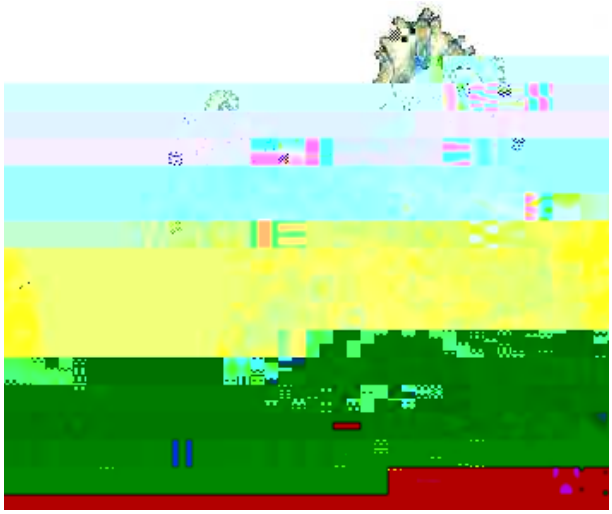
the octopus **manual**

Electronic Structure
Molecular Dynamics
Excited-State Dynamics
Recipes-Generator
March 2002



Male Hapalochlaena lunulata (top),
and female Hapalochlaena lunulata (bottom).
Photograph by Roy Caldwell.

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2 Authors, Collaborators and Acknowledgements.

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3 Introduction

3.1 Description of octopus

octopus is a program aimed at the ab initio virtual experimentation on electron/ion dynamics in external electromagnetic fields of arbitrary intensity, shape and frequency in a hopefully ever increasing range of systems types. Its main characteristics are:

- Electrons are described quantum-mechanically within the Density-Functional Theory (DFT) for the ground-state whereas the excitation spectra is computed using time-dependent form (TDDFT) by performing simulations in time.
- The electron-nucleus interaction is described within the pseudo-potential approximation. Nuclei are described classically as point particles.
- Wave-functions are expanded in a real-space grid. The kinetic energy operator is computed with a high-order finite difference method. FFTs are used in part of the calculations. Time and grid spacing are related by imposing a stable time-evolution.
- Forces on the ions are computed through the Ehrenfest theorem. Extension to quant mechanical nuclear dynamics is in progress.
- Allows for spin-polarised calculations as well as non-collinear magnetism and spin-orbit effects.
- Computes photo-electron (energy and angle resolved) and photo-absorption spectra for different polarised external electromagnetic fields. Linear response calculations are a simple case of this general time-evolution procedure (see below).
- Includes non-linear electronic effects: high-harmonic generae9:

3.2 Time dependent density functional theory

Several reviews of time-dependent density function theory (TDDFT) and its applications have appeared recently, like the works by

determines the time-dependent

browse at http://nautilus.fis.uc.pt/cgi-bin/cvsweb.cgi/marques/octo

`absoft (i386)'
-O3 -YEXT_NAMES=LCS -YEXT_SFX=_

`absoft (opteron)'
-O3 -mcmodel=medium -m64 -cpu:host -YEXT_NAMES=LCS -YEXT_SFX=_

`NAG (opteron)'
-colour -kind=byte -mismatch_all -abi=64 -ieee=full -O4 -Ounroll=4

`pgi (opteron)'
-fast -mcmodel=medium -O4

`alpha' -align dcommons -fast -tune host -arch host -noautomatic

`xlf (IBM)'
-bmaxdata:0x80000000 -qmaxmem=-1 -qsuffix=f=f90 -Q -O5 -qstrict
-qtune=auto -qarch=auto -qhot -qipa

`sgi' -O3 -INLINE -n32 -LANG:recursive=on

You can now run the configure script (./configure**).** **You can use a fair amount of options to spice** octopus **to your own taste. To**

Section 6.1.7 [Verbose], pag pag Section [DebugLevel], pag pag 14,
tively).

Run make, and then makepag install. If everything went ne, you should now be able pag to pag Depending on the options passed
pre xes could be added to the generic name pag pag

Whatever went wron ron ron t o

5 The parser

All input options should be in

If octopus tries to a variable that is de nit()Tj 38.0945 0 Td (in)Tj 13.2981 0 Td (the)Tj /R43 10.90
todefault value. All variablese to le If you
0 Td (is)Tof13.298105 0 Tdthe)wTj 24.1973 0 Td (a)TjTj 19.5273 0 Td (inp)program40.7136 0 Td (triej 11.6182 4 0 Tdnot)

6 Input file options

`octopus` **has quite a few options, that we will subdivide in different groups. After the name of**

– **Oxygen labelled 'O'. Next number is the atomic mass (in atomic mass units), and third eld, the atomic number (8, inand'**

- columns 31-54 : The Cartesian coordinates. The Fortran format is '(3f8.3)'.
- columns 61-65 : Classical charge of the atom. The Fortran format is '(f6.2)'.

6.3.2 XYZCoordinates (string, 'coords.xyz')

If PDBCoordinates is not present, reads the atomic coordinates from the XYZ file XYZCoordinates. The XYZ format is very simple, as can be seem from this example for the CO molecule (in A).

```
2
CO molecule in equilibrium
    C  -0.56415   0.0   0.0
    O   0.56415   0.0   0.0
```

The first line of the file has an integer indicating the number of atoms. The second can contain comments that are simply ignored by octopus. Then there follows one line per each atom, containing the chemical species and the Cartesian coordinates of the atom.

6.3.3 Coordinates (block data)

If neither a XYZCoordinates nor a PDBCoordinates was found, octopus tries to read the coordinates for the atoms from the block Coordinates. The format is quite straightforward:

```
%Coordinates
  'C' | -0.56415 | 0.0 | 0.0 | no
  'O' |  0.56415 | 0.0 | 0.0 | no
%
```

The first line defines a Carbon atom at coordinates (-0.56415, 0.0, 0.0), that is not allowed to move during block obviously defines

6.3.6 RandomVelocityTemp (double, 0)

If this variable is present, octopus **will assign random velocities to the atoms following a Bolzmann distribution with temperature** RandomVelocityTemp**.**

– fourier_space: **Derivatives are calculated in reciprocal space. Obviously this case implies cyclic boundary conditions, so be careful.**

```
%Occupations
```

- random: **Each atomic magnetization density is randomly rotated.**
- user_defined: **The atomic magnetization densities are rotated so that the magnetization vector has the same direction as a vector provided**

6.8.12 EigenSolverFinalTolerance (double, 1.0e-14)

This is the final tolerance for the eigenvectors.

6.8.13 EigenSolverFinalToleranceIteration (integer, 7)

Determines how many iterations are needed to go from EigenSolverInitTolerance to EigenSolverFinalTolerance.

6.8.14 EigenSolverMaxIter (integer, 25)

6.10 Time Dependent

invoked as a means to approximate the evolution operator (TDEvolutionMethod = 0),
a different procedure is taken – it will be describ

where J_k are the Bessel functions of the first kind, and H has te be previously scaled to $[-1;1]$. See H. Tal-Ezer and R.

It may the be

– 10: **Shape is read from a file.**

If envelope=10**, the** t0 **parameter is substituted by a string that determines the name of the file. The format of this file should be three columns of real numbers: time, field and phase. Atomic units are assumed. The values for the laser field that the program will use are interpolated / extrapolated from this numerically defined function.**

6.10.8 TDGauge (integer, length)

In which gauge to treat the laser. Options are:

– length: **Length gauge.**

– velocity: **Velocity gauge.**

6.10.9 TDDeltaStrength (double, 0.0 a.u.)

When no laser is applied, a delta (in time) electric field with strength TDDeltaStrength **is applied. This is used to calculate the linear**

6.10.16 TDOutputLaser (logical, true)

If true, octopus outputs the laser field to the file "td.general/laser".

6.10.17 TDOutputElEnergy (logical, false)

If true, octopus outputs the different components of the electronic energy to the file td.general/el_energy.

6.10.18 TDOutputOccAnalysis (logical, false)

If true, outputs the projections of the time-dependent KohnSham

6.11.4 GOStep (double, 0.5)

Initial step for the geometry optimizer.

6.12.7 OutputAxisX (logical, false)

The values of the function on the x axis are printed. The string \.y=0,z=0" is appended to previous le names.

6.12.8 OutputAxisY (logical, false)

The values of the function on the y axis are printed. The string \.x=0,z=0" is appended to previous le names.

6.12.9 OutputAxisZ (logical, false)

6.12.8 isappended

The values of the function on the z axis are printed.

6.14.2 POLStaticField (double, 0.001 a.u.)

7.8 oct-make-st

make_st reads tmp/restart.static and replaces some of the Kohn-Sham states by Gaussians wave packets. The states which should be replaced are given in the %MakeStates section in the inp le and written to tmp/restart.static.new. (You probably want to copy that le to tmp/restart.static and use then CalculationMode=5 or 6.)

```
%MakeStates
  ik | ist | idtypesigma | x0 | k
%
```

The values stand for

- ik: The k point (or the spin, if spin-components=2) of the state
- ist: The state to be replaced
- id: The component of the state (if the wave functions have more one componen
omponents=3 is used).

wave packet; currently only 1 (Gaussian) is available

pend on the type chosen. For a Gaussian wave packet, de ned as

$$(x) = \frac{}{\sqrt{2}} e^{i k x \; x_0} e^{\left(\frac{}{2 \; 2} \right)};$$

they are:

- the width of the Gaussian
  - k: the k vector. In 3D use k1|k2|k3.
  - x : the coordinate where the Gaussian is initially centred. In 3D use x01|x02|x03.

7.9 oct-center-geo

7.10 wf.net

This is an OpenDX network, aimed at the visualization

8 Undocumented Variables

If you want to use these variables you will have to go to the code to let y

```
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
```

Follow now the steps of the previous example. Carbon and Hydrogen have a hgh-pbe.mpllo-2.14pseudo-pe.

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