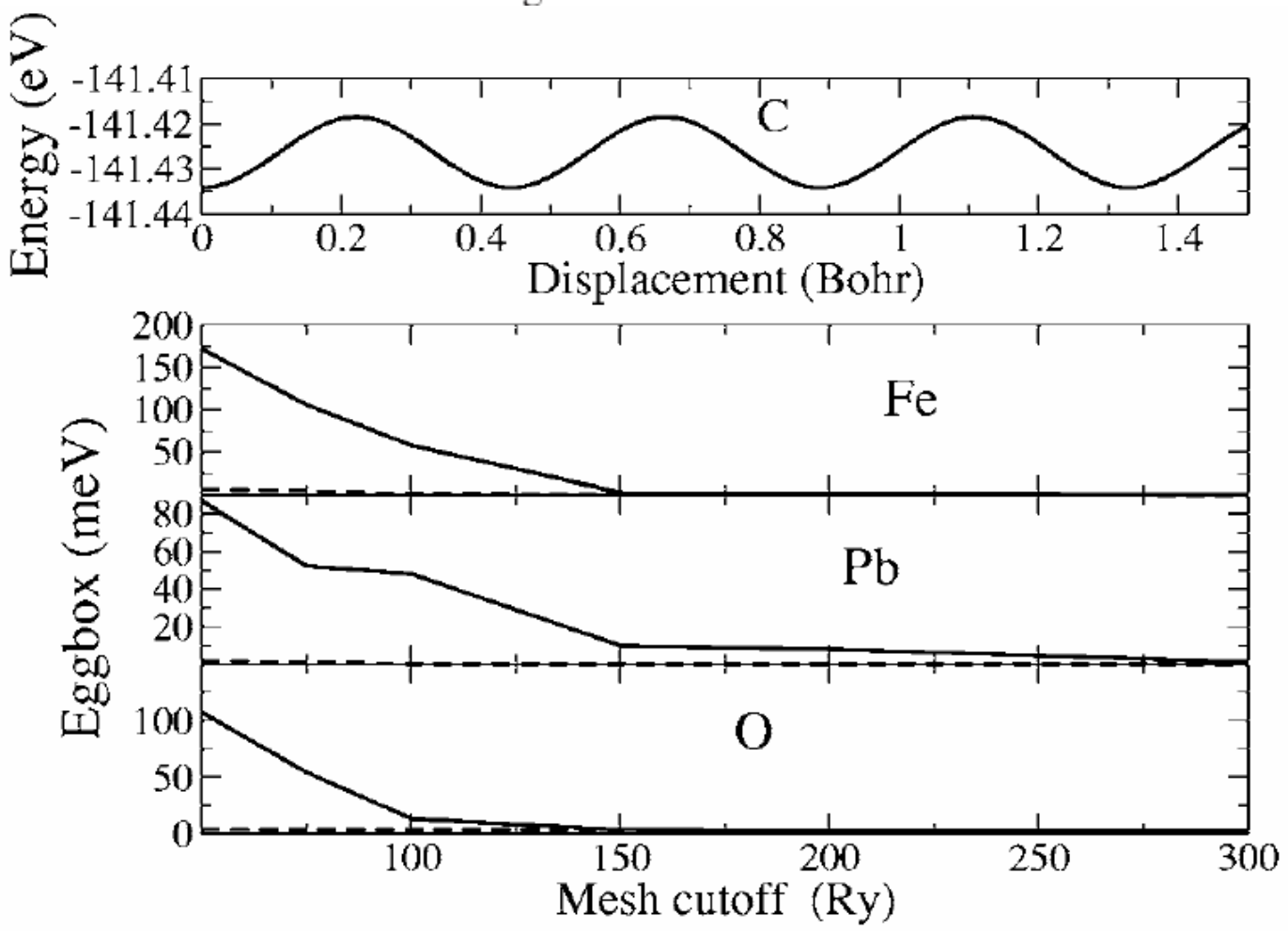
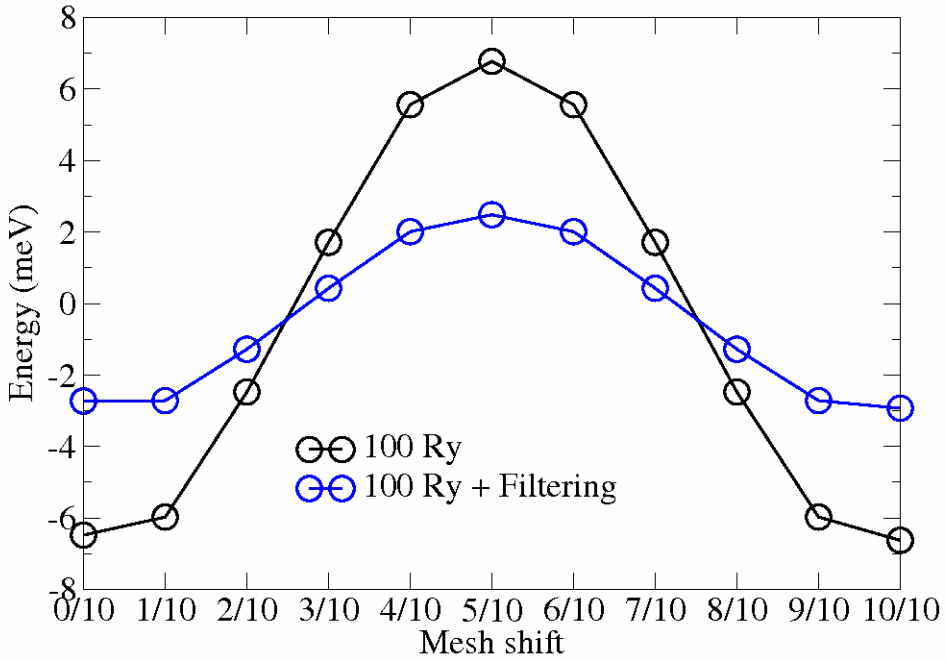


The war against the eggbox…
Solution 3: filtering the radial functions

```
PAO.Filter T            # Filter the Pseudo Atomic Orbitals?
VNA.Filter T            # Filter the Neutral Atom Potentials?
FilterCutoff 100 Ry     # Kinetic energy cutoff of plane waves used to
                        # filter all the atomic basis functions,
                        # the pseudo-core densities for partial core corrections,
                        # and the neutral-atom potentials.
                        # The FilterCutoff should be similar or lower
                        # than the MeshCutoff to avoid the eggbox effect
                        # on the atomic forces.
```



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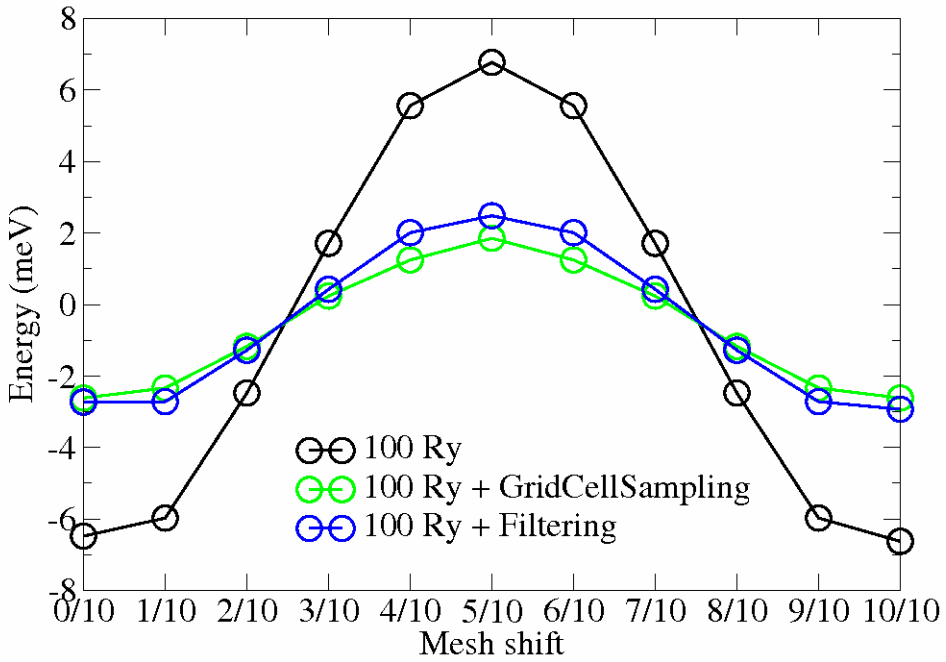

Filtering the radial functions produces, for this system, similar results than the grid cell sampling, although with a reduction in the CPU time

A fine comparison between the two methods, would require the study of the convergence of a relevant quantity (for instance, the frequence of a phonon) with respect the cutoff, evaluating the computational cost of each method