A

```
CalculationMode = gs_start

units = 'eVA'

Nitrogen_mass = 14.0
Nitrogen_z = 7

%Species
'N' | Nitrogen_mass | Nitrogen_z | 'tm2' | 1 | 0
%

XYZCoordinates = 'N.xyz'

ExtraStates = 1
%Occupations
2 | 1 | 1 | 1
%

BoxShape = sphere
radius = 5.0
spacing = 0.18

LocalPotentialSpace = real_space

TypeOfMixing = broyden
```

Input File 1: The Nitrogen atom

@ CalculationMode = gs_start
This variable de nes the run mode { please consult the man

The following two entries require some knowledge of what nonlocal pseudopotentials are,

```
Info: Performing initial LCAO calculation.
Info: LCAO basis dimension:      4
Eigenvalues [eV]
 #st   Eigenvalue    Occupation
   1   -17.420305       2.000000
   2    -6.377044       1.000000
   3    -6.377044       1.000000
   4    -6.377044       1.000000
Info: SCF using real wavefunctions.
Info: SCF mixing the density.
Info: Broyden mixing used. It can (i) boost your
```

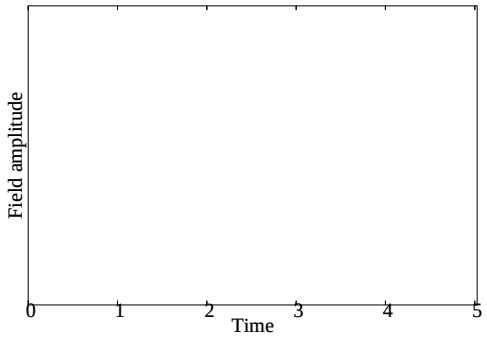
```
OutputWfs = yes
OutputWfsNumber = ``1-4''
OutputDX = yes
OutputAxisX = yes
OutputAxisY = yes
OutputAxisZ = yes
```

You will now notice that the convergence procedure is closed in only one iterar08y

this particular example, are shown in Figure 2. A rather good spacing for this Nitrogen pseudopotential seems to be 0.18A; probably

- **You may want to check how good the LDA vibrational frequency is;**

- **Next three columns (headed** `n.dip.(1)`**,** `n.dip.(2)` **and** `n.dip.(3)`**) represent the dipole**


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)"
%
%Coordinates
"He" | 0 | 0 | 0 | no
%
```

Input File 7: The 1D-modebf the Helium atom

A Visualizationwith OpenDX