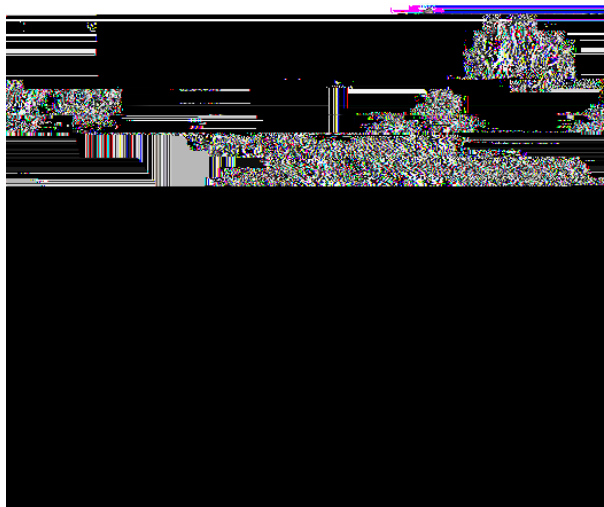


# the octopus manual

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Version 1.99devel

Electronic Structure  
Molecular Dynamics  
Excited-State Dynamics  
Recipes-Generator  
March 2005





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**The** octopus







The main developing team of this program is composed of:

- Miguel A. L. Marques (Donostia International Physics Center, San Sebastián, España)
-







the

determines the time-dependent density, just as in the Hohenberg-Kohn formalism the static ground state density is given by the minimum of the total energy ( $E[\rho]$  for  $\rho(r) \geq 0$ )<sup>2</sup>

## 2 Installation

Maybe somebody else installed the octopus for you. In that case, the files should be under some directory that we can call PREFIX: the executables in PREFIX/bin (e.g. if PREFIX=/usr/local, the main octopus executable is then /usr/local/bin/octopus); the documentation in info format in PREFIX/info (so that you may see it by typing info -f PREFIX/info/octopus.info if the info program is installed in your system); some sample files in PREFIX/share/octopus/samples; the pseudopotential files that octopus

5. gsl: Finally that someone had the nice idea of making a public sci



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

## 2.3 Different octopus executables



Whatever went wrong...: Up to now, we cannot really make a list of common errors. J/R3581.6163584



If octopus



#### 4.1.6 UnitsOutput

**the** octopus

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**4.4.6 DerivativesSpace (integer, real\_space)**

Defines in which space gradients and the Laplacian are calcul

### 4.5.3 ExtraStates

### 4.6.3 Local Potential Space (**integer**, **fourier\_space**)

If `fourier_space`

- OEP\_level = oep\_kli
- OEP\_level = oep\_ceda
- OEP\_level = oep\_full

#### 4.7.4 SICCorrection (integer, 0)

### 4.8 SCF



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This method amounts to a straightforward application of the



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## 5.8 oct-make-st

make\_st reads tmp/restart.static



## 6 Undocumented Variables

If you want to use these variableh you will have to go to the code to find out what they

## 7 Examples

### 7.0.1 Hello world

As a first example, we will create a simple program that prints "Hello world". The program is written in C and is located in the file `hello.c` in the directory `src`. The program is compiled and run as follows:

```

$ gcc -o hello hello.c
$ ./hello
Hello world

```

The output of the program is "Hello world". The program is a simple example of a program that prints a string to the standard output.





Info: SCF converged in 5 iterations  
Info: Deallocating rpsi.

C	0.000	-1.396	0.000
C	-1.209	-0.698	0.000

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