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1 Authors

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3 Installation

Maybe somebody else installed the octopus for you. In that case, the files should be under some

5. gsl: Finally that someone had the nice idea of making a public scientific library!
gsl still needs to grow,

3.3 Different octopus executables

By performing the standard install, you will get an executable called `octopus`, and a set of utility programs called `oct-something`.

4 The parser

All input options should be in a file called 'inp', in the directory octopus is run from. Alternatively, if this file is not found, standard input is read. For a fairly comprehensive example, just look at the file `OCTOPUS_HOME/share/samples/Na2` | if you installed the code (you did the `make install`), this file will also

If octopus tries to read a variable that is not defined in the input file, it automatically assigns to it a default value. All variables read at startup have a default value. If you are not sure of what the "4

5 Description

5.1 Mesh

`octopus` uses a grid in real space to solve the Kohn-Sham equations. The grid is equally-spaced, but the spacings can be different for each Cartesian

`\td.x`" directories, during evolution, where `\x`" stands for the iteration number at which each write is done. Note that if you wish to plot any function (`OutputKSPotential = yes`, etc.), at least one of the output formats should be enabled (`OutputPlaneX = yes`, `OutputDX = yes`, `OutputNETCDF = yes`, etc.). [This is not necessary if you wish to plot the geometry (`OutputGeometry = yes`)]. Note further that the data written by `OutputAxisX`, `OutputPlaneX` etc. has always the (side) length of the longest axis; this is independent from the chosen geometry. Data points which are inexistent in the actual geometry have the value zero in those files.

5.6 Spectrum calculations

Once octopus has been run, results

6.1.1 Debug

DebugLevel

Section: Generalities::Debug

Type: integer

Default: 1

This variable decides whether or not you want to send debugging mode, the memory it is using (only for the moment being, in Linux systems), and some other information. As a server developer, you have two options: (i) setting it to zero (or less than zero, in which case you do not run debugging mode (this is the default) or (ii)

6.1.3 Parallel

= "eVA", all physical values in the input files will be considered to be in eV and Angstroms.

UnitsOutput

Section: Generalities::Units

Type: string

Default: "a.u"

Same as "Units", but only refers to the values in the output files. That is, if UnitsInput = "eVA", all physical values in the output files will be considered to be in eV and Angstroms.

6.2 Geometry Optimization

GOMaxIter

Section: Geometry Optimization

Type: integer

Default: 200

Even if previous convergence criterium is not satisfied, minimum number of iterations /Rs.

will stop after this

GOMethod

Section: Geometry Optimization

Type: integer

Default: steep

Method by which the minimum

is performed.

Options :

steep (1): simple steepest descent.

GOSTep

Section: Geometry Optimization

Type: float

Default: 0.5

Stop at

Type: float

Default: 200

descent is not a 8.50 a.u. in

Even

Type: block

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

Options:

non_

refers to the radius of the cylinder if `VlocalCuto = 1`, to the thickness of the slab if `VlocalCuto =`

Type: integer

Default: lda_c_pz

Defines the correlation functional

Options:

gga_c_pbe (102): Perdew, Burke & Ernzerhof correlation

lda_c_pw (10): LDA: Perdew & Wang

lda_c_ob_pw (11): LDA: Ortiz correlation
(11): Defines the correlation functional

SICorrection**Section: Hamiltonian::XC****Type: integer****Default: sic_none**

This variable controls which Self Interaction Correction to use. Note that this correction will be applied

`root_newton (3): Newton method`

`root_laguerre (4): Laguerre method`

`root_watterstrom (5): Watterstrom method`

`RootSolverAbsTolerance`

mesh_log (3): Double logarithmic mesh

mesh_sinh (4): Sinh mesh

gauss_legendre (5): Gauss-Legendre mesh

SparskitAbsTolerance

Section: Math::Ge-eral

Type: oat

Default: 1e-8

Some Sparskit solver use an absolute tolerance as stopping

sk_cgnr (2): Conjugate Gradient Method (Normal Residual equation)
sk_bcg (3): Bi-Conjugate Gradient Method
sk_dbcg (4): BCG with partial pivoting
sk_bcgstab (5): BCG stabilized
sk_tfqmr (6): Transpose-Free Quasi-Minimum Residual method
sk_fom (7): Full Orthogonalization Method
sk_gmres (8): Generalized Minimum Residual method
sk_fgmres (9): Flexible version of Generalized Minimum Residual method

W

`curv_gygi (2)`: The deformation of the grid is done according to the scheme described by F. Gygi [F. Gygi and G.

Default: minimum

This variable decides the shape of the simulation box. Note that some incompatibilities apply:

will attempt to use a suitable default, but this is not always p

Which wavefunctions to print, in list form, i.e., "1-5" to print the first five states, "2,3" states,

Type: oat
Default: 1e-5

Absolute convergence of the density: $= \int d^3r (\rho_{out}(r) - \rho_{inp}(r))^2$. A zero value means do not use this criterion.

ConvAbsEv
Section: SCF::Convergence
Type: oat
Default: 0.0

Absolute convergence of the eigenvalues: $= \sum_{j=1}^{N_{occ}} |\epsilon_{out,j} - \epsilon_{inp,j}|$. A zero value means do not use this criterion.

ConvRelDens
Section: SCF::Convergence
Type: oat
Default: 0.0

Relative convergence of the density: $= \frac{1}{N} \int d^3r (\rho_{out}(r) - \rho_{inp}(r))^2$. N is the total number of electrons in the problem. A zero value means do not use this criterion.

ConvRelEv
Section: SCF::Convergence
Type: oat
Default: 0.0

Relative convergence of the eigenvalues: =

SCF

Determines the maximum number of iterations for the eigensolver (per state) { that is, if this number is reached, the diagonalization is stopped even if the desired tolerance was not achieved. Must be larger or equal than 1.

6.5.3 Mixing

perSteps

Section: SCF::Mixing

Type: integer

Default: 3

In the Broyden and in the GR-Pulay scheme, the new input c

6.6 States

CenterOfInversion

Section: States

Type: integer

Default: no

Only used in 1D periodic calculation to enforce the correspondig symmetry in the Brillouin Zone

Options:

no: The system has no center of inversion: use the whole BZ

yes (1): The system has a center of inversion: use half BZ

ElectronicTemperature

Section: States

Type: oat

Default: 0.0

If Occupations is not set, ElectronicTemperature is the temperature in the Fermi-Dirac function used to distribute the electrons among the existing states.

ExcessCharge

Section: States

Type: oat

Default: 0.0

The net charge of the system. A negative value means that we are adding electrons, while a positive value means that we are removing electrons.

and the value of the ExcessCharge variable. However, one may command octopus to put more states, which is necessary if one wants to use fractional occupational numbers, either fixed from the origin through the Occupations block by prescribing an electronic temperature with ElectronicTemperature.

kpoints is usually reduced exploiting the symmetries of the system. For example, the following input samples the BZ with 100 points in the xy plane of the reciprocal space

```
%NumberKPoints
10 | 10 | 1
%
```

Occupations

Section: States

Type: block

The occupation numbers of the orbitals can be fixed through the use of this variable.
For

The first line defines a Carbon atom at coordinates ("-0.56415", "0.0", "0.0"), that is *_not_* allowed to move during dynamical simulations. The second line has a similar meaning. This block obviously defines a Carbon monoxide molecule, if the input units are AA. Note that in this way it is possible to fix some of the atoms (this is not possible when specifying the coordinates through a "PDBCoordinates" or "XYZCoordinates" file). It is always possible to fix *_all_* atoms using the "MoveIons"

Note that some common pseudopotentials are distributed with the code in the directory OCTOPUS-HOME/share/PP/. To use these pseudopotentials you are not required to define them explicitly

If XYZVelocities is not present, octopus will try to fetch the initial atomic velocities from this block. If this block is not preseno

The "envelope" decides the shape of the enveloping function { see the manual for details. "tau0", "t0" and "tau1" are three parameters that decide on the temporal shape of the pulse { the exact details depend on the particular envelope.

TDDeltaStrengthMode
Section

It may be demonstrated that the order of the error of the algorithm is the same as the one that we would have by making use of the Exponential Midpoint Rule (EM, described below).

TDExpOrder

Section: Time Dependent::Propagation

Type: integer

Default: 4

For TDExponentialMethod **equal** standard **or** chebyshev, the order to which the exponential is expanded. For the Lanczos approximation, it is the maximum Lanczos-subspace dimension.

TDExponentialMethod

agation

Tech(yp)Tj 10olu (t::Pro3czo2091 Tf 3
26700(08030f (190924429 (5da9d (,)Tj,648299de (10.90911)Tfj 10.69550 Tdu(43)Tj11960882 D57ek35)Tj,6694009rically 0 T518.50)Tj

lanczos (2): Allows for larger time-steps. However, the larger the time-step, the longer the computational time per time-step. In certain cases, if the time-step is too large, the code will emit a warning whenever it considers that the evolution may not be properly proceeding { the Lanczos process did not conv

TDMaxim

td.general (256) function on the static (zero) projections of the time-dependent Kohn-Sham wavefunctions onto the static (zero) projections of the time-dependent angular (2): Outputs the angular momentum of

If SpecDampMode is set to "exp", the damping parameter of the exponential is fixed through this variable.

SpecDampMode

Section: Utilities::Optical Spectra

Type: integer

Default: polynomial

Decides which damping/ Itering is to be applied

Type: integer
Default: inertia

7 Undocumented Variables

If you want to use these variables you will have to go to the code to find out what they do. If you do it, please take the time to write a short description and send a patch of the manual to us ;) BTW, some of this Tj 34.3963 0 Td (some)Tj 28.2760 Td (y)TU

8 External utilities

A few small programs are generated along with `octopus`, for the purpose of post-processing the generated information. These utilities should all be run from the directory where `octopus` was run, so that it may see the input file, and the directories created by it.

8.1 `oct-sf`

This utility generates the dipole strength function of the given system. Its main input is the `td.general/multipoles` file. Output is written to a file called `spectrum`. This file is made of two columns: energy (in eV or a.u., depending on the units specified in the input file), and dipole strength function (in 1/eV, or 1/a.u., idem).

In

In

8.8 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 input

8.10 wf.net

This


```
functional: non-relativistic
Correlation family : LDA
functional: Perdew-Zunger
Info: Allocating rpsi.
Info: Random generating starting wavefunctions.
Info: Unnormalized total
```


Info: SCF converged in 5 iterations

Info: Deallocating rpsi.

Info: Calculation ended on 2003/03/17 at 03:50:04

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 much harder pseudo-potential than Sodium, so harder to have

H

.....	32
.....	53
.....	53

J

.....	23
-------	----

L

.....	34
.....	24
.....	31

M

.....	56
.....	56
.....	35
.....	37
.....	37
.....	45
.....	15
.....	19

N

.....	19
.....	38
.....	51

O

.....	39
.....	25
.....	25
.....	23
.....	32

.....	28
.....	37
.....	16
.....	51

X

.....	24
.....	32
.....	41
.....	43