2 Copying

The octopus Copying Conditions

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if you are using the Absoft Fortran 90 compiler on a linux machine. Also, if you have some of the required libraries in some unusual directories, these directories may be placed in the variable LDFLAGS (e.g., export LDFLAGS=$LDFLAGS:/opt/lib/).

The configuration script will try to find out which compiler you are using. Unfortunately, and due to the nature of the primitive language that octopus is programmed in, the automatic test fails very often. Often it is better to set the variable FCFLAGS

- `--with-fft-lib=<lib>`: **Instruct the** `configure` **script to look for the fftw library exactly in the waey that it is specified in the** `<lib>` **argument, i.e** `--with-fft-lib='-L/opt/lib -lfftw3'`.
- `--with-blas=<lib>`: **Instruct the** `configure` **script o look for the as library in the waey that it is specified in the**

3.3 Di□erent octopus executables

By performing the standard install, you will get an executable called `octopus`**, and a set of utility programs called** `oct-`**something. However, the code may be compiled di□erently in order to profit from special feautures (e.g parallel executables, etc). The following is**

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“td.x” directories, during evolution, where “x” stands for

6 Input Variables

octopus Has quite a few options, tHat we will subdivide in di erent groups. After tHe name of tHe option, its type and default value (wHen applicable) are given in parentHesis.

6.1 Generalities

- **CalculationMode**
  Section: Generalities
  Type: integer
  Defaoo
  - gs

6.1.2 IO

- **FlushMessages**
  Section: Generalities::IO
  Type

Type: block

This option is only used when `GuessMagnetDensity` **is set to** `user_defined`**. It provides a directis**

Options:

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- **PoissonSolverThreshold**

The calculation of the excitation spectrum of a system in the frequency-domain formulation of linear-response time-dependent density functional t

the

- **SparskitRelTolerance**
  Section: Math::General
  Type: float
  Default:

Type: float

This number determines the distance over which Euclidean coordinates are e esve

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Gillan, Chem. Phys. Lett. 325, 473 (2000)].

- **broyden**

in tun calcuated considering the nature of the species sup plied in the `Species` **block, an th valu of the** `ExcessCharge` **variable. However, one may command** `octopus`

- **SpinComponents**
  Section: States
  Type: integer
  Default: unpolarized

6.7.3 Velocities

- **RandomVelocityTemp**

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Default: 1

Fourier-space, and the latter in real space. The necessary transformations are performed with the FFT algorithm.

$$U_{SO}(t + \delta t, t) = \exp\{-$$

$$U_{EM}(t + \Delta t, t) = \exp\left[-i\Delta t H_{t+\frac{\Delta t}{2}}\right].$$

- magnus (5): Magnus Expansion (M4). This is o

Type: float
Default: 1e-5

An internal tolerance variable for the Lanczos method. The smaller, the more precisely the exponential is calculated, and also the bigger the dimen

- "-"

7 Undocumented Variables

8.8 oct-make-st

make_st **reads** tmp/restart.static

8.10 wf.net

This is an OpenDX network, aimed at the visualization of wave-functions. To be able to use it, you need to have properly installed the OpenDX program (get it at opendx.org), as well as the Chemistry extensions obtainable at the Cornell Theory Center (http://www.tc.cornell.edu/Services/Vis/dx/index.asp). Once these are working, you may follow a small tutorial on wf.net **by following next steps:**

- **Place in a directory the program wf.net, the (needed) auxiliary file wf.cfg, and the sample inp file that can all be found in** OCTOPUS-HOME**/util.**
- **Run** octopus**. The inp file used prescribes the calculation of the C atom in its ground state, in spin-polarized mode. It also prescribes that the wave-functions should be**

```
                functional: non-relativistic
      Correlation family    : LDA
                functional: Perdew-Zunger
Info: Allocating rpsi.
Info: Random generating starting wavefunctions.
Info: Unnormalized total charge =      0.998807
Info: Renormalized total charge =      1.000000
Info: Setting up Hamiltonian.
Info: Performing LCAO calculation.
Info: LCAO basis dimension:      1
      (not considering spin or k-points)
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.102098       1.000000
Info: SCF using real wavefunctions.
Info: Broyden mixing used. It can (i) boost pour convergence,
      (ii) do nothing special, or (iii) totally screw up the run.
      Good luck!
Info: Converged =     0
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.102975       1.000000      (2.8E-02)
Info: iter =    1 abs_dens = 0.53E-03 abs_ener = 0.60E+00

Info: Converged =     0
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.102477       1.000000      (1.4E-03)
Info: iter =    2 abs_dens = 0.43E-03 abs_ener = 0.65E-05

Info: Converged =     1
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.102419       1.000000      (5.1E-04)
Info: iter =    3 abs_dens = 0.39E-04 abs_ener = 0.20E-06

Info: Converged =     1
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.10249886(9)0.296       1.000000      (8.5E-05)
Info: iter =    4 abs_dens = 0.24E-04 abs_ener = 0.52E-08

Info: Converged =     1
Eigenvalues [H]
   #   Eigenvalue    Occupation      Error (1)
   1    -0.10249886(9)0.297       1.000000      (1.5E-06)
Info: iter =    5 abs_dens = 0.14E-05 abs_ener = 0.36E-10
```

```
C  0.000 -1.396  0.000
C -1.209 -0.698  0.000
C -1.209  0.698  0.000
H  0.000  2.479  0.000
H  2.147  1.240  0.000
H  2.147 -1.240  0.000
H  0.000 -2.479  0.000
H -2.147 -1.240  0.000
H -2.147  1.240  0.000
```

W

X