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1 Authors

The main developing team of this program is composed of:

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3 Installation

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

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

the octopus 2.0rc1 man

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.

4 The parser

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

is 3.05 consider Ti 37.52.70 I Td 70
If octopus tries to read a variable that is not de ned in the input le, it automatically assigns to it a default value. All Madia 20 read 7 ot Toju 2000 to value 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 di erent 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, OutputDX = yes, OutputDX = yes, 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 les.

5.6 Spectrum calculations

Once octopus has been run, results

6.1.1 Debug

DebugLevel

Section: Generalities::Debug

Type: integer Default: 1

exits the subroutines, what is the memory it is using decides wether or and atorwife you want in a send a bague point fonde, the memory it using confer the moment being in Liftuy systems) and some other the developers and nearly interest of the properties (i) setting it to zero, to or less than zero, in which case you do not ortruin debugging mode (this is the default) subjudited to Td (are) Tj 18.6872 0 Td (only) Tj 23.8363 0 Td (prin) Tj 19.1564 0 Td (ted) Tj 18.6872 0 Td (ded) Td (ded) Tj 18.6872 0 Td (ded) Tj 18.6872 0 Td (ded) Td (ded) Tj 18.6872 0 Td (ded) Td (

6.1.3 Parallel

= "eVA", all physical values in the input les 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 les. Thao is, if UnitsInput = "eVA", all physical values in the output les will be considered to be in eV and Angstroms.

6.2 Geometry Optimization

GOMaxIter

Section: Geometry Optimization

Type: integer Default: 200

Even if previous congence criterium is not satis ed, minion

will stop after this

 $number\ of\ iterTj\ /Rs.$

GOMethod

Section: Geometry Optimization

Type: integer Default: steep

Method by which the minion

is performed.

Opti/Rs:

steep (1): simple steepest descent.

GOStep

Section: Geometry Optimization

Type: oat Default: 0.5

Seype pT

Type: oat Default: 200

descen isnosa8.50aultin

Even

Type: block

This option is only used when GuessMagnetDensi ty is set to user_defi ned. It provides

Options:

non_

21

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

Type: integer Default: Ida_c_pz

De nes the correlation functional

Options:

gga_c_pbe (102): Perdew, Burke & Ernzerhof correlation

Ida_c_pw (10): LDA: Perdew & Wang

Ida_c_ob_pw (11): LDA: Ortiz con(fe16): R20411111 pulk 32 10.9091 Tf -235.887 -15.72 Td ()Tj /R69 1

SICorrection

Section: Hamiltonian::XC

Type: integer Default: sic_none

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

will be applyed

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.

the octopus 2.0rc1 manual

Default: minimum

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

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

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

Type: oat Default: 1e-5

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

ConvAbsEv

Section: SCF::Convergence

Type: oat Default: 0.0

Absolute convergence of the eigenvalues: $= \sum_{j=1}^{P} j^{out}$ inp j. A zero value means do not use this criterion.

ConvRelDens

Section: SCF::Convergence

Type: oat Default: 0.0

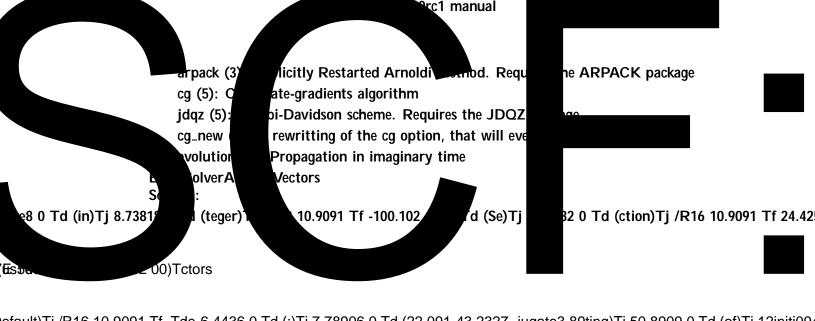
Relative convergence of the density: $=\frac{R}{N}d^3r(^{out}(r)^{inp}(r))^2$. N is the total number of electrons in the problem. A zero value means do not use this criterion.

ConvRelEv

Section: SCF::Convergence

Type: oat Default: 0.0

Relative convergence of the eigenvalues: =



efault)Tj /R16 10.9091 Tf Tde-6.4436 0 Td (:)Tj 7.78906 0 Td (22 091-43.2327 -jugate3.89ting)Tj 50.8909 0 Td (of)Tj 12initi094

Chapter 6: Input Variables

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
Section: SCF::Mixing

Type: integer Default: 3

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

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, Electronic Temperature 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, whi(y)Tj 28t36254atuTel (fa)This specifically supprinted by the system of the system. A negative value means that we are adding electrons, whi(y)Tj 28t36254atuTel (fa)This specifically specifical

and the value of the ExcessCharge variable. However, one may command octopus to put mory states, which isecessary if one wants to use fractional occupational numbers, either xed from the origin through the Occupations block by prescribing an electronic temperature with Electronic Temperature.

Bringd1**990as4Ris553**12edird)**(njræk)(tij) 273-3496358**j2120**1.5702(9)012j3 2179.025613**007toddg(d))tej 15.7149.080 11Td (an)n)Tj1 T4h8582 0 Ttcd (**5te) Tj** 6.04.69107 103.31982

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

Occupations Section: States Type: block

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

The rst line de nes 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 de nes a Carbon monoxide molecule, if the input units are AA. Note that in this way it is pssible to x some of the atoms (this is not pssible when specifying the coordinates through a "PDBCoordinates" or "XYZCoordinates" le). It is always pssible to x _all_atoms using the "Movelons"

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 de ne 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

the octopus

the external potential that we know at all times since it is imposed to the system by us (e.g. a laser eld): $V(t) = V_{int}(t) + V_{ext}(t)$. Then we de ne to be V to be the sum of $V_{ext}(t + t=2)$ and the internal potential built from the wavefunctions after applying the righw kinetic term of the equation, expf i t=2Tg.

It may the be demonstrated that the order of the error of the algorithm is the same that the one that we would have by making use of the Exponential Midpoint Rule (EM, described beln \(\frac{7}{4}\) bu636 0 Td (ed) Tj 13.6),8.9164 2(ed) Tj 13.j 17.9672 0 Td (algor SO7.9672 3 Td (the context of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of the algorithm is the same that the order of the error of th

agation

TDExpOrder

Section: Time Dependent::Propagation

Type: integer Default: 4

For TDExponential Method equal standard or chebyshev, the order to which the exponential is expanded. For the Lanczos approximation, it is the maximum Lanczos-

subspace dimension.

TDExponentialMethodev

nTeah(yp)Tj 10olu (t::Pro3czo2091 Tf 3

2 6Toobr(08a1BOTcf (1900921Lat297(5dta@cff(,)319).6648299205fe T(st0a9900911)Tffj 1139.69985500 TTobb17(480))Tfjj11966481802 T050Teb1315(01971,66694900994riscally 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

e-functions to the le td. getdepotupro(256) functions to the uthe uttatith (zeprotions) of the time-dependent angular (2): Outputs the angular momentum of

If SpecDampMode is set to "exp", the damping parameter of the exponential is xed 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 nd 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 le, 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 /mul ti pol es le. Output is written to a le called spectrum. This le is made of two columns: energy (in eV or a.u., depending on the units speci ed in the input le), and dipole strength function (in 1/eV, or 1/a.u., idem).

In

8.8 oct-make-st

 $\label{lem:make_st_reads} $$ make_st_reads tmp/restart. static and replaces some of the Kohn-Sham states by Gaussians wave packets. The states which should be replaced are given in the $$ 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

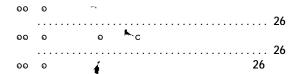
```
C 0.000 -1.396 0.000
C -1.209 -0.698 0.000
H 0.000 2.479 0.000
H 2.147 1.240 0.000
H 2.147 -1.240 0.000
H 0.000 -2.479 0.000
H -2.147 -1.240 0.000
H -2.147 1.240 0.000
```

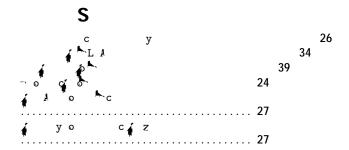
Follow now the steps of the previous example. Carbon and Hydrogen have a much harder pseudo-potential than Sodium, solanderyilal have

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