# A short tutorial on the octopus code

**[Tutorial based on the 1.4 version]**

**May 21, 2005**

```
                    Running octopus, version 1.4
             (build time - Mon Jan 24 16:22:00 CET 2005)

                The octopus is swimming in g32 (Linux)
Info: Calculation started on 2005/01/26 at 19:01:22
Info: Octopus will run in 3 dimension(s)
Info: Octopus will treat system as periodic in 0 dimension(s)
Info: Boundary conditions: zero wave-functions
Info: Reading pseudopotential from file:
      '/home/alberto/software/octopus/1.4a/share/octopus/PP/TM2/N.ascii'
      Calculating atomic pseudo-eigenfunctions for specie N ....
      Done.
Info: l =  0 component used as local potential
  Type = sphere
  Radius  [A] =   5.000
  Spacing [A] = ( 0.180, 0.180, 0.180)    volume/point [A^3] =  0.00583
  # inner mesh =  89727
  Grid Cutoff [eV] =  1160.595
Info: Derivatives calculated in real-space
Info: Local Potential in Real Space.
Info: Using FFTs with spherical cutoff
      to solve Poisson equation
Info: FFT allocated with size ( 125, 125, 125) in slot  1
Info: Poisson Cutoff Radius [A] =    11.250000
Info: Exchange and correlation
      Exchange    : LDA  - non-relat.
      Correlation : LDA  - PZ81
Info: Allocating rpsi.
```

```
Info: Performing initial LCAO calculation.
Info: LCAO basis dimension:      4
Eigenvalues [eV]
 #st    Eigenvalue    Occupation
```

```
System name: system

Mesh:
  Type = sphere
  Radius  [A] =   5.000
  Spacing [A] = ( 0.180, 0.180, 0.180)    volume/point [A^3] =  0.0
```

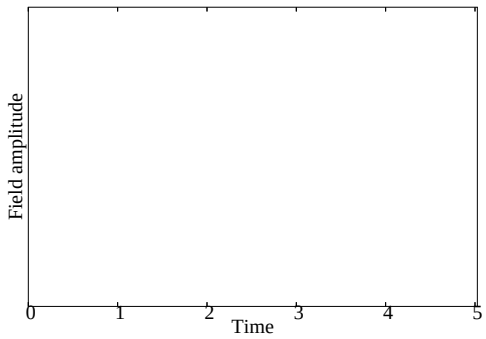
```
OutputWfs = yes
OutputWfsNumber = ‘‘1-4’’
OutputDX = yes
OutputAxisX = yes
OutputAxisY = yes
OutputAxisZ = yes
```

**You will now notice that the convergence procedure is closed in only one iteration; the reason is that**

**Exercise 1:**

† **You may investigate the e□ects of the di□erent SCF related va**

- **Next three columns (headed**


Field amplitude
0
1
2
3
4
5
Time

```
SystemName="He"
CalculationMode = gs_start
Dimensions=2
NonInteractingElectrons = yes
radius = 10
spacing = 0.1
OutputWfs = yes
OutoutPlaneZ = yes
%Species
"He" | 4 | 1 | "-2/(1+x^2)^(1/2)-2/(1+y^2)^(1/2)+1/(1+(x-y)^2)^(1/2)"
```