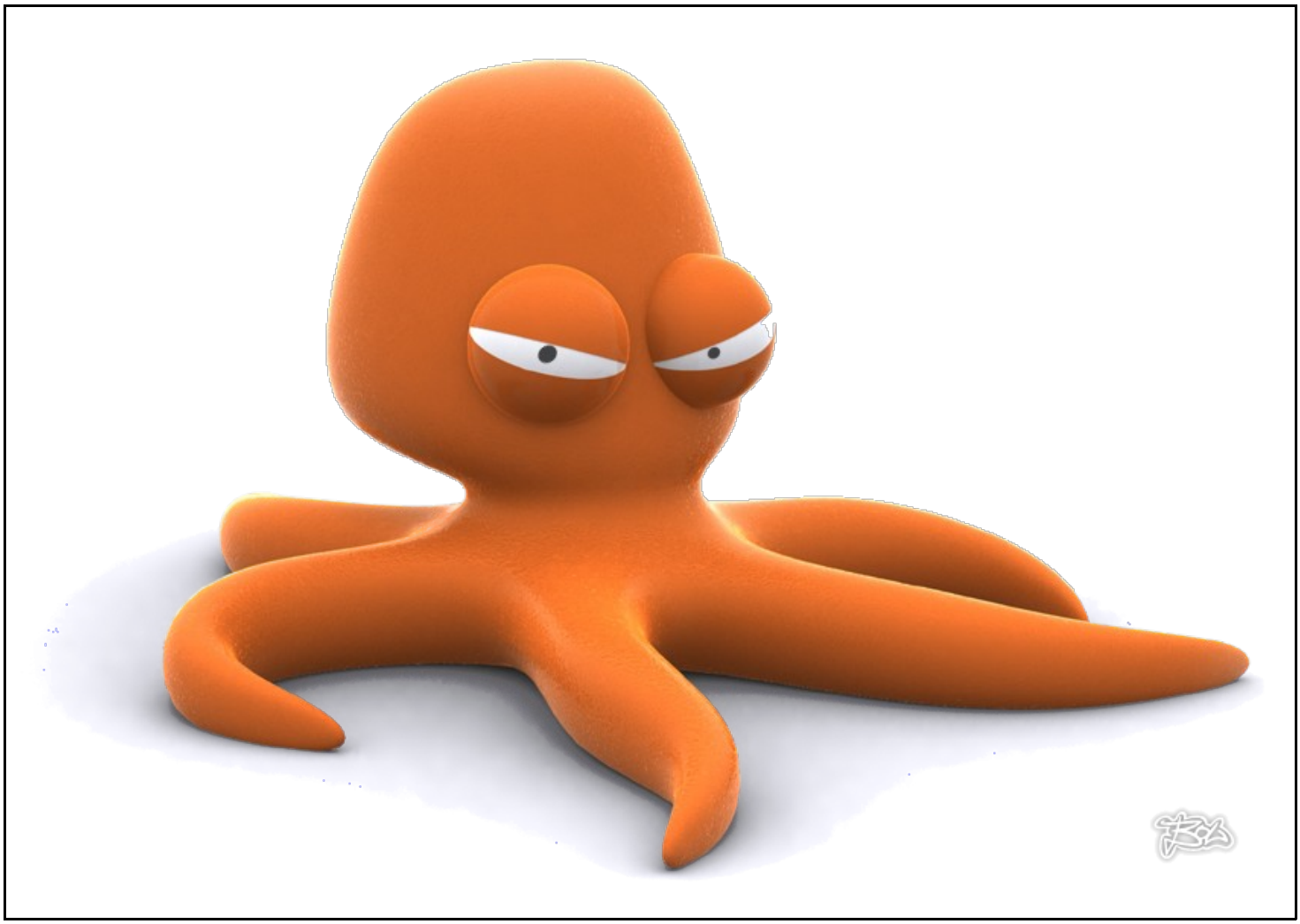


Version 6.0

(From the OctopusWiki)

Alberto Castro
Angel Rubio
Carlo Andrea Rozzi
Florian Lorenzen
Heiko Appel
Micael Oliveira
Miguel A. L. Marques
Xavier Andrade - **David A. Strubbe**

Contents

If you are going to collaborate, please check Writing Documentation.
If you want to know what you can do check for open tickets: [1]
If you want to print or download the whole manual there is a PDF version available.

About This Manual

Copying

This manual is for Octopus 6.0, a first principles, electronic structure, excited states, time-dependent density functional theory program.

You can find a copy of the Free Documentation License here

Reading this manual

If you are new to Octopus it is recommended that you read this manual sequentially. To read this manual you need some basic knowledge of Density Functional Theory (DFT) and Time Dependent Density Functional Theory (TDDFT), also a bit of numerical methods may be useful.

The way to tell what to do Octopus is through input variables, each one of this variable has its proper documentation describing what it does and what are the possible values that it can take. All this documentation of the variables is contained in the Reference Manual Appendix. That information is complementary to this manual, here we will only give a brief description of the function of each variable and we will leave the details for the Reference Manual. If you are reading an electronic version of this manual, all references to input variables will be marked as hyperlinks, opening that link will take you a page with the reference documentation for that variable.

There are some styles used in this documents: "proper names" (like Fortran), "**`files and directories`**" (like **`inp`** or **`/tmp/`**), "*`commands`*" (like *`ls`*) and "`input file text`" (like `a=0.5`).

Getting help

If you need help using Octopus, you have any doubts about the content of this manual or you want to contact us for any reason, please do it so through the octopus users mailing list.

Contributing

This manual is developed using a Wiki, this means that you can directly cooperate with it. You can always find the original version in http://www.tddft.org/programs/octopus/wiki/index.php/Manual.

Previous Manual - Next Manual:About Octopus

Back to Manual <p class=newpage>

About Octopus

Octopus is a software package for density-functional theory (DFT), and time-dependent density functional theory (TDDFT).

Developers

The main development team of this program is composed of:

- Joseba Alberdi
- Xavien Andrade
- Alberto Castro
- Tilman Dannert
- Umberto De Giovannini
- Alain Delgado
- Nicole Helbig
- Hannes Huebener
- Joaquim Jornet-Somoza
- Ask Larsen
- Irina Lebedeva
- Miguel A. L. Marques
- Fernando Nogueira
- Micael Oliveira
- Carlo Andrea Rozzi
- Angel Rubio
- Ravindra Shinde
- Jose R. F. Sousa
- David Strubbe
- Iris Theophilou
- Alejandro Varas
- Matthieu Verstraete
- Philipp Wopperer

Former developers:

- Heiko Appel
- Fulvio Berardi
- Johanna Fuks
- David Kammerlander
- Kevin Krieger
- Florian Lorenzen
- Danilo Nitsche
- Roberto Olivares-Amaya
- Arto Sakko
- Axel Thimm
- Jessica Walkenhorst
- Jan Werschnik

Other contributors are:

- Sebastien Hamel
    - ♦ parallel version of oct-excite
- Eugene S. Kadantsev
    - ♦ linear response code

Introduction

Octopus is a pseudopotential real-space package aimed at the simulation of the electron-ion dynamics of one-, two-, and three-dimensional ?nite systems subject to time-dependent electromagnetic ?elds. The program is based on time-dependent density-functional theory (TDDFT) in the Kohn-Sham scheme. All quantities are expanded in a regular mesh in real space, and the simulations are performed in real time. The program has been successfully used to calculate linear and non-linear absorption spectra, harmonic spectra, laser induced fragmentation, etc. of a variety of systems. The fundamentals of DFT and TDDFT can be found, e.g., in the books [1]and [2]. All information about the octopus package can be found in its homepage, http://www.tddft.org/programs/octopus/, and in the articles [3]and [4].

The main advantage of real-space methods is the simplicity and intuitiveness of the whole procedure. First of all, quantities like the density or the wave-functions are very simple to visualize in real space. Furthermore, the method is fairly simple to implement numerically for 1-, 2-, or 3-dimensional systems, and for a variety of different boundary conditions. For example, one can study a finite system, a molecule, or a cluster without the need of a super-cell, simply by imposing that the wave-functions are zero at a surface far enough from the system. In the same way, an infinite system, a polymer, a surface, or bulk material can be studied by imposing the appropriate cyclic boundary conditions. Note also that in the real-space method there is only one convergence parameter, namely the grid-spacing, and that decreasing the grid spacing always improves the result.

Unfortunately, real-space methods suffer from a few drawbacks. For example, most of the real-space implementations are not variational, i.e., we may find a total energy lower than the true energy, and if we reduce the grid-spacing the energy can actually increase. Moreover, the grid breaks translational symmetry, and can also break other symmetries that the system may possess. This can lead to the artificial lifting of some degeneracies, to the appearance of spurious peaks in spectra, etc. Of course all these problems can be minimized by reducing the grid-spacing.

History

Octopus is based on a fixed-nucleus code written by George F. Bertsch and K. Yabana to perform real-time dynamics in clusters [5]and on a condensed matter real-space plane-wave based code written by A. Rubio, X. Blase and S.G. Louie [6]. The code was afterwards extended to handle periodic systems by G.F. Bertsch, J.I. Iwata, A. Rubio, and K. Yabana [7]. Contemporaneously there was a major rewrite of the original cluster code to handle a vast majority of finite systems. At this point the cluster code was named tddft.

This version was consequently enhanced and beautified by A. Castro (at the time Ph.D. student of A. Rubio), originating a fairly verbose 15,000 lines of Fortran 90/77. In the year 2000, M. Marques (aka Hyllios, aka António de Faria, corsário português), joined the A. Rubio group in Valladolid as a postdoc. Having to use tddft for his work, and being petulant enough to think he could structure the code better than his predecessors, he started a major rewrite of the code together with A. Castro, finishing version 0.2 of tddft. But things were still not perfect: due to their limited experience in Fortran 90, and due to the inadequacy of this language for anything beyond a HELLO WORLD program, several parts of the code were still clumsy. Also the idea of GPLing the almost 20,000 lines arose during an alcoholic evening. So after several weeks of frantic coding and after getting rid of the Numerical Recipes code that still lingered around, Octopus was born.

The present released version has been completely rewritten and keeps very little relation to the old version (even input and output files) and has been enhanced with major new flags to perform various excited-state dynamics in finite and extended systems. The code will be updated frequently and new versions can be found here.

If you find the code useful for you research we would appreciate if you give reference to this work and previous ones.

Contributing to Octopus

If you have some free time, and if you feel like taking a joy ride with Fortran 90, just drop us an email. You can also send us patches, comments, ideas, wishes, etc. They will be included in new releases of octopus.

If you found a have a bug, please report it to our Bug Tracking System:
http://www.tddft.org/trac/octopus/newticket

The Octopus Copying Conditions

This program is ?free?; this means that everyone is free to use it and free to redistribute it on a free basis. What is not allowed is to try to prevent others from further sharing any version of this program that they might get from you.

Specifically, we want to make sure that you have the right to give away copies of the program, that you receive source code or else can get it if you want it, that you can change this program or use pieces of them in new free programs, and that you know you can do these things.

To make sure that everyone has such rights, we have to forbid you to deprive anyone else of these rights. For example, if you distribute copies of the program, you must give the recipients all the rights that you have. You must make sure that they, too, receive or can get the source code. And you must tell them their rights.

Also, for our own protection, we must make certain that everyone finds out that there is no warranty for this program. If these programs are modified by someone else and passed on, we want their recipients to know that what they have is not what we distributed, so that any problems introduced by others will not reflect on our reputation.

The precise conditions of the license are found in the General Public Licenses that accompany it.

Please note that Octopus distribution normally comes with some external libraries that are not covered by the GPL license, please see the Copying Appendix for the copying conditions or these packages.

1. ? *A Primer in Density Functional Theory*, C. Fiolhais, F. Nogueira, and M.A.L. Marques (editors), Springer Berlin Heidelberg New York, (2006), ISBN: 3-540-03082-2
2. ? *Time-dependent Density Functional Theory*, M. A. L. Marques and C. A. Ullrich and F. Nogueira and A. Rubio and K. Burke and E. K. U. Gross (editors), Springer Berlin Heidelberg New York, (2006), ISBN: 3-540-35422-0
3. ? M.A.L. Marques, A. Castro, G. F. Bertsch, and A. Rubio, *octopus: a first principles tool for excited states electron-ion dynamics*, Comp. Phys. Comm. **151** 60 (2003)
4. ? A. Castro, H. Appel, M. Oliveira, C. A. Rozzi, X. Andrade, F. Lorenzen, M.A.L. Marques, E. K. U. Gross, and A. Rubio, *octopus: a tool for the application of time-dependent density functional theory*, Phys. Stat. Sol. (b) **243** 2465 (2006)
5. ? G.F. Bertsch and K. Yabana, *Time-dependent local-density approximation in real time*, Phys. Rev. B **54** 4484 (1996)
6. ? A. Rubio, X. Blase, and S.G. Louie, *Ab Initio Photoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters*, Phys. Rev. Lett. **77** 247 (1996)
7. ? G.F. Bertsch, J.I. Iwata, A. Rubio, and K. Yabana, *Real-space, real-time method for the dielectric function*, Phys. Rev. B **62** 7998 (2000)

Previous Manual:Octopus - Next Manual:Installation

Back to Manual <p class=newpage>

Installation

Maybe somebody else installed 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 in **`/usr/local/bin/octopus`**); the pseudopotential files that Octopus will need in **`PREFIX/share/octopus/PP/`**, etc.

However, you may be unlucky and that is not the case. In the following we will try to help you with the still rather unfriendly task of compiling and installing the `octopus`.

Instructions for Specific Architectures

See step-by-step instructions for some specific supercomputers and generic configurations (including Ubuntu and Mac OSX). If the system you are using is in the list, this will be the easiest way to install. Add entries for other supercomputers or generic configurations on which you have successfully built the code.

Dowloading

Download the latest Octopus version here: Octopus 6.0.

Binaries

If you want to install Octopus in a Debian-based Linux box (Debian or Ubuntu, you might not need to compile it; we release binary packages for some platforms. Keep in mind that these packages are intended to run on different systems and are therefore only moderately optimized. If this is an issue you have to compile the package yourself with the appropriate compiler flags and libraries (see below).

Download the appropiate **.deb** file from the downloads page for the current version. Install it (using root access) with the command below, using the appropriate filename you downloaded:

```
$ dpkg -i octopus_package.deb
```

Source code

If you have a different system from those mentioned above or you want to compile Octopus you need to get the source code file (**.tar.gz** file) and follow the compilation instructions below.

Building

Quick instructions

For the impatient, here is the quick-start:

```
$ tar xzf octopus-6.0.tar.gz
 $ cd octopus-6.0
 $ ./configure
 $ make
 $ make install
```

This will probably *not* work, so before giving up, just read the following paragraphs.

Slow instructions

There is an appendix with detailed instructions on how to compile Octopus and the required libraries from scratch -- you only need to do this if you are unable to install from a package manager or use per-built libraries.

Long instructions

The code is written in standard Fortran 95, with some routines written in C (and in bison, if we count the input parser). To build it you will need both a C compiler (gcc works just fine and it is available for almost every piece of silicon), and a Fortran 95 compiler. You can check in the Compilers Appendix which compilers Octopus has been tested with. This appendix also contains hints on potential problems with certain platform/compiler combinations and how to fix them.

Requirements

Besides the compiler, you will also need:

make
: most computers have it installed, otherwise just grab and install the GNU make.

cpp
: The C preprocessor is heavily used in Octopus to preprocess Fortran code. It is used for both C (from the CPP variable) and Fortran (FCCPP). GNU cpp is the most convenient but others may work too. For more info, see Preprocessors.

Libxc
: The library of exchange and correlation functionals. It used to be a part of Octopus, but since version 4.0.0 it is a standalone library and needs to be installed independently. For more information, see the Libxc page. Octopus 4.0.0 and 4.0.1 require version 1.1.0 (not 1.2.0 or 1.0.0). Octopus 4.1.2 requires version 2.0.x or 2.1.x, and won't compile with 2.2.x. (Due to bugfixes from libxc version 2.0 to 2.1, there will be small discrepancies in the testsuite for `functionals/03-xc.gga_x_pbea.inp` and `periodic_systems/07-tb09.test`). Octopus 5.0.0 supports libxc versions 2.0.x, 2.1.x and 2.2.x. Please note: The Libxc testsuite prior to 2.1 will report some errors in most cases. This is not something to worry about.

FFTW
: We have relied on this great library to perform Fast Fourier Transforms (FFTs). You may grab it from the FFTW site. You require FFTW version 3.

LAPACK/BLAS
: Our policy is to rely on these two libraries as much as possible on these libraries for linear-algebra operations. If you are running Linux, there is a fair chance they are already installed in your system. The same goes to the more heavy-weight machines (alphas, IBMs, SGIs, etc.). Otherwise, just grab the source from netlib site.

GSL
: Finally someone had the nice idea of making a public scientific library! GSL still needs to grow, but it is already quite useful and impressive. Octopus uses splines, complex numbers, special functions, etc. from GSL, so it is a must! If you don't have it already installed in your system, you can obtain GSL from the GSL site. You will need version 1.9 or higher. Version 4.0 of Octopus (and earlier) can only use GSL 1.14 (and earlier). A few tests will fail if you use GSL 1.15 or later. Version 5.0.0 of Octopus (and earlier) can only use GSL 1.16 or earlier, due to a bug in our configure script.

Perl
: During the build process Octopus runs several scripts in this language. It's normally available in every modern Unix system.

Optional libraries

There are also some optional packages; without them some parts of Octopus won't work:

MPI
: If you want to run Octopus in multi-tentacle (parallel) mode, you will need an implementation of MPI. MPICH or Open MPI work just fine in our Linux boxes.

PFFT
: We rely on this great library for highly scalable parallel Poisson solver, based on Fast Fourier Transforms (FFTs). You may grab it from the M. Pippig's site. You also require FFTW version 3.3 compiled with MPI and with a small patch by M. Pippig (also available there).

NetCDF
: The Network Common Dataform library is needed for writing the binary files in a machine-independent, well-defined format, which can also be read by visualization programs such as OpenDX

GDLib
: A library to read graphic files. See Tutorial:Particle in an octopus. (The simulation box in 2D can be specified via `BoxShapeImage`.) Available from http://www.libgd.org/

SPARSKIT
: Library for sparse matrix calculations. Used for one propagator technique.

ETSF I/O
: An input/output library implementing the ETSF standardized formats, requiring NetCDF, available at [2]. Versions 1.0.2, 1.0.3, and 1.0.4 are compatible with Octopus (though 1.0.2 will produce a small discrepancy in a filesize in the testsuite). It must have been compiled with the same compiler you are using with Octopus. To use ETSF_IO, include this in the `configure` line, where `$DIR` is the path where the library was installed:

```
--with-etsf-io-prefix="$DIR"
```

LibISF
: (version 5.0.0 and later) To perform highly scalable parallel Poisson solver, based on BigDFT 1.7.6, with a cheap memory footprint. You may grab it from the BigDFT site. You require BigDFT version 1.7.6 compiled with MPI, following these instructions: installation instructions . Probably, you have to manually copy the files "libwrappers.a" and "libflib.a" to the installation "/lib" directory. To configure Octopus, you have to add this configure line:

```
 --with-isf-prefix="$DIR"
```

Unpacking the sources

Uncompress and untar it (*gzip -cd octopus-6.0.tar.gz*). In the following, **OCTOPUS-SRC/** denotes the source directory of Octopus, created by the *tar* command.

The **OCTOPUS-SRC/** contains the following subdirectories of interest to users:

doc/
: The documentation of Octopus, mainly in HTML format.

liboct_parser/
: The C library that handles the input parsing.

share/PP/
: Pseudopotentials. In practice now it contains the Troullier-Martins (PSF and UPF formats) and Hartwigsen-Goedecker-Hutter pseudopotential files.

share/util/
: Currently, the *utilities* include a couple of IBM OpenDX networks (**mf.net**), to visualize wavefunctions, densities, etc.

testsuite/
: Used to check your build. You may also use the files in here as samples of how to do various types of calculations.

src/
: Fortran90 and C source files. Note that the Fortran90 files have to be preprocessed before being fed to the Fortran compiler, so do not be scared by all the # directives.

Development version

You can get the development version of Octopus by downloading the nightly distribution from http://www.tddft.org/programs/octopus/download/octopus-night.tar.gz

You can also get the current version with the following command (you need the subversion package):

```
$ svn co http://www.tddft.org/svn/octopus/trunk
```

Before running the configure script, you will need to run the GNU autotools. This may be done by executing:

```
$ cd trunk
 $ autoreconf -i
```

Note that you need to have working recent versions of the automake and autoconf. In particular, the configure script may fail in the part `checking for Fortran libraries of mpif90` for `autoconf` version 2.59 or earlier. The solution is to update `autoconf` to 2.60 or later, or manually set `FCLIBS` in the `configure` command line to remove a spurious apostrophe.

Please be aware that the development version may contain untested changes that can affect the execution and the results of Octopus, especially if you are using new and previously unreleased features. So if you want to use the development version for production runs, you should at least contact Octopus developers.

You can also use the current release branch, which is the released version with only important bugfixes added, and is the source of minor revision numbers (e.g. 4.0.1).

http://www.tddft.org/programs/octopus/download/octopus-night.5.0.x.tar.gz or

```
$ svn co http://www.tddft.org/svn/octopus/branches/5.0.x
```

Configuring

Before configuring you can (should) set up a couple of options. Although the configure script tries to guess your system settings for you, we recommend that you set explicitly the default Fortran compiler and the compiler options. Note that configure is a standard tool for Unix-style programs and you can find a lot of generic documentation on how it works elsewhere.

For example, in bash you would typically do:

```
$ export FC=abf90
 $ export FCFLAGS="-O -YEXT_NAMES=LCS -YEXT_SFX=_"
```

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` by hand, check the Compilers Appendix page for which flags have been reported to work with different Fortran compilers.

You can now run the configure script

```
$ ./configure
```

You can use a fair amount of options to spice Octopus to your own taste. To obtain a full list just type *`./configure --help`*. Some commonly used options include:

`--prefix=`**`PREFIX/`**
: Change the base installation dir of Octopus to **`PREFIX/`**. **`PREFIX/`** defaults to the home directory of the user who runs the configure script.

`--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. You can also use the `FFT_LIBS` environment variable.

`--with-pfft-prefix=`**`DIR/`**
: Installation directory of the PFFT library.

`--with-pfft-lib=`**`<lib>`**

Instruct the configure script to look for the PFFT library exactly in the way that it is specified in the **<lib>** argument. You can also use the `PFFT_LIBS` environment variable.

`--with-blas=`**<lib>**
Instruct the configure script to look for the BLAS library in the way that it is specified in the **<lib>** argument.

`--with-lapack=`**<lib>**
Instruct the configure script to look for the LAPACK library in the way that it is specified in the **<lib>** argument.

`--with-gsl-prefix=`**DIR/**
Installation directory of the GSL library. The libraries are expected to be in **DIR/lib/** and the include files in **DIR/include/**. The value of **DIR/** is usually found by issuing the command *`gsl-config --prefix`*.

`--with-libxc-prefix=`**DIR/**
Installation directory of the Libxc library.

If you have problems when the configure script runs, you can find more details of what happened in the file config.log in the same directory.

Compiling and installing

Run *`make`* and then *`make install`*. The compilation may take some time, so you might want to speed it up by running *`make`* in parallel (*`make -j`*). If everything went fine, you should now be able to taste Octopus.

Depending on the value given to the --prefix=**PREFIX/** given, the executables will reside in **PREFIX/bin/**, and the auxiliary files will be copied to **PREFIX/share/octopus**. The sample input files will be copied to **PREFIX/share/octopus/samples**.

Testing your build

After you have successfully built Octopus, to check that your build works as expected there is a battery of tests that you can run. They will check that Octopus executes correctly and gives the expected results (at least for these test cases). If the parallel version was built, the tests will use up to 6 MPI processes, though it should be fine to run on only 4 cores. (MPI implementations generally permit using more tasks than actual cores, and running tests this way makes it likely for developers to find race conditions.)

To run the tests, in the sources directory of Octopus use the command

```
$ make check
```

or if you are impatient,

```
$ make check-short
```

which will start running the tests, informing you whether the tests are passed or not. For examples of job scripts to run on a machine with a scheduler, please see Manual:Specific_architectures.

If all tests fail, maybe there is a problem with your executable (like a missing shared library).

If only some of the tests fail, it might be a problem when calling some external libraries (typically blas/lapack). Normally it is necessary to compile all Fortran libraries with the same compiler. If you have trouble, try to look for help in the Octopus mailing list.

Previous Manual:About Octopus - Next Manual:Input file

Back to Manual <p class=newpage>

Basics

<p class=newpage>

The input file

Octopus uses a single input file from which to read user instructions to know what to calculate and how. This page explains how to generate that file and what is the general format. The Octopus parser is a library found in the **liboct_parser** directory of the source, based on bison and C. You can find two (old) separate release versions of it at the bottom of the Releases page.

Input file

Input options should be in a file called **inp**, in the directory Octopus is run from. This is a plain ASCII text file, to create or edit it you can use any text editor like emacs, vi, jed, pico, gedit, etc. For a fairly comprehensive example, just look at the tutorial page Tutorial:Nitrogen_atom.

At the beginning of the program, the parser reads the input file, parses it, and generates a list of variables that will be read by Octopus (note that the input is case-independent). There are two kind of variables: scalar values (strings or numbers), and blocks (that you may view as matrices).

Scalar Variables

A scalar variable `var` can be defined by:

```
var = exp
```

`var` can contain any alphanumeric character plus _, and `exp` can be a quote-delimited string, a number (integer, real, or complex), a variable name, or a mathematical expression. Complex numbers are defined as `{real, imag}`. Real numbers can use scientific notation with `e` or `E` (no `d` or `D`, Fortran people), such as `6.02e23`. Variable names are not case-sensitive, and you must not redefine a previously defined symbol -- especially not the reserved variables `x, y, z, r, w, t` which are used in space- or time-dependent expressions, where `w` is the 4th space coordinate when operating in 4D.

Mathematical expressions

The parser can interpret expressions in the input file, either to assign the result to a variable, or for defining functions such as a potential in the `Species` block or a time-dependent function in the `TDFunctions` block. The arguments can be numbers or other variables.

Arithmetic operators

`a+b`
: addition

`a-b`
: subtraction

`-a`
: unary minus

`a*b`
: multiplication

`a/b`
: division

`a^b`
: exponentiation

Logical operators

Logical operation will return 0 for false or 1 for true. You can exploit this to define a piecewise expression, e.g. "`2 * (x <= 0) - 3 * (x > 0)`" (although the `step` function may also be used). The comparison operators (except ==) use only the real part of complex numbers.

`a < b`
: less than

`a <= b`
: less than or equal to ($\leq$)

`a > b`
: greater than

`a >= b`
: greater than or equal to ($\geq$)

`a == b`
: equal to

`a && b`
: logical and

`a || b`
: logical or

`!a`
: logical not

Functions

`sqrt(x)`
: The square root of `x`.

`exp(x)`
: The exponential of `x`.

`log(x)` or `ln(x)`
: The natural logarithm of `x`.

`log10(x)`
: Base 10 logarithm of `x`.

`logb(x, b)`
: Base `b` logarithm of `x`.

`{x, y}`
: The complex number $x + iy$.

`arg(z)`
: Argument of the complex number `z`, arg(z), where $-\pi < \arg(z) <= \pi$.

`abs(z)`
: Magnitude of the complex number `z`, $|z|$.

`abs2(z)`
: Magnitude squared of the complex number `z`, $|z|^2$.

`logabs(z)`
: Natural logarithm of the magnitude of the complex number `z`, $\log|z|$. It allows an accurate evaluation of $\log|z|$ when $|z|$ is close to one. The direct evaluation of `log(abs(z))` would lead to a loss of precision in this case.

`conjg(z)`
: Complex conjugate of the complex number `z`, $z^* = x - iy$.

`inv(z)`
: Inverse, or reciprocal, of the complex number `z`, $\frac{1}{z} = \frac{x - iy}{x^2 + y^2}$.

`sin(x)`, `cos(x)`, `tan(x)`, `cot(x)`, `sec(x)`, `csc(x)`
: The sine, cosine, tangent, cotangent, secant and cosecant of `x`.

`asin(x)`, `acos(x)`, `atan(x)`, `acot(x)`, `asec(x)`, `acsc(x)`
: The inverse (arc-) sine, cosine, tangent, cotangent, secant and cosecant of `x`.

`atan2(x,y)`
: = atan(y / x).

`sinh(x)`, `cosh(x)`, `tanh(x)`, `coth(x)`, `sech(x)`, `csch(x)`
: The hyperbolic sine, cosine, tangent, cotangent, secant and cosecant of `x`.

`asinh(x)`, `acosh(x)`, `atanh(x)`, `acoth(x)`, `asech(x)`, `acsch(x)`
: The inverse hyperbolic sine, cosine, tangent, cotangent, secant and cosecant of `x`.

`min(x, y)`
: The minimum of `x` and `y`.

`max(x, y)`
: The maximum of `x` and `y`.

`step(x)`
: The Heaviside step function in `x`. This can be used for piecewise-defined functions.

`erf(x)`
: The error function $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2}$.

`realpart(z)`
: The real part of the complex number `z`.

`imagpart(z)`
: The imaginary part of the complex number `z`.

`floor(x)`
: The largest integer less than the real number `x`.

`ceiling(x)`
: The smallest integer greater than the real number `x`.

These mathematical operations are all based on the GSL library and are defined in `symbols.c` and `grammar.y`.

References

- https://www.gnu.org/software/gsl/manual/html_node/Properties-of-complex-numbers.html
- https://www.gnu.org/software/gsl/manual/html_node/Complex-arithmetic-operators.html
- https://www.gnu.org/software/gsl/manual/html_node/Error-Function.html
- https://www.gnu.org/software/libc/manual/html_node/Rounding-Functions.html
- https://www.gnu.org/software/gsl/manual/html_node/Representation-of-complex-numbers.html

Predefined variables

There are some predefined constants for your convenience:

`pi`
: `3.141592653589793`.

`e`
: The base of the natural logarithms.

`false` or `no`
: False.

`true` or `yes`
: True.

`i`
: The imaginary unit *i*, *i.e.* `{0, 1}`

Blocks

Blocks are defined as a collection of values, organised in row and column format. The syntax is the following:

```
%var
   exp | exp | exp | ...
   exp | exp | exp | ...
   ...
 %
```

Rows in a block are separated by a newline, while columns are separated by the character | or by a tab. There may be any number of lines and any number of columns in a block. Note also that each line can have a different number of columns. Values in a block don't have to be of the same type.

Comments

Everything following the character # until the end of the line is considered a comment and is simply cast into oblivion.

Environment variables

You can also set variables using the environment, which can be helpful in scripting.

Default values

If Octopus tries to read a variable that is not defined in the input file, it automatically assigns to it a default value (there are some cases where Octopus cannot find a sensible default value and it will stop with an error). All variables read (present or not in the input file) are output to the file **`exec/parser.log`**. If you are not sure of what the program is reading, just take a look at it.

We recommend you to keep the variables in the input file to a minimum: *do not write a variable that will be assigned its default value*. The default can change in newer versions of Octopus and old values might cause problems. Besides that, your input files become difficult to read and understand.

Documentation

Each input variable has (or should have) its own documentation explaining what it does and the valid values it may take. This documentation can be obtained online or it can also be accessed by the oct-help command.

Experimental features

Even in the stable releases of Octopus there are many features that are being developed and are not suitable for production runs. To protect users from inadvertly using these parts they are declared as *Experimental*.

When you try to use one of these experimental functionalities Octopus will stop with an error. If you want to use it you need to set the variable `ExperimentalFeatures` to `yes`. Now Octopus will only emit a warning.

By setting `ExperimentalFeatures` to `yes` you will be allowed to use parts of the code that are not complete or not well tested and most likely produce wrong results. If you want to use them for production runs you should contact the Octopus developers first.

Good practices

In order to ensure compatibility with newer versions of Octopus and avoid problems, keep in mind the following rules of good practice when writing input files:

- Although input variables that take an option as an input can also take a number, the number representation makes the input file less readable and it is likely to change in the future. So **avoid using numbers instead of values**. For example

```
Units = ev_angstrom
```

must always be used instead of

```
Units = 3
```

- **Do not include variables that are not required in the input file**, especially declarations of values that are just a copy of the default value. This makes the input file longer, less readable and, since defaults are likely to change, it makes more probable that your input file will have problems with newer versions of Octopus. Instead rely on default values.

- **Avoid duplicating information in the input file**. Use your own variables and the mathematical-interpretation capabilities for that. For example, you should use:

```
m = 0.1
c = 137.036
E = m*c^2
```

instead of

```
m = 0.1
c = 137.036
E = 1877.8865
```

In the second case, you might change the value of `m` (or `c` if you are a cosmologist) while forgetting to update `E`, ending up with an inconsistent file.

Previous Manual:Installation - Next Manual:Running Octopus

Back to Manual <p class=newpage>

Running Octopus

Input

In order to run, Octopus requires an input file that *must* be called **`inp`**. Depending on your input file there are other files that you might need, like pseudopotentials or coordinate files (we will discuss this later in this manual).

The rest of the files that are required are part of the Octopus installation; if Octopus is correctly installed they should be available and Octopus should know where to find them. With Octopus you can't just copy the binary between systems and expect it to work.

Executing

To run Octopus you just have to give the *`octopus`* command in the directory where you have your input file. While running, Octopus will display information on the screen. If you want to capture this information you can send the output to a file, let's say **`out.log`**, by executing it like this:

```
$ octopus > out.log
```

This captures only the normal output. If there is a warning or an error, it will be still printed on the screen. To capture everything to a file, run

```
$ octopus >& out.log
```

If you want to run Octopus in the background, append `&` to the last command.

Output

While running, Octopus will create several output files, all of them inside subdirectories in the same directory where it was run. The files that contain the physical information depend on what Octopus is doing and they will be discussed in the next chapter.

One directory that is always created is **`exec/`**, this file contains information about the Octopus run. Here you will find the **`parser.log`** file, a text file that contains *all* the input variables that were read by Octopus, both the variables that are in the input file and the variables that took default values; in the second case they are marked by a comment as `#default`. This file is very useful if you want to check that Octopus is correctly parsing a variable or what are the default values that it is taking.

Clean Stop

If you create a file called **`stop`** in the running directory, Octopus will exit gracefully after finishing the current iteration. May not work for gcm, invert_ks, casida, td_transport, one_shot run modes. You can use this to prevent possible corruption of restart information when your job is killed by a scheduler, by preemptively asking Octopus to quit automatically in a job script like this:

```
#PBS -l walltime=4:10:00
mpirun $HOME/octopus/bin/octopus_mpi &> output &
sleep 4h
touch stop
wait
```

or more sophisticatedly like this:

```
MIN=`qstat -a $PBS_JOBID | awk '{wall=$9} END {print $9}' | awk -F: '{min=($1*60)+$2; print min}
sh ~/sleep_stop.sh stop $((MIN-10))m > sleepy &
mpirun $HOME/octopus/bin/octopus_mpi &> output
```

with auxiliary script `sleep_stop.sh`:

```
#!/bin/bash
if [ $# -ne 2 ]; then
   echo "Usage: sleep_stop.sh FILENAME TIME"
else
   echo "Time until $1 created: $2"
   rm -f $1
   sleep $2
   touch $1
fi
```

Restarting

Another directory that will created is **`restart/`**; in this directory Octopus saves the information from the calculation that it is doing. This information can be used in the following cases:

- If Octopus is stopped without finishing by some reason, it can restart from where it was without having to do all work again.
- If after the calculation is done (or even if it was stopped), the user wants to do the same simulation with some different parameters, Octopus can save some work by starting from the restart information.
- There are some calculations that require the results of other type of calculation as an input; in this case it uses the files written in **`restart/`** by the previous calculation (we will discuss this case later, when we talk about the different calculation modes).

Sometimes it's not desired to restart a calculation, but to start it from the very beginning. Octopus can be instructed to do so by setting the input variable `fromScratch` to `yes`.

Previous Manual:Input file - Next Manual:Units

Back to Manual <p class=newpage>

Units

Before entering into the physics in Octopus we have to address a very important issue: *units*. There are different unit systems that can be used at the atomic scale: the most used are atomic units and what we call "convenient" units. Here we present both unit systems and explain how to use them in Octopus.

Atomic Units

Atomic units are a Gaussian system of units (by "Gaussian" it means that the vacuum dielectric constant has no dimensions and is set to be $\epsilon_0 = \frac{1}{4\pi}$), in which the numerical values of the Bohr radius, the electronic charge, the electronic mass, and the reduced Planck's constant are set to one:

$$(1) \qquad a_0 = 1; e^2 = 1; m_e = 1; \hbar = 1.$$

This simplifies formulae (although some may feel it presents a serious hazard for dimensional analysis, interpretation and understanding of formulae, and physics in general. But this is just a personal taste). This sets directly two fundamental units, the atomic units of length and of mass:

$$(2) \qquad \mathrm{au}_{\mathrm{length}} = a_0 = 5.2917721 \times 10^{-11}\ \mathrm{m}; \quad \mathrm{au}_{\mathrm{mass}} = m_e = 9.1093819 \times 10^{-31}\ \mathrm{kg}.$$

Since the squared charge must have units of energy times length, we can thus set the atomic unit of energy

$$(3) \qquad \mathrm{au}_{\mathrm{energy}} = \frac{e^2}{a_0} = 4.3597438 \times 10^{-18}\ \mathrm{J},$$

which is called Hartree, Ha. And, since the energy has units of mass times length squared per time squared, this helps us get the atomic unit of time:

$$(4) \qquad \mathrm{Ha} = m_e \frac{a_0^2}{\mathrm{au}_{\mathrm{time}}^2} \rightarrow \mathrm{au}_{\mathrm{time}} = a_0 \sqrt{\frac{m_e}{\mathrm{Ha}}} = \frac{a_0}{e}\sqrt{m_e a_0} = 2.4188843 \times 10^{-17}\,\mathrm{s}.$$

Now the catch is: what about Planck's constant? Its dimensions are of energy times time, and thus we should be able to derive its value by now. But at the beginning we set it to one! The point is that the four physics constants used ($a_0, m_e, e^2, \hbar$) are not independent, since:

$$(5) \qquad a_0 = \frac{\hbar^2}{m_e \frac{e^2}{4\pi\epsilon_0}}.$$

In this way, we could actually have derived the atomic unit of time in an easier way, using Planck's constant:

$$(6) \qquad \hbar = 1\ \mathrm{Ha}\,\mathrm{au}_{\mathrm{time}} \Rightarrow \mathrm{au}_{\mathrm{time}} = \frac{\hbar}{\mathrm{Ha}} = \frac{\hbar a_0}{e^2}\,.$$

And combining (6) and (5) we retrieve (4).

Convenient Units

Much of the literature in this field is written using Ångströms and electronvolts as the units of length and of energy, respectively. So it may be "convenient" to define a system of units, derived from the atomic system of units, in which we make that substitution. And so we will call it "convenient".

The unit mass remains the same, and thus the unit of time must change, being now $\hbar/\mathrm{eV}$, with $\hbar = 6.582\,1220(20) \times 10^{-16}$ eV s.

Units in Octopus

By default Octopus reads and writes atomic units; you can switch to convenient units by setting the variable `Units` to `ev_angstrom`. If you prefer different units for input and output, there are the variables `UnitsInput` and `UnitsOutput`.

Mass Units

An exception for units in Octopus is mass units. When dealing with the mass of ions, atomic mass units (amu) are always used. This unit is defined as 1 / 12 of the mass of the ^{12}C atom. In keeping with standard conventions in solid-state physics, effective masses of electrons are always reported in units of the electron mass (*i.e.* the atomic unit of mass), even in the eV-Å system.

Charge Units

In both unit systems, the charge unit is the electron charge *e* (*i.e.* the atomic unit of charge).

Unit Conversions

Converting units can be a very time-consuming and error-prone task when done by hand, especially when there are implicit constants set to one, as in the case of atomic units. That is why it's better to use as specialized software like Gnu Units.

In some fields, a very common unit to express the absorption spectrum is Mb. To convert a strength function from 1/eV to Mb, multiply by $\pi h c r_e$, with $r_e = e^2/(m_e c^2)$. The numerical factor is 109.7609735.

Previous Manual:Running Octopus - Next Manual:Physical System

Back to Manual <p class=newpage>

Physical System

The first thing that Octopus has to know is the physical system you want to treat. To do this you have specify a group of species and their positions.

Dimensions

Octopus can work in a space with 1, 2 or 3 dimensions. You can select the dimension of your system with the `Dimensions` variable.

Species

An Octopus species is very generic and can be a nucleus (represented by pseudopotentials or by the full Coulomb potential), a jellium sphere or even a user-defined potential. The information regarding the atomic species goes into the `Species` block.

Pseudopotentials

The many-electron Schroedinger equation can be greatly simpli?ed if electrons are divided in two groups: valence electrons and inner core electrons. The electrons in the inner shells are strongly bound and do not play a signi?cant role in the chemical binding of atoms, thus forming with the nucleus an inert core. Binding properties are almost completely due to the valence electrons, especially in metals and semiconductors. This separation implies that inner electrons can be ignored, reducing the atom to an inert ionic core that interacts with the valence electrons. This suggests the use of an e?ective interaction, a pseudopotential, that gives an approximation to the potential felt by the valence electrons due to the nucleus and the core electrons. This can signi?cantly reduce the number of electrons that have to be dealt with. Moreover, the pseudo wave functions of these valence electrons are much smoother in the core region than the true valence wave functions, thus reducing the computational burden of the

calculations.

Modern pseudopotentials are obtained by inverting the free atom Schroedinger equation for a given reference electronic con?guration, and forcing the pseudo wave functions to coincide with the true valence wave functions beyond a certain cuto? distance. The pseudo wave functions are also forced to have the same norm as the true valence wave functions, and the energy pseudo eigenvalues are matched to the true valence eigenvalues. Di?erent methods of obtaining a pseudo eigenfunction that satis?es all these requirements lead to di?erent non-local, angular momentum dependent pseudopotentials. Some widely used pseudopotentials are the Troullier and Martins potentials, the Hamann potentials, the Vanderbilt potentials and the Hartwigsen-Goedecker-Hutter potentials. The default potentials used by Octopus are of the Troullier and Martins type, although you can also opt for the HGH potentials.

Octopus comes with a package of pseudopotentials and the parameters needed to use them. If you want to have a look you can find them under **`PREFIX/share/octopus/PP`**. These pseudopotentials serve to define many species that you might wish to use in your coordinates block, e.g. a helium atom, "He". If you are happy to use these predefined pseudopotentials, you do not need to write a species block.

However it is also possible to define new species to use in your coordinates block by adding a `Species` block. You can check the documentation of that variable for the specific syntax. With this block you may specify the format of your file that contains a pseudopotential and parameters such as the atomic number, or you may define an algebraic expression for the potential with the user-defined potential. A user defined potential should be finite everywhere in the region where your calculation runs.

If you want to search other repositories on the web or create your own pseudopotentials, check the pseudopotentials page. Save the pseudopotential file in the same directory as the inp file and specify its format with the species block.

All-Electron Nucleus

The potential of this species is the full Coulomb potential

$$V\left(\vec{r}\right) = \frac{1}{\left|\vec{R}_i - \vec{r}\right|} \ .$$

The main problem to represent this potential is the discontinuity over $\vec{R}_i$. To overcome this problem we do the following:

- First we assume that atoms are located over the closest grid point.
- Then we calculate the charge density associated with the nucleus: a delta distribution with the value of the charge at this point and zero elsewhere.
- Now we solve the Poisson equation for this density.

In this way we get a potential that is the best representation of the Coulomb potential for our grid (we will discuss about grids later) and is continuous in $\vec{R}_i$ (the value is the average of the potential over the volume associated with the grid point).

The main problem is that the requirement of having atoms over grid points is quite strong: it is only possible for a few systems with simple geometries and you can't move the atoms. Also the Coulomb potential is very hard, which means you will need a very small spacing, and as you have to consider both core and valence electrons, this species is only suitable for atoms or very small molecules.

User Defined

It is also possible to define an external, user-defined potential in the input file. All functions accepted by the parser can be used. Besides that, one can use the symbols *x*, *y*, *z*, and *r*. In this way it is trivial to calculate model systems, like harmonic oscillators, quantum dots, etc.

Coordinates

For each instance of a species (even for user-defined potentials), you have to specify its position inside the simulation box. To do this you can use the `Coordinates` block which describes the positions inside of the input file or one of the `XYZCoordinates` or `PDBCoordinates` variables, that specify an external file, in xyz or PDB format respectively, from where the coordinates will be read.

Before using a geometry with Octopus we recommend that you center it. For this you can use the oct-center-geom utility.

Velocities

If you are going to do ion dynamics you may want to have an initial velocity for the particles. You have several choices for doing this:

- Don't put anything in the input file; particles will have zero initial velocity.
- Give them a random velocity according to a temperature (in degrees Kelvin) given by the `RandomVelocityTemp` variable.
- Explicitly give the initial velocity for each particle, either through the `Velocities` block or from a pseudo-xyz file detailed by the variable `XYZVelocities`.

Number of Electrons

Each species adds enough electrons to make the system neutral. If you want to add or remove electrons you can specify the total charge of your system with the `ExcessCharge` variable (a negative charge implies to add electrons).

Previous Manual:Units - Next Manual:Hamiltonian

Back to Manual <p class=newpage>

Hamiltonian

Octopus is based upon Density Functional Theory in the Kohn-Sham formulation. The Kohn-Sham Hamiltonian is the main part of this formulation; in this section we describe how the Hamiltonian is treated in Octopus and what

are the variables that control it.

Introduction

Although the Hohenberg-Kohn theorem states that DFT is exact, the Kohn-Sham method of reducing an interacting many-particle problem to a non-interacting single-particle problem introduces an approximation: the exchange-correlation term.

Ground-State DFT

The Kohn-Sham method of DFT assumes that, for each interacting ground-state density $n(r)$, there exists a non-interacting electron system with the same ground-state density. The interacting ground state is obtainable through the solution of the Kohn-Sham equations

$$\left[-\frac{\nabla^2}{2} + v_{\rm KS}[n](r)\right]\varphi_i(r) = \varepsilon_i\varphi_i(r)$$

The notation $v_{\rm KS}[n]$ means that the Kohn-Sham potential, $v_{\rm KS}$, has a functional dependence on n, the electronic density, which is defined in terms of the Kohn-Sham wave-functions by

$$n(r) = \sum_i^{\rm occ} |\varphi_i(r)|^2 \ .$$

The potential $v_{\rm KS}$ is defined as the sum of the external potential (normally the potential generated by the nuclei), the Hartree term, and the exchange-correlation (xc) potential

$$v_{\rm KS}[n](r) = v_{\rm ext}(r) + v_{\rm Hartree}[n](r) + v_{\rm xc}[n](r) \ .$$

Due to the functional dependence on the density, these equations form a set of nonlinear coupled equations. The standard procedure to solve it is iterating until self-consistency is achieved.

The total energy of the electronic system is given by

$$E_{\rm elec}[n] = T_s[n] + \int d^3r\ n(r)v_{\rm ext}(r) + E_{\rm Hartree}[n] + E_{\rm x}[n] + E_{\rm c}[n]$$

where $T_s[n]$ is the non-interacting kinetic energy, $v_{\rm ext}$ is the external potential, and $E_{\rm x,c}[n]$ are the exchange (x) and correlation (c) energies. The second term is called the "external energy" in the code. In practice, from the solution of the Kohn-Sham equations, we can evaluate the energy via the eigenvalues as

$$E_{\rm elec}[n] = \sum \epsilon_i - \int d^3r\ n(r)v_{\rm xc}(r) - E_{\rm Hartree}[n] + E_{\rm x}[n] + E_{\rm c}[n]$$

where $v_{\rm xc}[n]$ is the exchange-correlation potential. To find the total energy of the entire system, we additionally include ion-ion interaction and ionic kinetic energy.

$E_{xc} = E_x + E_c$ is an unknown object and includes all the non-trivial many-body e?ects required to make KS theory exact. Several approximations to E_{xc} have been proposed. The most used is the local density approximation (LDA). In this approximation $E_{xc}[n(r)]$ is taken to be the exchange and correlation energy of a homogeneous electron gas with density $n = n(r)$. Although there exists an exact expression for the exchange energy in this model, the exact value of the correlation energy is known only in the limit of very high densities. Ceperley and Alder did a Monte Carlo simulation of the homogeneous electron gas at several densities. Several parameterizations of the correlation energy for any density were then obtained interpolating the Monte Carlo results. One particularly simple parameterization was proposed by Perdew and Zunger, and this option may be used by Octopus. You can, of course, choose other xc functionals (`XCFunctional`), via the extensive library provided by Libxc.

Time-dependent DFT

Time-dependent density-functional theory (TDDFT) extends the basic ideas of ground-state density-functional theory (DFT) to the treatment of excitations and of more general time-dependent phenomena. TDDFT can be viewed as an alternative formulation of time-dependent quantum mechanics but, in contrast to the normal approach that relies on wave-functions and on the many-body Schrödinger equation, its basic variable is the one-body electron density, $n(r,t)$. The advantages are clear: The many-body wave-function, a function in a $3N$-dimensional space (where N is the number of electrons in the system), is a very complex mathematical object, while the density is a simple function that depends solely on the 3-dimensional vector r. The standard way to obtain $n(r,t)$ is with the help of a fictitious system of non-interacting electrons, the Kohn-Sham system. The final equations are simple to tackle numerically, and are routinely solved for systems with a large number of atoms. These electrons feel an effective potential, the time-dependent Kohn-Sham potential. The exact form of this potential is unknown, and has therefore to be approximated.

The time-dependent Kohn-Sham equations are

$$i\frac{\partial}{\partial t}\varphi_i(r,t) = \left[-\frac{\nabla^2}{2} + v_{\rm KS}(r,t)\right]\varphi_i(r,t)$$

The density of the interacting system can be obtained from the time-dependent Kohn-Sham orbitals

$$n(r,t) = \sum_i^{\rm occ} |\varphi_i(r,t)|^2 \ .$$

The time-dependent Kohn-Sham equations, having the form of a one-particle equation, is fairly easy to solve numerically. We stress, however, that the Kohn-Sham equation *is not* a mean-field approximation: If we knew the exact Kohn-Sham potential, $v_{\rm KS}$, we would obtain the exact Kohn-Sham orbitals, and from these the correct density of the system. The Kohn-Sham potential is conventionally separated in the following way

$$v_{\rm KS}(r,t) = v_{\rm ext}(r,t) + v_{\rm Hartree}(r,t) + v_{\rm xc}(r,t) \ .$$

The first term is again the external potential. The Hartree potential accounts for the classical electrostatic interaction between the electrons

$$v_{\mathrm{Hartree}}(r,t) = \int d^3r' \frac{n(r,t)}{|r-r'|} \ .$$

The time-dependence of the exchange and correlation potential introduces the need for an approximation beyond the one made in the time-independent case. The simplest method of obtaining a time-dependent xc potential consists in assuming that the potential is the time-independent xc potential evaluated at the time-dependent density, i.e.,

$$v_{\mathrm{xc}}^{\mathrm{adiabatic}}(r,t) = \tilde{v}_{\mathrm{xc}}[n](r)|_{n=n(t)} \ ,$$

This is called the adiabatic approximation. If the time-independent xc potential chosen is the LDA, then we obtain the so-called adiabatic local density approximation (ALDA). This approximation gives remarkably good excitation energies but su?ers from the same problems as the LDA, most notably the exponential fall-o? of the xc potential. If a strong laser pushes the electrons to regions far from the nucleus, ALDA should not be expected to give an accurate description of the system. Other options for the time-dependent xc potential are orbital-dependent potentials like the exact exchange functional (EXX) (usually in the Krieger-Li-Iafrate (KLI) approximation).

Occupations

You can set the occupations of the orbitals by hand, using the `Occupations`.

External Potential

You can add an external uniform and constant electric or magnetic field, set by the `StaticElectricField` or `StaticMagneticField`. If you want to add a more general potential, you can do it using a user-defined `Species`.

If you got the coordinates from a PDB file, you can add the potential generated by the point charges defined there by setting the `ClassicalPotential` variable to yes.

Electron-Electron Interaction

You can neglect this term by setting `TheoryLevel = independent_particles` variable. This implies that both the Hartree and exchange-correlation terms will not be calculated.

Exchange and correlation potential

Octopus does not distinguish, for the moment, between ground-state DFT xc functionals, and time-dependent DFT functionals. In other words, in all cases the *adiabatic* approximation is assumed. In mathematical terms, we may formalize this in the following way: let *n* be the time-dependent density, a function living in the four-dimensional space-time world. We will call $n_t(\vec{r}) = n(\vec{r},t)$, the electronic density at time t, a function in the three-dimensional space. An exchange and/or correlation *energy* functional E^{α} in ground state DFT may then be used to build an *adiabatic* exchange and/or correlation *action* functional in the following way:

$$A^\alpha[n] = \int_{t_0}^{t_f} \mathrm{d}\tau E^\alpha[n_\tau] \,,$$

The time-dependent potential functional is then:

$$v^\alpha[n](\vec{r},t) \equiv \frac{\delta A^\alpha}{\delta n(\vec{r},t)} = \frac{\delta E^\alpha}{\delta n_t(\vec{r})} = v^{\alpha(\mathrm{GS})}[n_t](\vec{r}) \,.$$

We use the distinct notation $v^\alpha[n](\vec{r},t)$ and $v^{\alpha(\mathrm{GS})}[n_t](\vec{r})$ to stress that the exchange and correlation potential in TDDFT -- the former -- and the exchange and correlation potential in GS-DFT -- the latter -- are in principle two conceptually different objects, which coincide only thanks to the adiabatic approximation. This is the reason why we may actually only refer to the functionals in the GS-DFT context.

We may classify the xc functionals contained in the Octopus code following John Perdew's Jacob's Ladder scheme:

- LDA rung: A functional α belonging to the LDA rung depends only on the electronic density (on the spin density in spin-polarized or spinors cases). Moreover, it has a *local* dependency on the density, i.e.:

$$E^\alpha_{\mathrm{LDA}} = E^\alpha_{\mathrm{LDA}}[n] = \int \mathrm{d}^3 r e^\alpha_{\mathrm{LDA}}(n(\vec{r})) \,.$$

The potential may be then derived by functional derivation:

$$v^\alpha_{LDA}[n](\vec{r}) = \frac{\delta E^\alpha_{\mathrm{LDA}}}{\delta n(\vec{r})} = \frac{\mathrm{d}e^\alpha_{\mathrm{LDA}}}{\mathrm{d}n}(n(\vec{r})) \,.$$

- GGA rung: A functional α belonging to the GGA rung depends on the electronic density, and also on its gradient. Moreover, it also has a *local* dependency (actually, the GGA is very often called a *semi-local* functional due to this).

$$E^{\alpha(\mathrm{GGA})} = E^{\alpha(\mathrm{GGA})}[n, \vec{\nabla} n] = \int \mathrm{d}^3 r e^\alpha_{\mathrm{GGA}}(n(\vec{r}), \vec{\nabla} n(\vec{r})) \,.$$

- meta-GGA rung:

- OEP rung: This is the family of functionals which are defined in terms of the occupied Kohn-Sham orbitals, $\{\varphi_i\}_{i=1}^N$. These are in fact the only *non-local* functionals. The name of the rung, OEP, stands for "optimized-effective-potential", the reason being that in general this is the method used to derive the potential from the energy functional (direct functional derivation is in this case not possible). A more suitable name would be orbital-dependent functionals.

Octopus comes with several Exchange and Correlation potentials, including several flavours of LDA, GGA and OEP. You can choose your favorites by setting the variable `XCFunctional`. (Note that until Octopus <= 2.1 the exchange-correlation functional was chosen with the variables `XFunctional` and `CFunctional`.)

When using OEP Exchange, the variable `OEPLevel` controls the level of approximation required.

You can also include Self-Interaction Correction (SIC), controlled by the variable `SICCorrection`.

Relativistic Corrections

The variable `RelativisticCorrection` allows one to choose the relativistic correction to be used. Up to now only spin-orbit coupling (`RelativisticCorrection` = `spin_orbit`) is implemented.

Spin-orbit Coupling

The spin-orbit coupling as it is implemented in Octopus is included in the pseudo-potentials. These can either be HGH pseudo-potentials or Troullier-Martins-like pseudo-potentials. In the later case the pseudo-potentials need to be generated from fully relativistic calculations and their fully separable form is given by:

$$\hat{v}_{KB} = v_{local} + \sum_{l,j,m_j} \frac{|\varphi^{PP}_{ljm_j} \delta v^{PP}_{lj} >< \varphi^{PP}_{ljm_j} \delta v^{PP}_{lj}|}{< \varphi^{PP}_{ljm_j} | \delta v^{PP}_{lj} | \varphi^{PP}_{ljm_j} >}$$

Since the angular part of the pseudo wave-functions $\varphi^{PP}_{ljm_j}$ are spherical spinors the wave-functions should be complex spinors and so the `SpinComponents` needs to be set to `non_collinear`. This is also true for HGH pseudo-potentials.

Note that currently Octopus is only able to read j-dependent Troullier-Martins-like pseudo-potentials that are provided in the UPF file format.

Previous Manual:Physical System - Next Manual:Discretization

Back to Manual <p class=newpage>

Discretization

Besides all the approximations we have to do, no computer can solve an infinite continuous problem. We have to discretize our equations somehow. Octopus uses a grid in real space to solve the Kohn-Sham equations. That is, functions are represented by their value over a set of points in real space. Normally the grid is equally spaced, but also non-uniform grids can be used. The shape of the simulation region may also be tuned to suit the geometric configuration of the system.

Grid

In Octopus functions are represented by a set of values that correspond to the value of the function over a set of points in real space. By default these points are distributed in a uniform grid, which means that the distance

between points is a constant for each direction. It is possible to have grids that are not uniform, but as this is a bit more complex we will discuss it later.

In this scheme, the separation between points, or spacing, is a critical value. When it becomes large the representation of functions gets worse and when it becomes small the number of points increases, increasing memory use and calculation time. This value is equivalent to the energy cutoff used by plane-wave representations.

In Octopus you can choose the Spacing of your simulation by the `Spacing` variable. If you set this as a single value it will give the same spacing for each directions (for example `Spacing=0.3`). If you want to have different spacings for each coordinate you can specify `Spacing` as a block of three real values.

If you are working with the default pseudopotential species of Octopus they come with a recommended `Spacing` value and you don't need to give it in the input file. Normally this default values are around 0.4 [b] (~0.2 [Å]), but you may need smaller spacing in some cases. Do not rely on these default values for production runs.

Double grid (experimental)

The double-grid technique is a method to increase the precision of the representation of the pseudopotentials in the grid that has been recently integrated in Octopus (not available in Octopus 2.1 and previous versions). To activate this technique, set the variable `DoubleGrid` to `yes`. The use of a double grid increases the cost of the transfer of the potential to the grid, but as in most cases this is done only a few times per run, the overhead to the total computation time is negligible. The only exception is when the atoms are displaced while doing a time-dependent simulation, where the double grid can severely increase the computation time.

Box

We also have to select a finite domain of the real space to run our simulation, which is known as the simulation box. Octopus can use several kinds of shapes of box. This is controlled by the variable `BoxShape`. Besides standard shapes Octopus can take shapes given by a user-defined function or even by an image.

The way to give the size of the simulation box changes for each shape, but for most of them it is given by the variable `Radius`.

Zero boundary conditions

By default Octopus assumes zero boundary conditions, that is, wavefunctions and density are zero over the boundary of the domain. This is the natural boundary condition when working with finite systems.

In this case choosing an adequate box size is very important: if the box is too small the wavefunctions will be forced to go to zero unnaturally, but if the box is too large, a larger number of points is needed, increasing calculation time and memory requirements.

Previous Manual:Hamiltonian - Next Manual:Output

Back to Manual <p class=newpage>

Output

At first you may be quite happy that you have mastered the input file, and Octopus runs without errors. However, eventually you (or your thesis advisor) will want to learn something about the system you have managed to describe to Octopus.

Ground-State DFT

Octopus sends some relevant information to the standard output (which you may have redirected to a file). Here you will see energies and occupations of the eigenstates of your system. These values and other information can also be found in the file **`static/info`**.

However Octopus also calculates the wavefunctions of these states and the positions of the nuclei in your system. Thus it can tell you the density of the dipole moment, the charge density, or the matrix elements of the dipole moment operator between different states. Look at the values that the `Output` variable can take to see the possibilities.

For example, if you include

```
Output = wfs_sqmod + potential
```

in your **`inp`** file, Octopus will create separate text files in the directory **`static`** with the values of the square modulus of the wave function and the local, classical, Hartree, and exchange/correlation parts of the Kohn-Sham potential at the points in your mesh.

You can specify the formatting details for these input files with the `OutputFormat` variable and the other variables in the `Output` section of the Reference Manual. For example, you can specify that the file will only contain values along the x, y, or z axis, or in the plane x=0, y=0, or z=0. You can also set the format to be readable by the graphics programs OpenDX, gnuplot or MatLab. OpenDX can make plots of iso-surfaces if you have data in three-dimensions. However gnuplot can only make a 3-d plot of a function of two variables, i.e. if you have the values of a wavefunction in a plane, and 2-d plots of a function of one variable, i.e. the value of the wavefunction along an axis.

Time-Dependent DFT

Optical Properties

A primary reason for using a time-dependent DFT program is to obtain the optical properties of your system. You have two choices for this, linear-response theory *a la* Jamorski, Casida & Salahub [1], or explicit time-propagation of the system after a perturbation, a la Yabana & Bertsch [2]. You may wish to read more about these methods in the paper by Castro et al.[3]

Linear-Response Theory

Linear-response theory is based on the idea that a small (time-dependent) perturbation in an externally applied electric potential $v(r,)$ will result in a (time-dependent) perturbation of the electronic density $(r,)$ which is linearly related to the size of the perturbation: $\delta\rho(r,\omega) = \int d^3r' \chi(r,r';\omega)\delta v(r,\omega)$. Here, obviously,

the time-dependence is Fourier-transformed into a frequency-dependence, . The susceptibility, (*r*,*r*';), is a density-density response function, because it is the response of the charge density to a potential that couples to the charge density of the system. Because of this, it has poles at the excitation energies of the many-body system, meaning that the induced density also has these poles. One can use this analytical property to find a related operator whose eigenvalues are these many-body excitation energies. The matrix elements of the operator contain among other things: 1) occupied and unoccupied Kohn-Sham states and energies (from a ground state DFT calculation) and 2) an exchange-correlation kernel, $f_{xc}(r,r',\omega) = \frac{\delta v_{xc}[n(r,\omega)]}{\delta n(r',\omega)} \mid_{\delta v_{ext}=0}$.

Casida's equations are a full solution to this problem (for real wavefunctions). The Tamm-Dancoff approximation uses only occupied-unoccupied transitions. The Petersilka approximation uses only the diagonal elements of the Tamm-Dancoff matrix, *i.e.* there is no mixing of transitions.[4]It takes only a little more time to calculate the whole matrix, so Petersilka is provided mostly for comparison.

These methods are clearly much faster (an order of magnitude) than propagating in time, but it turns out that they are very sensitive to the quality of the unoccupied states. This means that it is very hard to converge the excitation energy, because one requires a very large simulation box (much larger than when propagating in real time).

Electronic Excitations by Means of Time-Propagation

See Manual:Time_Dependent#Delta_kick:_Calculating_an_absorption_spectrum.

References

1. ? Christine Jamorski, Mark E. Casida, and Dennis R. Salahub, *Dynamic polarizabilities and excitation spectra from a molecular implementation of time-dependent density-functional response theory: N2 as a case study*, J. Chem. Phys. 5134-5147 (1996)
2. ? K. Yabana, G. F. Bertsch, *Time-dependent local-density approximation in real time*, Phys. Rev. B 4484 - 4487 (1996)
3. ? Alberto Castro, Heiko Appel, Micael Oliveira, Carlo A. Rozzi, Xavier Andrade, Florian Lorenzen, M. A. L. Marques, E. K. U. Gross, Angel Rubio, *octopus: a tool for the application of time-dependent density functional theory*, physica status solidi (b) **243** 2465-2488 (2006)
4. ? Petersilka, M. and Gossmann, U. J. and Gross, E. K. U., *Excitation Energies from Time-Dependent Density-Functional Theory*, Phys. Rev. Lett. **76** 1212--1215 (1996)

Previous Manual:Discretization - Next Manual:Troubleshooting

Back to Manual <p class=newpage>

Symmetry

There is not much use of symmetry in Octopus.

In finite systems, you will get an analysis just for your information, but which will not be used anywhere in the code. It is of this form (*e.g.* for silane):

```
***************************** Symmetries *****************************
Symmetry elements : 4*(C3) 3*(C2) 3*(S4) 6*(sigma)
Symmetry group    : Td
**********************************************************************
```

Many symmetries will in fact be broken by the real-space mesh. Since it is always orthogonal, it will break three-fold rotational symmetry of benzene, for example.

In periodic systems, you will also get an analysis, *e.g* like this for bulk silicon in its 8-atom convention cell:

```
***************************** Symmetries *****************************
Space group No.227
 International: Fd -3 m
 International(long): Fd -3 m _1
 Schoenflies: Oh^7
 Multiplicity: 192
Point group
 International: m -3 m
 Schoenflies: Oh
Identity has a fractional translation     0.500000    0.500000    0.000000
Identity has a fractional translation     0.500000    0.000000    0.500000
Identity has a fractional translation     0.000000    0.500000    0.500000
Disabling fractional translations. System appears to be a supercell.
Info: The system has    24 symmetries that can be used.
**********************************************************************
```

The analysis is done by the library spglib. The comments on fractional translations and supercell are due to the use of the conventional cell, since the 2-atom primitive cell does not have orthogonal lattice vectors and therefore cannot be used in Octopus currently.

For large systems, the symmetry analysis might be very time-consuming; in rare cases, the symmetry analysis might crash and stop the calculation. In either situation, you can use the variable `SymmetriesCompute` to turn off the symmetry analysis. You can manually identify a direction in which symmetry is broken with `SymmetryBreakDir`, which is appropriate for the case that an external field is applied in a particular direction.

Symmetries are used in two ways for periodic systems: first, to reduce the set of k-points needed. This behavior is controlled by `KPointsUseSymmetries`. For high-symmetry systems, this can make a dramatic reduction in the time required for a calculation. For example, in our silicon example, if we set

```
%KPointsGrid
 4   | 4   | 4
 0.5 | 0.5 | 0.5
%
```

we will obtain not 4×4×4 = 64 k-points but only 4:

```
   4 k-points generated from parameters :
 ------------------------------------------------
    n =    4    4    4      s =  0.50  0.50  0.50

 index |    weight    |             coordinates              |
     1 |     0.125000 |    0.125000    0.125000    0.125000  |
     2 |     0.375000 |    0.125000    0.125000    0.375000  |
     3 |     0.375000 |    0.375000    0.375000    0.125000  |
```

```
    4 |     0.125000 |    0.375000    0.375000    0.375000  |
```

The density and other scalar quantities are straightforwardly computed from the density due to each k-point and the weight; the same has been done for some vector quantities such as the gradients used in GGA functionals and the forces.. Note, however, that the proper calculation of more complicated tensorial properties such as the response functions in the Sternheimer calculation modes have not been implemented with symmetry. You can also use the symmetry operations to symmetrize the density, via `SymmetrizeDensity`. In general, you should beware of use of symmetries for partially periodic systems (*e.g.* wire or sheet geometry) for which some problems have been found.

The use of symmetry for reducing the number of calculations needed for obtaining absorption spectra by time-propagation is discussed here: Tutorial:Optical_Spectra_from_TD:Symmetries

---

Previous Manual:Output - Next Manual:Troubleshooting

Back to Manual <p class=newpage>

Troubleshooting

If Octopus works properly on your system (i.e. you can recreate the results in the tutorial) but you have troubles using it for your own work, here are some things to try. Please feel free to add your own ideas here.

Read parser.log

If you look at the file **`exec/parser.log`**, it will tell you the value of the variables that you set with the **`inp`** file, as well as all the variables which are taking their default value. This can sometimes be helpful in understanding the behavior of the program.

Use OutputDuringSCF

If you add `OutputDuringSCF` = `yes` to your input file, you can examine the results of each iteration in the Self Consistent Field calculation. So if you also have the variable `Output` set to `Output` = `density + potential`, both the electron density and the Kohn-Sham, bare, exchange-correlation and Hartree potentials will be written to a folder (called, e.g., `scf.0001`) after each SCF iteration.

Set DebugLevel

Set the variable `Debug` to 1 for some extra diagnostic info and a stack trace with any fatal error, 2 to add a full stack strace, and 99 to get a stack trace from each MPI task when running in parallel.

Previous Manual:Symmetry - Next Manual:Ground State

Back to Manual <p class=newpage>

Calculations

<p class=newpage>

Ground State

The ground-state electronic density in a Kohn-Sham (KS)-based electronic-structure code such as Octopus is obtained after a self-consistent process that attempts to solve the KS equations.

Kohn-Sham Ground State

In essence, the problem is the following: at a given iteration step, one departs from an approximate solution ? some KS eigenfunctions ψ_j^{inp}, eigenvalues ϵ_j^{inp} and density ^{inp}, which determines a KS ?input? Hamiltonian. By diagonalizing this Hamiltonian, one obtains the corresponding ?output? eigenfunctions, eigenvalues, and density. This density (or, alternatively, the corresponding Kohn-Sham potential) is then used to build a new input Hamiltonian, that will be diagonalized in the next iteration step. This cycle is considered to be closed, and the solution achieved, when the input and output are similar enough that some convergence criterion is fulfilled. In our case, we have allowed for four different criteria, to be defined below. The self-consistent procedure will stop either when the first of the convergence criterions is fulfilled, or when a maximum number of iterations has been performed.

Mixing

The output density (or potential) of a given iteration is not used directly to construct the Kohn-Sham potential for the following iteration. Instead, it is "mixed" with some densities (or potentials) of previous iteration steps. The manner in which this mixing is produced is determined by the variables `MixingScheme`, `Mixing`, `MixField` and `MixNumberSteps`.

Convergence

After each iteration Octopus checks whether some convergence criterion is met. One criterion is that the error in the electron density be smaller than some threshold. Of course, the true electron density is not known, so this "error" is really the change in the density since the last iteration: $\epsilon = \int \mathrm{d}^3 r |\rho^{out}(\mathbf{r}) - \rho^{inp}(\mathbf{r})|.$ We call this criterion `ConvAbsDens`.

However, since the density is proportional to the number of electrons *N*, this absolute criterion is not very transferable between different system sizes. Therefore the default criterion to use is `ConvRelDens`, in which the relative density, $\frac{\rho}{N}$, is used rather than the absolute density. $\epsilon = \frac{1}{N} \int \mathrm{d}^3 r |\rho^{out}(\mathbf{r}) - \rho^{inp}(\mathbf{r})|.$ By default we use a value of `1e-5`.

The other convergence variables `ConvAbsDens`, `ConvAbsEv`, and `ConvRelEv` are set to `0`, indicating that they will not be used as criteria for convergence.

These other available criteria use errors defined as follows:

ConvAbsEv: The change in each eigenvalue is found and the sum of these changes must be smaller than the threshold.

$$\epsilon = \sum_{j=1}^{N_{occ}} |\epsilon_j^{out} - \epsilon_j^{inp}|.$$

ConvRelEv: The eigenvalues are scaled by the number of electrons, otherwise as above.

$$\epsilon = \frac{1}{N} \sum_{j=1}^{N_{occ}} |\epsilon_j^{out} - \epsilon_j^{inp}|.$$

To use them, set the relevant variable equal to a number indicating your desired error. Set the other three convergence variables to zero.

Eigensolver

In each iteration of the self-consistency problem described above, Octopus must diagonalize the Kohn-Sham input Hamiltonian to obtain the output eigenfunctions and eigenvalues. This diagonalization is done by the eigensolver, also an iterative procedure. There are several options for the iterative scheme used to diagonalize the Hamiltonian, which are specified in the documentation for the variable Eigensolver. You may specify the threshhold for considering this iterative diagonalization finished with the variable EigensolverTolerance. The variable EigensolverMaxIter sets a maximum number of steps in the diagonalization, so that if it is reached, the diagonalization is considered finished even if some of the eigenvectors are not fully converged.

During each self-consistent field cycle iteration Octopus reports the eigenvalues it has obtained by diagonalizing the Hamiltonian, and how many of those eigenvectors are fully converged.

```
********************** SCF CYCLE ITER #    3 ************************
 etot =  4.52092631E+00 abs_ev   =  7.91E+02 rel_ev   =  4.28E+01
                        abs_dens =  5.16E-01 rel_dens =  1.43E-02
Matrix vector products:   3669
Converged eigenvectors:      6
Eigenvalues [H]
 #st  Spin   Eigenvalue     Occupation       Error
   1   --    -1.288198       2.000000      (7.2E-07)
   2   --    -0.830676       2.000000      (1.0E-06)
   3   --    -0.826885       2.000000      (8.8E-07)
   4   --    -0.808297       2.000000      (6.2E-07)
...
```

It is not too important whether the eigenvectors are not converged in the SCF steps, only whether they are converged at the end.

LCAO

Since the solution of the ground-state problem is done iteratively, we need an initial guess; a set of initial Kohn-Sham orbitals. If we are doing the calculation with pseudopotentials (as opposed to model potentials defined by the user), we can use the pseudo-orbitals that are used to generate the pseudopotential. By default, the program will fill the initial guess states with pseudo-orbitals. Whether or not this is done is determined by the variable

LCAOStart. The guess density is the sum of the atomic densities.

Note, however, that those pseudo-orbitals are not passed directly to the iterative cycle. Instead, the code performs an initial diagonalization with the Hamiltonian generated by the guess density. Therefore, the SCF cycle is started with the linear combination of those atomic orbitals, with the coefficients that result of that diagonalization (LCAO stands for linear combination of atomic orbitals). In other words, the first step of the SCF cycle is performed inside the LCAO subspace, whereas the following steps are performed in the full space.

This diagonalization will typically be done with a number of pseudo-orbitals that is larger than the number that will be used later in the KS SCF cycle. Once we diagonalize that LCAO matrix, we take the lowest lying eigenstates to proceed with the calculation. There is some default number of pseudo-orbitals that will be used, but one can change it making use of variable LCAODimension.

If you set SCFinLCAO, the LCAO calculation will be performed self-consistently. Or, in other words, the whole SCF cycle will be done inside the LCAO subspace.

Unoccupied states

This is CalculationMode =unocc. The purpose of this run mode is to calculate higher lying Kohn-Sham orbitals. For that purpose, it reads the restart information from a converged previous ground-state calculation, and builds the corresponding Hamiltonian. Then, it calculates the unoccupied eigenvalues and eigenfunctions. The number of unoccupied orbitals calculated is given by the ExtraStates.

Previous Manual:Troubleshooting - Next Manual:Time-Dependent

Back to Manual <p class=newpage>

Time-Dependent

Time evolution

When CalculationMode = td, the code performs the time-propagation of the electronic orbitals and – if required – the ionic positions. The latter task does not pose major algorithmical problems (the usual Verlet algorithms deal with that task); however the best way to propagate a Schrödinger-like equation is still unclear. Due to this fact, we provide with a rather excessive selection of possibilities for that purpose. Before describing the set of variables necessary to specify the way in which the time evolution is to be performed, it is worth making a brief introduction to the problem.

We are concerned with a set of Schrödinger-like equations for the electronic orbitals $\psi_j(t)$:

$$i\frac{\partial}{\partial t}\psi_j(t) = H(t)\psi_j(t)$$

$$\psi_j(t=0) = \psi_j^{(0)}$$

Because this equation is linear (the time derivative and the Hamiltonian are both linear operators), one may formally define a linear ?evolution? operator, $U(T,t)$, which transforms the initial vector into the solution at time T:

$$\psi_j(T) = U(T,0)\psi_j^{(0)}$$

Moreover, there is the formally exact expression for the evolution operator

$$\psi_j(T) = \mathcal{T}\text{exp}\left\{-i\int_0^T d\tau H(\tau)\right\}\psi_j^{(0)},$$

where $\mathcal{T}\text{exp}$ is the time-ordered exponential, which is a short-hand for:

$$\psi_j(T) = \left\{\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_0^t d\tau_1\cdots\int_0^t d\tau_n H(\tau_1)\cdots H(\tau_n)\right\}\psi_j^{(0)}$$

If the Hamiltonian commutes with itself at different times, we can drop the time-ordering product, and leave a simple exponential. If the Hamiltonian is time-independent, which makes it trivially self commuting, the solution is simply written as:

$$\psi_j(T) = \text{exp}\left\{-iTH\right\}\psi_j^{(0)}.$$

Unfortunately, this is not the case for TDDFT when the system is exposed to external time-dependent perturbations like electric and magnetic fields or pulsed lasers. But even without an external time-dependency, there remains the intrinsic time-dependency of the Kohn-Sham Hamiltonian, which is built “self-consistently” from the varying electronic density.

The first step to tackle this problem is to split the propagation of the long interval $[0,T]$ into N smaller steps by utilizing the group property

$$U(T,t) = U(T,t')U(t',t)$$

of the time-evolution operator. This yields the following time discretization:

$$U(T,0) = \prod_{i=0}^{N-1} U(t_i+\Delta t, t_i),$$

where $t_0 = 0$, $t_N = T$, $\Delta t = T/N$. So at each time step we are dealing with the problem of performing the short-time propagation:

$$\psi_j(t+\Delta t) = U(t+\Delta t,t)\psi_j(t) = \mathcal{T}\text{exp}\left\{-i\int_t^{t+\Delta t} d\tau H(\tau)\right\}\psi_j(t).$$

In this way, one can monitor the evolution in the interior of $[0, T]$. In fact, the possibility of monitoring the evolution is generally a requirement.

This requirement imposes a natural restriction on the maximum size of Δt : if $\omega_{\max}$ is the maximum frequency that we want to discern, Δt should be no larger than $\approx 1/\omega_{\max}$. Below this $\Delta t_{\max}$, we are free to choose Δt considering performance reasons: technically, the reason for the discretization is two-fold: the time-dependence of H is alleviated, and the norm of the exponential argument is reduced (the norm increases linearly with Δt).

Since we cannot drop the time-ordering product, the desired algorithm cannot be reduced, in principle, to the calculation of the action of the exponential of an operator over the initial vector. Some algorithms tailored to approximate the evolution operator, in fact, do not even need to peform such operator exponentials. Most of them, however, do rely on the calculation of one or more exponentials, such as the ones used by Octopus. This is why in principle we need to specify two different issues: the “evolution method”, and the “exponential method”. In other words: we need an algorithm to approximate the evolution operator $U(t + \Delta t, t)$ – which will be specified by variable `TDPropagator` – and, if this algorithm requires it, we will also need an algorithm to approximate the exponential of a matrix operator $\exp\{A\}$ – which will be specified by variable `TDExponentialMethod`.

Propagators for the time-dependent Kohn-Sham equations

In the following, we describe the propagators available in Octopus for the time-dependent Kohn-Sham equations. These propagators solve the problem of approximating the orbitals $\psi_j(t + \Delta t)$ from the knowledge of $\psi_j(\tau)$ and $H(\tau)$ for $0 \leq \tau \leq t$. Some methods require the knowledge of the Hamiltonian at some points τ in time between t and $t + \Delta t$.

This quantity can be approximated by the following procedure:

1. Approximate $H(\tau)$ through extrapolation of a polynomial fit to a certain number of previous time steps.
2. Propagate $\psi_j(t)$ to get $\psi_j(t + \Delta t)$.
3. Calculate $H(t + \Delta t)$ from the orbitals $\psi_j(t + \Delta t)$.
4. Interpolate the required $H(\tau)$ from $H(t)$ and $H(t + \Delta t)$.
5. Repeat the steps 2 to 4 until self-consistency is reached.

In Octopus, however, the above scheme is dropped for performance reasons and only step 1 is implemented, via a second-order extrapolation, except for the first two steps where the extrapolation obviously cannot be trusted. Instead, we rely on a sufficiently small Δt .

Midpoint rules

The implicit midpoint rule or Crank-Nicolson method (`TDPropagator`=`crank_nicolson`) calculates the exponential of the Hamiltonian by a first-order Padé approximation. The Hamiltonian is evaluated at $t + \Delta t/2$ and the integral is dropped:

$$U_{\mathrm{CN}}(t+\Delta t,t)=\frac{1-i\frac{\Delta t}{2}H(t+\Delta t/2)}{1+\frac{\Delta t}{2}H(t+\Delta t/2)}$$

The calculation of the matrix fraction is transformed into the solution of the linear system

$$L\psi_j(t+\Delta t)=b$$

with the known quantities

$$L=1+i\frac{\Delta t}{2}H(t+\Delta t/2)$$

and

$$b=\left\{1-i\frac{\Delta t}{2}H(t+\Delta t/2)\right\}\psi_j(t).$$

The Crank-Nicolson scheme is unitary and preserves time-reversal symmetry.

A similar but similar scheme is the exponential midpoint rule (`TDPropagator`=`exp_mid`), which is unitary and time-reversal-symmetry-preserving, but has the drawback that it requires fairly small time steps:

$$U_{\mathrm{EM}}(t+\Delta t,t)=\exp\left\{-i\Delta tH(t+\Delta t/2)\right\}$$

Magnus expansions

Magnus expansion (`TDPropagator`=`magnus`) is the most sophisticated propagation implemented in Octopus. According to Magnus, there exists an operator $\Omega(t+\Delta t,t)$ for which holds

$$U(t+\Delta t,t)=\exp\left\{\Omega(t+\Delta t,t)\right\}$$

given by the series

$$\Omega(t+\Delta t,t)=\sum_{k=1}^{\infty}\Omega_k(t+\Delta t,t)$$

that converges at least for some local environment of t.

The operators $\Omega_k(t+\Delta t,t)$ are generated with the recursive procedure

$$\Omega_k(t+\Delta t,t)=\sum_{l=0}^{k-1}\frac{B_l}{l!}\int_t^{t+\Delta t}S_k^l(\tau)d\tau,$$

$$S_1^0(\tau) = -iH(\tau), \quad S_k^0 = 0 \text{ for } k > 1,$$

$$S_k^j(\tau) = \sum_{m=1}^{k-l} \left[\Omega_m(t+\Delta t, t), S_{k-m}^{l-1}(\tau)\right] \text{ for } 1 \le l \le k-1,$$

where B_l are Bernoulli numbers.

In Octopus we have implemented a fourth-order Magnus expansion, which means that the operator series is truncated to second order and the integrals are calculated by a second-order quadrature formula. The resulting operator is

$$\Omega_{M(4)}(t+\Delta t, t) = -i\frac{\Delta t}{2}\left[H(t_1) + H(t_2)\right] - \frac{\sqrt{3}\Delta t^2}{12}\left[H(t_2), H(t_1)\right]$$

with the quadrature sampling points $$t_{1,2} = t + \left[\frac{1}{2} \mp \frac{\sqrt{3}}{6}\right]\Delta t$$.

With a modified Hamiltonian

$$H_{M(4)}(t, \Delta t) = \overline{H}(t, \Delta t) + i\left[T + v_{\text{ext}}^{\text{nonlocal}}(t), \overline{\Delta V}(t, \Delta t)\right],$$

$$\overline{H}(t, \Delta t) = T + \frac{1}{2}\left[V_{\text{KS}}(t_1) + V_{\text{KS}}(t_2)\right],$$

$$\overline{\Delta V}(t, \Delta t) = \frac{\sqrt{3}}{12}\Delta t\left[V_{\text{KS}}(t_1) - V_{\text{KS}}(t_1)\right]$$

the propagator takes the form

$$U_{M(4)}(t+\Delta t, t) = \exp\left\{-i\Delta t H_{M(4)}(t, \Delta t)\right\}.$$

Note that only the nonlocal components of the Kohn-Sham Hamiltonian contribute to the commutator and, furthermore, that we make the assumption that the nonlocal potential $v_{\text{ext}}^{\text{nonlocal}}(t)$ does not vary significantly in the interval $[t, t+\Delta t]$. This nonlocal component stems from the ionic pseudopotentials. Consequently, its variation is caused by the ionic movement, which is negligible on the electronic time scale determining Δt.

Time-reversal-symmetry based propagation

Due to time-reversal symmetry, propagating backwards by $\Delta t/2$ starting from $\psi_j(t+\Delta t)$ should lead to the same result as propagating forwards by $\Delta t/2$ starting from $\psi_j(t)$. Using the simplest approximation to the evolution operator, we end up with the condition

$$\exp\left\{+i\frac{\Delta t}{2}H(t+\Delta t)\right\}\psi_j(t+\Delta t) = \exp\left\{-i\frac{\Delta t}{2}H(t)\right\}\psi_j(t)$$

Rearranging the terms gives an approximation for the propagator:

$$U_{\mathrm{ETRS}}(t+\Delta t, t) = \exp\left\{-i\frac{\Delta t}{2}H(t+\Delta t)\right\}\exp\left\{-i\frac{\Delta t}{2}H(t)\right\}$$

This *enforced time-reversal symmetry* method is available in Octopus by setting (TDPropagator=etrs).

It is worthwhile to give a sidenote on the approximation of $H(t+\Delta t)$: for the etrs method the Hamiltonian at time $t+\Delta t$ is not extrapolated, but rather built from the density $n' = \sum_j |\psi'_j(t+\Delta t)|^2$, which, in turn, is calculated from the orbital estimate

$$\psi'_j(t+\Delta t) = \exp\left\{-i\Delta t H(t)\right\}\psi_j(t).$$

There exists, however, also a variant TDPropagator=aetrs *(approximated enforced time-reversal symmetry)* that performs a second-order polynomial extrapolation of $H(t-k\Delta t)$, $k=0,1,2$, to get $H(t+\Delta t)$, which is about 40 % faster than etrs.

Approximations to the exponential of an operator

Most of the evolution methods described in the previous section require the calculation of the exponential of a matrix. Before going into the details of the TDExponentialMethod that Octopus provides, one general difficulty deserves mentioning.

In principle, we would like to calculate $\exp\{A\}v$ by first calculating $\exp\{A\}$ and then applying this result to any vector v. Unfortunately, the size of our Hamiltonian matrix is of the order $\approx 10^5$ which forbids its full storage in matrix form. Apart from that, methods to calculate the exponential of a matrix explicitly are limited to a few thousand matrix elements. For this reason, we have to turn to iterative solutions that calculate $\exp\{A\}v$, for a particular vector v.

Polynomial expansions

The simplest possibility is to use the definition of the exponential of a matrix

$$\exp\{A\} = \sum_{k=0}^{\infty}\frac{1}{k!}A^k$$

to get the approximation of order k (TDExponentialMethod=taylor):

$$\mathrm{taylor}_N\left\{A, v\right\} = \sum_{k=0}^{N} \frac{1}{k!} A^k v$$

$\mathrm{taylor}_N\left\{A, v\right\}$ amounts to the expansion of the exponential in the standard polynomial base $\left\{1, x, x^2, \ldots\right\}$.

Experience shows that the choice $k = 4$ gives particularly good results for our TDDFT implementation.

The standard polynomial basis is not the only possibility; Octopus also implements the expansion of the exponential in the Chebyshev basis (`TDExponentialMethod`=`chebyshev`):

$$\mathrm{cheb}_N\left\{A, v\right\} = \sum_{k=0}^{N} c_k T_k(A) k v$$

with T_k being the Chebyshev polynomial of order k.

The truncation N for both these expansions can be set by the input variable `TDExpOrder`.

Krylov-subspace projection

The Krylov subspace of order N for a given operator A and vector v is defined as

$$\mathcal{K}_N\left\{A, v\right\} = \mathrm{span}\left\{v, Av, A^2 v, \ldots, A^{N-1} v\right\}.$$

The idea is to find the element of $\mathcal{K}_N\left\{A, v\right\}$ that optimally approximates $\exp\left\{A\right\}$ in a least-squares sense. It can be proven that this is given by

$$\beta V_N (V_N^T \exp\left\{A\right\} V_N) e_1$$

with $V_N = [v_1, \ldots, v_N]$ being an orthonormal basis of $\mathcal{K}_N\left\{A, v\right\}$ calculated with the Lanczos procedure. To get rid of the exponential, the approximation

$$V_N^T \exp\left\{A\right\} V_N \approx \exp\left\{V_N^T A V_N\right\}$$

is introduced. The object $H_N = V_N^T A V_N$ is also a result of the Lanczos procedure and of the small dimension $k \times k$ which allows for direct calculation of the remaining exponential. So, we have

$$\mathrm{lanczos}_N\left\{A, v\right\} = V_N \exp\left\{H_N\right\} e_1,$$

which can be selected by setting `TDExponentialMethod`=`lanczos`. When actually calculating the exponential, Octopus recursively generates the quantities H_N and V_N until some convergence criterion –

controlled by TDLanczosTol – is met or the order exceeds the maximum allowed order controlled by TDExpOrder. In the latter case, a warning is written. Care should be taken in choosing the convergence parameter small enough to avoid faulty evolutions.

Performing a time-propagation

To actually perform a time-propagation, a necessary prerequisite is to have the ground-state density (see Ground State) of the system under consideration.

Then, the CalculationMode has to be set to td.

Besides the already mentioned input variables concerning the propagation method, two more important parameters have to be set: TDTimeStep and TDMaxSteps. The first one sets Δt , the second sets the number of iterations. It is convenient to define these two variables like this:

```
T  = 0.1     # Length of propagation.
dt = 0.002   # Length of time step.

TDMaximumIter = T/dt
TDTimeStep = dt
```

In the absence of a perturbation, the system's total energy should be a constant. This check to determine a reasonable time step has to be done before any other calculation.

The relevant parts of Octopus' output might look like

```
  Iter            Time        Energy     Elapsed Time
     1       0.002000   -541.542073         4.800
     2       0.004000   -541.542073         4.560
     3       0.006000   -541.542073         3.880
     .
     .
     .
    48       0.096000   -541.542073         7.420
    49       0.098000   -541.542073         7.620
    50       0.100000   -541.542073         7.490
```

The energy is printed in the third column and should remain constant. In general, larger time steps are desirable to shorten computational propagation time but keep in mind that the size of the time step limits to the maximum frequency you will be able to observe, and, consequently, also any external perturbation to which you might wish to expose the system.

External fields

Delta kick: Calculating an absorption spectrum

To obtain the linear optical absorption spectrum of the system, we follow the scheme proposed by Yabana and Bertsch, and excite all frequencies of the system by giving some small momentum ($\mathcal{K}$) to the electrons. This is achieved by transforming the ground-state wavefunctions according to:

$$\varphi_i(r, \delta t) = e^{i\mathcal{K}z}\varphi_i(r, 0)\,,$$

and then propagating these wavefunctions for some (finite) time. The spectrum can then be obtained from the expression for the dipole strength function $S(\ )$:

$$S(\omega) = \frac{2\omega}{\pi} \mathcal{I}m\alpha(\omega) \,,$$

where the dynamical polarizability, $(\ )$, is essentially the Fourier transform of the dipole moment of the system $d(t)$:

$$\alpha(\omega) = \frac{1}{\mathcal{K}} \int dt \; e^{i\omega t} \left[d(t) - d(0) \right] \,.$$

With this definition, the Thomas-Reiche-Kuhn f-sum rule for the number of electrons, N, is given by the integral:

$$N = \int d\omega \; S(\omega) \,.$$

This sum rule can be used to check the quality of the calculations. Another check is energy conservation, which TDDFT respects when no external field is applied.

To obtain a spectrum with such a recipe in Octopus one has to follow the steps:

1. Choose a system of linearly independent (can be non-orthogonal) axes (defined by the variable `TDPolarization`). The defaults are the 3 Cartesian axes.
2. Add an electric kick using the variable `TDDeltaStrength`. Its value should be small so that we remain in the linear regime, but large enough to avoid numerical errors.
3. Run a time-dependent simulation for the 3 independent directions. This involves running Octopus 3 times, changing the value of `TDPolarizationDirection` each time. After each run, move the file `td.general/multipoles` to `td.general/multipoles.X<tt>, where <tt>X` is 1, 2, or 3.
4. Run the utility oct-propagation_spectrum.

Lasers

To calculate non-linear optical properties, we follow the evolution of the system under the influence of a laser field that is treated in the dipole approximation (although this constraint can be removed). The harmonic emission spectrum can then be calculated from the acceleration of the dipole moment:

$$H(\omega) \propto \left| \int dt \; e^{i\omega t} \frac{d^2}{dt^2} d(t) \right|^2 \,.$$

During the propagation, charge density is absorbed at the boundaries of the simulation region, either by an imaginary absorbing potential or a mask function. In the first case, we add to the Kohn-Sham potential a term

$$V_{\rm eff}(r,t) = V_{\rm KS}(r,t) - iV_{\rm abs}(r) \,,$$

where V_{abs} is zero in the inner region of the simulation box, and rises smoothly till the edges. By adjusting both the height and the shape of the potential, we can select which momenta are absorbed and prevent the unwanted reflections at the boundary. When using a mask, the wavefunction is multiplied in each time-step by a function which is 1 in the inner simulation region and gradually goes to 0 at the borders:

$$\varphi(r,t) \to M(r)\varphi(r,t)\,.$$

The absorbed charge can be interpreted as an ionization probability and can be used to estimate the photo-electron spectra. The box size has to be big enough so that the physical system is not perturbed by the absorbing boundaries. Note that the wavefunctions are no longer normalized as the system slowly gets charged.

Symmetries

The dynamic polarizability (trivially related to optical absorption) is, in its most general form, a 3x3 tensor. The reason is that we can shine light on the system polarized in any of the three Cartesian axes, and for each of these three cases measure how the dipole of the molecule oscillates along the three Cartesian axes. This usually means that to obtain the full dynamic polarizability of the molecule we usually need to apply 3 different perturbations along x, y, z, by setting TDPolarizationDirection to 1, 2, or 3.

However, if the molecule has some symmetries, it is in general possible to reduce the total number of calculations from 3 to 2, or even 1. This is explained in detail here. To use this formalism in Octopus, you can use the variables TDPolarization, TDPolarizationDirection, TDPolarizationEquivAxes, and TDPolarizationWprime. The block TDPolarization defines a basis (not necessarily orthogonal) chosen to maximize the number of equivalent axes, and TDPolarizationDirection, and TDPolarizationWprime are vectors specified in that basis. Let us give a couple of examples.

The methane molecule has T_d symmetry, which means that the response is identical for all directions. This means that we only need one propagation to obtain the whole tensor. This propagation can be performed in any direction we wish. So we could use the input

```
%TDPolarization
 1 | 0 | 0
 0 | 1 | 0
 0 | 0 | 1
%
TDPolarizationDirection = 1
TDPolarizationEquivAxes = 3
%TDPolarizationWprime
 0 | 0 | 1
%
```

Note that we could have omitted the blocks TDPolarization and TDPolarizationWprime in the previous input file, as these are their default values.

Now let us look at a linear molecule. In this case, you might think that we need two calculations to obtain the whole tensor, one for the direction along the axis of the molecule, and another for the axis perpendicular to the molecule. The fact is that we need only one, in a specially chosen direction, so that our field has components both along the axis of the molecule and perpendicular to it. Let us assume that the axis of the molecule is oriented along

the *x*-axis. Then we can use

```
%TDPolarization
 1/sqrt(2) | -1/sqrt(2) | 0
 1/sqrt(2) |  1/sqrt(2) | 0
 1/sqrt(2) |  0         | 1/sqrt(2)
%
TDPolarizationDirection = 1
TDPolarizationEquivAxes = 3
%TDPolarizationWprime
 0 | 0 | 1
%
```

You should try to convince yourself that the three axes are indeed equivalent and linearly independent.

Finally, let us look at a general planar molecule (in the *xy* plane). In principle we need only two calculations (reduced to one if more symmetries are present, as for benzene). In this case we chose one of the polarization axes on the plane, and the other two rotated 45 degrees out of plane:

```
%TDPolarizationDirection
 1/sqrt(2) | 0 | 1/sqrt(2)
 1/sqrt(2) | 0 |-1/sqrt(2)
 0         | 1 | 0
%

TDPolarizationEquivAxes = 2
```

In this case, we need two runs, one for `TDPolarizationDirection` equal to 1, and another for it equal to 3. Note that if there are fewer than 3 equivalent axes, `TDPolarizationWprime` is irrelevant.

Previous Manual:Ground_State - Next Manual:Casida

Back to Manual <p class=newpage>

Casida Linear Response

Mark Casida's formulation of Linear-Response TDDFT allows calculations of the excitation energies of a finite system. For small molecules, this is normally the fastest way to calculate them.

To perform a Casida calculation you first need a ground-state calculation and a calculation of unoccupied states; then you run the code with `CalculationMode`=`casida`.

This is an input file for a linear-response calculation of the nitrogen dimer, found at **`SHARE/testsuite/linear_response/01-casida.*`**.

```
%CalculationMode
gs | unocc | casida
"ground_state_" |  "unocc_states_" | "lrtddft_"
1 | 2 | 3
%
```

```
FromScratch = yes

bond_length = 2.0744

%Coordinates
"N" |  -bond_length/2 |  0.0 |  0.0 | no
"N" |   bond_length/2 |  0.0 |  0.0 | no
%

%Species
"N" | 14.0067000 | tm2 | 7 | 2 | 0
%

BoxShape = sphere

Radius = 12.0
Spacing = 0.36

SpinComponents = unpolarized

XFunctional = lda_x
CFunctional = lda_c_vwn

MaximumIter = 200
ConvRelDens = 1e-5

LCAOStart = lcao_full
LCAODimension = 18

EigenSolver = cg_new
EigenSolverInitTolerance = 1e-2
EigenSolverFinalTolerance = 1e-5
EigenSolverFinalToleranceIteration = 6
EigenSolverMaxIter = 20
unocc_states_EigenSolverMaxIter = 1000

TypeOfMixing = broyden

NumberUnoccStates = 9

PoissonSolver = fft_corrected
```

Previous Manual:Time-Dependent - Next Manual:Linear_Response

Back to Manual <p class=newpage>

Sternheimer Linear Response

Octopus can calculate dynamic polarizabilities and first-order hyperpolarizabilites in a linear-response scheme using the Sternheimer equation. It is also possible to calculate optical spectra with this technique, but it is slower than time-evolution.

Ground state

The first thing we will need for linear response is a Ground State calculation. Unlike the Casida approach, when using the Sterheimer equation you needn't do a unoccupied-states calculation. To improve the convergence of the linear-response calculation, it is better to use tightly converged wavefunctions. For example, you can add these parameters to your gs calculation:

```
EigenSolverFinalTolerance = 1e-10
ConvRelDens = 1e-9
```

Input

The CalculationMode for polarizability calculations is em_resp. The main parameter you have to specify is the frequency of the perturbation, given by the EMFreqs block. You can also add an imaginary part to the frequency by setting the variable EMEta. Adding a small imaginary part is required if you want to get the imaginary part of the polarizability or to calculate polarizabilities near resonance; a reasonable value is 0.1 eV.

To get the hyperpolarizabilties, you also have to specify the variable EMHyperpol with the three coefficients with respect to the base frequency; the three values must sum to zero.

Output

After running, for each frequency in the input file, Octopus will generate a subdirectory under **em_resp/**. In each subdirectory there is a file called **alpha** that contains the real part of the polarizability tensor $_{ij}$ and the average polarizability

$$\bar{\alpha} = \frac{1}{3}\sum_{i=1}^{3}\alpha_{ii}$$

The imaginary part is written to file **eta**. If > 0, there is also a file called **cross_section_tensor** that contains the photo-absorption cross section tensor for that frequency, related to the imaginary part of the polarizability ($\sigma = \frac{4\pi\omega}{c}\mathrm{Im}\alpha$).

The hyperpolarizability will be in a file called **beta** at the base frequency, containing all the 27 components and some reduced quantities:

$$\beta_{||i} = \frac{1}{5}\sum_{j=1}^{3}(\beta_{ijj} + \beta_{jij} + \beta_{jji}) \ .$$

Optionally, Born charges can also be calculated.

Finite differences

In this mode only static polarizability can be obtained. The calculation is done by taking the numerical derivative of the energy with respect to an external static and uniform electric field. To use this, run with ResponseMethod =finite_differences. Octopus will run several ground-state energy calculations and

then calculate the polarizability using a finite-differences formula for the derivative. The results will be in the **em_resp_fd** directory. Hyperpolarizability and Born charges can also be calculated.

Previous Manual:Casida - Next Manual:Optimal Control

Back to Manual <p class=newpage>

Optimal Control

Tutorial on basic Optimal Control Theory

Previous Manual:Linear Response - Next Manual:Geometry Optimization

Back to Manual <p class=newpage>

Geometry Optimization

To perform a geometry optimization with Octopus one should set the `CalculationMode` to `go`. The method to be used should be set using the variable `GOMethod`. Note that most of the methods use the minimization routines from GSL.

The stopping criteria can be set with the variables `GOTolerance` and `GOMinimumMove`. Then minimization will be stopped when all forces on ions are smaller than `GOTolerance` or when all species coordinates change less than `GOMinimumMove` during one minimization step. If none of the previous criteria is matched after a number of minimization steps equal to `GOMaxIter`, then the minimization will be stopped with an error message.

After each minimization step taken by the GSL algorithms Octopus will write the current geometry to a file named **go.XXXX.xyz** (XXXX is the iteration number) in the directory **geom**. As an extra information, the title of the xyz file (second line) contains the total energy.

Note that Octopus is not particularly optimized to perform geometry optimizations and many times, if the stopping criteria are too small, the GSL routines will return an error message stating that they were unable to improve the solution.

At the end of the run, if the minimization was successful, the minimized geometry will be written to a file named **min.xyz** in the working directory.

Previous Manual:Optimal Control - Next Manual:Visualization

Back to Manual <p class=newpage>

Visualization

Every given number of time iterations, or after ground-state calculations, some of the functions that characterise the system may be written to disk so that they may be analized. Files are written within **static/** output directory after the self-consistent field, or within **td.x/** directories, during evolution, where ?x? stands for the iteration

number at which each write is done.

The function that you want to plot is selected by the `Output` variable and the output format is chosen by the `OutputFormat`.

dx

This is an OpenDX network, aimed at the visualization of wavefunctions. To be able to use it, you need to have properly installed the OpenDX program, as well as the Chemistry extensions developed at the Cornell Theory Center. Please take a look here to see how to obtain and install this software. Unfortunately, since this software is old and unmaintained, you are likely to have trouble installing.

Once these are working, you may follow the tutorial for the benzene molecule.

XCrySDen

Atomic coordinates (finite or periodic), forces, and functions on a grid can be plotted with the free program XCrySDen. Its XSF format also can be read by V_Sim and Vesta. Beware, these all probably assume that your output is in Angstrom units (according to the specification), so use UnitsOutput = eV_Angstrom, or your data will be misinterpreted by the visualization software.

CUBE

The Gaussian cube format (http://paulbourke.net/dataformats/cube/) can be output, and can be read by VMD, XCrysDen, Avogadro, and other software. Beware: these all seem to assume the output is in atomic units, so use UnitsOutput = atomic, or your data will be misinterpreted by the visualization software. This is despite the fact that the CUBE specification has a way of identifying the units used. VMD ignores it (http://www.ks.uiuc.edu/Research/vmd/plugins/molfile/cubeplugin.html) and will actually (version 1.9) will crash with a memory allocation error if it sees the negative number of voxels that marks the file as using Angstroms.

PDB

Everything is supposed to be in Angstroms: http://deposit.rcsb.org/adit/docs/pdb_atom_format.html

XYZ

Generally considered to be in Angstroms: http://openbabel.org/wiki/XYZ_%28format%29, https://en.wikipedia.org/wiki/XYZ_file_format, https://www.molpro.net/info/2012.1/doc/manual/node100.html, http://departments.icmab.es/leem/siesta/Documentation/Manuals/siesta-3.1-manual/node32.html

---

Previous Manual:Geometry Optimization - Next Manual:Advanced ways of running Octopus

Back to Manual <p class=newpage>

Advanced ways of running Octopus

Parallel Octopus

Octopus can be run in multi-tentacle (parallel) mode if you have configured it that way when you compiled and installed it. There are four possible parallelization strategies: domains, states, spin/*k*-points, and electron-hole pairs (only for Casida). You do not need to specify in the input file what kind of parallelization strategy you want to use as Octopus can find reasonable defaults. However, the experienced user may want to tune the corresponding variables.

Parallel in States

The first strategy is parallel in states. This means that each processor takes some states and propagates them independently of the others.

To use this include

```
ParStates = auto
```

in your input file.

This is clearly the most efficient (and simplest) way of parallelizing the code if the number of states is much larger than the number of processors available (which is usually the case for us). You can expect a more or less linear speed-up with number of processors until you reach around 5 states/processor. Beyond this it starts to saturate.

Parallel in Domains

When running parallel in "domains", Octopus divides the simulation region (the box) into separate regions (domains) and assigns each of of these to a different processor. This allows it not only to speed up the calculation, but also to divide the memory among the different processors. The first step of this process, the splitting of the box, is in general a very complicated process. Note that we are talking about a simulation box of an almost arbitrary shape, and of an arbitrary number of processors. Furthermore, as the communication between processors grows proportionally to the surface of the domains, one should use an algorithm that divides the box such that each domain has the same number of points, and at the same time minimizes the total area of the domains. Octopus uses the METIS library to make this domain decomposition of the space, METIS is included in the source code of Octopus and will be used by default.

So for example, if you are planning to run the ground state of Na there's only one choice:

```
ParDomains = auto
```

Octopus will then partition the real-space mesh and compute the resulting pieces on different nodes. Later when you plan to do time propagations you have more choices at hand. You could run only parallel in states

```
ParStates = auto
ParDomains = no
```

or in domains (as above), or you can decide to employ both parallelization strategies

```
ParStates = auto
ParDomains = auto
```

Problems with parallelization

The parallelization is only effective if a sufficiently large amount of load is given to each node. Otherwise communication dominates. In that case one should do the calculation in serial. This happens, for example, if you attempt to do parallelization in real-space domains, but your grid does not have too many points. If the code detects that the number of points per node is not large enough, it gives the warning:

```
** Warning:
** From node =    0
** I have less elements in a parallel group than recommended.
** Maybe you should reduce the number of nodes
```

Compiling and running in parallel

The steps to compile and use Octopus in parallel are:

1) use the --enable-mpi in the configuration script

2) give to Octopus the libraries, etc. necessary to compile a parallel code. When you install mpich in your system, it creates a series of programs called mpicc, mpif77, mpif90, etc. These are wrappers that call the specific compiler with the appropriate flags, libraries, etc. This means that to compile Octopus in parallel you'll need mpif90. Please check that this is present in your system (perhaps in /usr/local/bin if you compiled mpich from the sources). Octopus will try to find this compiler, but it may not be able to find it for several reasons:

- mpif90 is _not_ in the path.
- there is another f90 compiler specified by the user/system. This means that if you have the variable FC defined when you run the configure script, Octopus will use the fortran compiler specified by that variable, and will not try to find mpif90. Then, the configuration fails.

```
export FC=<whatever path>/mpif90
export FCFLAGS=<whatever flags>
./configure --enable-mpi
```

It is wise to also set the `FCFLAGS`, as Octopus cannot tell which fortran compiler you are using if you compile with mpif90.

3) Now you just have to run Octopus in parallel (this step depends on your actual system, you may have to use mpirun or mpiexec to accomplish it).

In some run modes (e.g., `td`), you can use the multi-level parallelization, i.e., to run in parallel in more than one way at the same time. In the `td` case, you can run parallel in states and in domains at the same time. In order to fine-tune this behavior, please take a look at the variables `ParStates`, `ParDomains`, `ParKPoints`, and `ParOther`. In order to check if everything is OK, take a look at the output of Octopus in the "Parallelization" section. This is an example:

```
************************* Parallelization ***************************
```

```
Octopus will run in *parallel*
Info: Number of nodes in par_states  group:     8 (      62)
Info: Octopus will waste at least  9.68% of computer time
************************************************************************
```

In this case, Octopus runs in parallel only in states, using 8 processors (for 62 states). Furthermore, some of the processors will be idle for 9.68% of the time (this is not that great, so maybe a different number of processors would be better in this case).

Passing arguments from environment variables

Octopus can also read input variables from the environment variables of the shell. This is especially useful if you want to call Octopus from scripts or if you want to pass one-time arguments when running Octopus.

To activate this feature you must first set `OCT_PARSE_ENV` to some value, for example in sh/bash

```
$ export OCT_PARSE_ENV=1
```

After that, to pass an input variable to Octopus, you must prepend the name of the variable by `'OCT_'`, for example:

```
$ export OCT_Radius=10
```

After that you can run Octopus as usual.

You can also pass the variables in the same command line:

```
$ OCT_PARSE_ENV=1 OCT_Radius=10 octopus
```

If you set a variable both from the input file and as a environment variable, the environment variable takes precedence. Be careful with this behaviour. Blocks are not supported (suggestions as how to elegantly put a block inside of environment variables are welcome).

There is an additional environment variable `OCTOPUS_SHARE` that can be set to specify the location of the `variables` file used by the parser. If this environment variable is not set, the default is as set by the configure script, namely `prefix/share/octopus`. You can set this to something else if necessary, for example to handle moving an executable from one machine to another, where the original path does not exist on the new machine.

Examples

For example this is a simple script that helps to determine the optimal Radius of the simulation box (an **`inp`** file with the rest of the parameters has to be provided):

```
export OCT_PARSE_ENV=1
for OCT_Radius in `seq 5 16`
do
  export OCT_Radius
  octopus >& out-$OCT_Radius
  energy=`grep Total static/info  | head -1 | cut -d "=" -f 2`
```

```
  echo $OCT_Radius $energy
done
```

Previous Manual:Visualization - Next Manual:External utilities:oct-analyze_projections

Back to Manual <p class=newpage>

Utilities

<p class=newpage>

oct-analyze_projections

Manual:External utilities:oct-analyze projections <p class=newpage>

oct-atomic_occupations

This script prints out to standard output the electronic configuration of a given atom, and the way in which this electronic configuration should be reflected in the `Occupations` block of a corresponding Octopus input file.

Options

`-s species`

species should be the atomic symbol (e.g. Na, Au, etc).

`-h`

Show a brief summary of command line options.

Examples

```
$ oct-atomic_occupations -s Na

$ oct-atomic_occupations -s Ti_sc

$ for x in \$(cat /usr/share/octopus/PP/defaults | awk '{print \$1}')
> do oct-atomic_occupations -s $x
> done
```

Previous Manual:External utilities:oct-analyze_projections - Next Manual:External utilities:oct-casida_spectrum

Back to Manual <p class=newpage>

oct-casida_spectrum

NAME

oct-casida_spectrum - Broadens the linear-response spectra from the Casida run mode.

SYNOPSIS

oct-casida_spectrum

[oct-casida_spectrum does not read standard input: all standard input will be simply ignored. An input file named **inp** must be present in the running directory. Also, oct-casida_spectrum accepts no command line arguments, since there is not a standard way to do this with Fortran 90.]

DESCRIPTION

This program is one of the Octopus utilities.

It post-processes the files **casida/casida**, **casida/petersilka** and **casida/eps_diff**, that contain the excitation energies and oscillator strengths.

The parameters of the spectrum can be set using the variables CasidaSpectrumBroadening, CasidaSpectrumMinEnergy, CasidaSpectrumMaxEnergy, and CasidaSpectrumEnergyStep.

Previous Manual:External utilities:oct-atomic_occupations - Next Manual:External utilities:oct-center-geom

Back to Manual <p class=newpage>

---

oct-center-geom

NAME

oct-center-geom - Centers a molecule's geometry

SYNOPSIS

oct-center-geom

[oct-center-geom does not read the standard input: all standard input will be simply ignored. An input file named **inp** must be present in the running directory. Also, oct-center-geom accepts no command-line arguments, since there is not a standard way to do this with Fortran 90.]

DESCRIPTION

This program is one of the Octopus utilities.

It reads the coordinates defined in the **inp** file, and constructs an output xyz file, that will be called **adjusted.xyz** file, that describes the same system but in which the atomic coordinates are centered, and (optionally) has the axes aligned.

To control the orientation of the centered molecule there are two parameters: MainAxis and AxisType.

Do not forget then to change your input file to use this file instead of your old geometry (by changing XYZCoordinates='adjusted.xyz').

Be careful with units, this utility honours the Units, UnitsInput and UnitsOutput variables, so the **adjusted.xyz** file will be in the specified output units.

Previous Manual:External utilities:oct-casida_spectrum - Next Manual:External utilities:oct-check_deallocs

Back to Manual <p class=newpage>

---

oct-check_deallocs

Manual:External utilities:oct-check deallocs <p class=newpage>

---

oct-conductivity

Manual:External utilities:oct-conductivity <p class=newpage>

---

oct-convert

Name

oct-convert - Octopus utility to read obj files and write in many different file formats

Description

This executable gives the ability to read files written during the ground-state or time-dependent execution

Example

You can run ground-state and time-dependent execution of the benzene example.

Then, we have to add this to the inp file, if we want to have the ground state density in DX format:

```
Output = density
OutputFormat = dx
ConvertFolder = 'restart/gs'
ConvertFilename = 'density'
ConvertIterateFolder = no
```

To convert the restart wave-functions (from 1 to 10) of a td run:

```
Output = density
OutputFormat = dx
ConvertIterateFolder = no
ConvertFilename = ' '
ConvertStart = 1
ConvertEnd   = 10
ConvertFolder = 'restart/td/'
```

If we want to convert the densities of the time-dependent executions, from files td.0000001 to td.0000010:

```
Output = density
OutputFormat = dx
ConvertIterateFolder = yes
ConvertStart = 1
ConvertEnd   = 10
```

Previous Manual:External utilities:oct-conductivity - Next Manual:External utilities:oct-dielectric-function

Back to Manual <p class=newpage>

---

oct-dielectric-function

Manual:External utilities:oct-dielectric-function <p class=newpage>

---

oct-display_partitions

NAME

oct-display_partitions - Graphical representation of the mesh partitions.

SYNOPSIS

oct-display_partitions

[oct-display_partitions does not read the standard input: all standard input will be simply ignored. Also, oct-display_partitions accepts no command line arguments.]

DESCRIPTION

This program is one of the octopus utilities.

It is a script to use gnuplot to plot the partitioning of the mesh. The files **TO DO** **mesh_partition.???** as produced in **debug/mesh_partition** by the Octopus debug mode have to be present in the current working directory when this script is invoked. The plot can be found in the file **mesh_partitions.png**. This script generates a gnuplot-script called **mesh_partitions_index.gp** which is stored in the current working directory and can be loaded into gnuplot manually. With:

```
$ gnuplot> load mesh_partitions_index.gp
 $ gnuplot> set term x11
 $ gnuplot> replot
```

the plot can be reproduced and shown on the screen so that rotating and zooming is possible.

Previous Manual:External utilities:oct-dielectric-function - Next Manual:External utilities:oct-harmonic-spectrum

Back to Manual <p class=newpage>

---

oct-harmonic-spectrum

NAME

oct-harmonic-spectrum - Calculates the harmonic spectrum.

SYNOPSIS

```
oct-harmonic-spectrum
```

[oct-harmonic-spectrum does not read the standard input: all standard input will be simply ignored. An input file named **inp** must be present in the running directory. Also, oct-harmonic-spectrum accepts no command line arguments, since there is not a standard way to do this with Fortran 90.]

DESCRIPTION

This program is one of the Octopus utilities.

TO DO MISSING SHORT DESCRIPTION OF THE PROGRAM

Previous Manual:External utilities:oct-display_partitions - Next Manual:External utilities:oct-help

Back to Manual <p class=newpage>

---

oct-help

Oct-help is a utility to helps you to write input files. It has been available since version 3.0. Oct-help has two modes:

search

```
$ oct-help search string
```

In this mode oct-help will print all variable names that contain *string* in their name.

show

```
$ oct-help show variable
```

In this mode oct-help will print the documentation for the indicated variable.

Previous Manual:External utilities:oct-harmonic-spectrum - Next Manual:External utilities:oct-infrared_spectrum

Back to Manual <p class=newpage>

---

oct-infrared_spectrum

Manual:External utilities:oct-infrared spectrum <p class=newpage>

---

oct-local_multipoles

Manual:External utilities:oct-local multipoles <p class=newpage>

---

oct-oscillator-strength

Manual:External utilities:oct-oscillator-strength <p class=newpage>

---

oct-photoelectron_spectrum

Manual:External utilities:oct-photoelectron spectrum <p class=newpage>

---

oct-propagation_spectrum

NAME

oct-propagate_spectrum - Calculates the absorption cross section tensor from the results of a time-propagation run.

SYNOPSIS

```
oct-propagate_spectrum
```

[oct-propagate_spectrum does not read the standard input: all standard input will be simply ignored. An input file named **inp** must be present in the running directory. Also, oct-propagate_spectrum accepts no command line arguments, since there is not a standard way to do this with Fortran 90.]

DESCRIPTION

This program is one of the Octopus utilities.

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 the input file, the user may set the PropagationSpectrumTransform (this should be set to ?sine? for proper use), the PropagationSpectrumDampMode (recommended value is ?polynomial?, which ensures fulfilling of the N-sum rule), the PropagationSpectrumStartTime, the PropagationSpectrumEndTime, the PropagationSpectrumEnergyStep, and the PropagationSpectrumMaxEnergy.

Previous Manual:External utilities:oct-photoelectron_spectrum - Next Manual:External utilities:oct-run_periodic_table

Back to Manual <p class=newpage>

---

oct-run_periodic_table

NAME

oct-run_periodic_table - run octopus for atoms

SYNOPSIS

oct-run_periodic_table [option] ...

DESCRIPTION

This script is one of the octopus utilities.

Simple script to run octopus for all atoms in the periodic table for which pseudopotentials are available.

`-h`

Show this message

`-n`

Run in dry run mode (show what would be executed)

`-s species`

Run octopus for given species.

`-a`

Run octopus for all atoms

`-r`

Do a restart, i.e. do not use `fromScratch`=yes.

`-t temperature`

Run with electronic temperature.

`-e no_states`

Use extra states

`-x octopus_executable`

`-d defaults_file_for_pseudopotentials`

EXAMPLES

The following command would run the octopus executable to calculate the He atom.

```
$  oct-run_periodic_table -s He -x octopus
```

Previous Manual:External utilities:oct-propagation_spectrum - Next Manual:External utilities:oct-run_regression_test.pl

Back to Manual <p class=newpage>

---

oct-run_regression_test.pl

NAME

oct-run_regression_test.pl - Script to create and run octopus regression tests

SYNOPSIS

```
oct-run_regression_test.pl [ option ] ... [ file ] ...
```

DESCRIPTION

This script is one of the octopus utilities.

This script can be used to generate and run the octopus regression tests.

`-n`

Dry run. Don't run the test. Only print what would be executed.

`-v`

Run in verbose mode. Useful for debugging the script.

`-h`

Show a brief summary of command line options.

`-e *file*`

Specify the name of the Octopus executable. The default is octopus.

`-c *file*`

Create a template for a Octopus regression test. This should always be used if you create a new regression test.

`-f *file*`

This option specifies the input file for a regression test.

`-d *directory*`

Use *directory* as working directory. The default is a randomly generated directory in /tmp.

`-i`

Print content of the octopus inputfile which is used for the current test to stdout.

`-p`

Preserve working directory. Don't clean up the temporary working directory after the run.

EXAMPLES

To create a template for a regression test run e.g.

```
$ oct-run_regression_test.pl -c finite_systems_3d/sodium.test
```

Running a test can be achieved with

```
$ oct-run_regression_test.pl -f finite_systems_3d/sodium.test
```

If a test run fails it might be useful for bug tracing to preserve the working directory of this run and to print out the input file

```
$ oct-run_regression_test.pl -pi -f finite_systems_3d/sodium.test
```

Run a MPI test with a local directory as working directory

```
$ oct-run_regression_test.pl -d./tmp -f benzene.test -e `pwd`/../src/octopus-mpi
```

Previous Manual:External utilities:oct-run_periodic_table - Next Manual:External utilities:oct-run_testsuite.sh

Back to Manual <p class=newpage>

oct-run_testsuite.sh

NAME

oct-run_testsuite - Script to run the octopus testsuite.

SYNOPSIS

```
oct-run_testsuite [ option ] ...
```

DESCRIPTION

This script is one of the octopus utilities.

This script runs the octopus testsuite.

`-h`

Prints out a short help message.

`-n`

Run in dry mode (show what would be executed).

`-f`

Run full testsuite.

`-l`

Local run.

`-p prefix`

Installation prefix [default: /usr]

`-m address` Mail report to address

EXAMPLES

TO DO MISSING EXAMPLES

Previous Manual:External utilities:oct-run_regression_test.pl - Next Manual:External utilities:oct-vdW_c6

Back to Manual <p class=newpage>

oct-vdW_c6

Manual:External utilities:oct-vdW_c6 <p class=newpage>

oct-vibrational_spectrum

This utility calculates the vibrational spectrum from a molecular-dynamics run.

What this utility does is to read the velocity from the **`td.general/coordinates`** and calculate the Velocity Autocorrelation Function:

$$C_v(t) = \sum_{i=1}^{N_{atoms}} \vec{v}_i(t) \cdot \vec{v}_i(t_0) \ ,$$

afterward a cosinusoidal envelope is added, to make the periodic extension of the function continuous and then the spectrum is calculated by taking the Fourier transform of the function. On exit, two files are generated **`td.general/velocity_autocorrelation`** and **`td.general/vibrational`**.

This utility honours the variables `PropagationSpectrumStartTime` and `PropagationSpectrumEndTime` to control the time of sampling. Note that the velocity in the initial time must be different from zero, or C_v will be identically zero.

As a discrete Fourier tranform is used, this utility can take several minutes to process a large run. If Octopus was compiled with OpenMP support, this utility can run in several threads.

Previous Manual:External utilities:oct-vdW_c6 - Next Manual:External utilities:oct-xyz-anim

Back to Manual <p class=newpage>

oct-xyz-anim

NAME

oct-xyz-anim - Constructs an "animated" xyz file from a time-propagation file where the atoms were allowed to move

SYNOPSIS

```
oct-xyz-anim
```

[oct-xyz-anim does not read the standard input: all standard input will be simply ignored. An input file named **inp** must be present in the running directory. Also, oct-xyz-anim accepts no command line arguments, since there is not a standard way to do this with Fortran 90.]

DESCRIPTION

This program is one of the Octopus utilities. It reads out the **td.general/coordinates** file, and makes a movie in XYZ format, called 'movie.xyz'.

Previous Manual:External utilities:oct-vibrational_spectrum - Next Manual:Deprecated_Utilities

Back to Manual <p class=newpage>

Deprecated Utilities

Some utilities present in older version of octopus have superseded by other utilities or integrated into the main code, in this section you can find how to replace them.

octopus_cmplx

Not exactly a utility, now there is no complex version of the code, the main executable *octopus* can calculate real or complex wavefunctions depending of the requirements of input file.

oct-sf

This utility was replaced by *oct-propagation_spectrum*.

oct-cross-section

This utility was replaced by *oct-propagation_spectrum*.

oct-hs-mult and oct-hs-acc

These utilities were replaced by *oct-harmonic-spectrum*.

oct-excite

This utility was used to calculate the excitation spectrum within linear response. It no longer exists because the linear-response formalism calculations are now done by the main code, by making use of the "casida" run mode. See Manual:Calculation Modes:Casida

oct-make-st

This utility was used to replace some of the Kohn-Sham states in the restart directory by Gaussians wave packets. This sort of operation can now be done using the UserDefinedStates variable.

oct-rotatory_strength and oct-rsf

This utility has been removed. It is replaced by a new PropagationSpectrumType in **oct-propagation_spectrum**.

Previous Manual:External utilities:oct-xyz-anim - Next Manual:Examples:Hello world

Back to Manual <p class=newpage>

Examples

<p class=newpage>

Hello World

As a first example, we will take a sodium atom. With your favourite text editor, create the file **inp**.

```
CalculationMode = gs
%Coordinates
    'Na' | 0.0 | 0.0 | 0.0
%
```

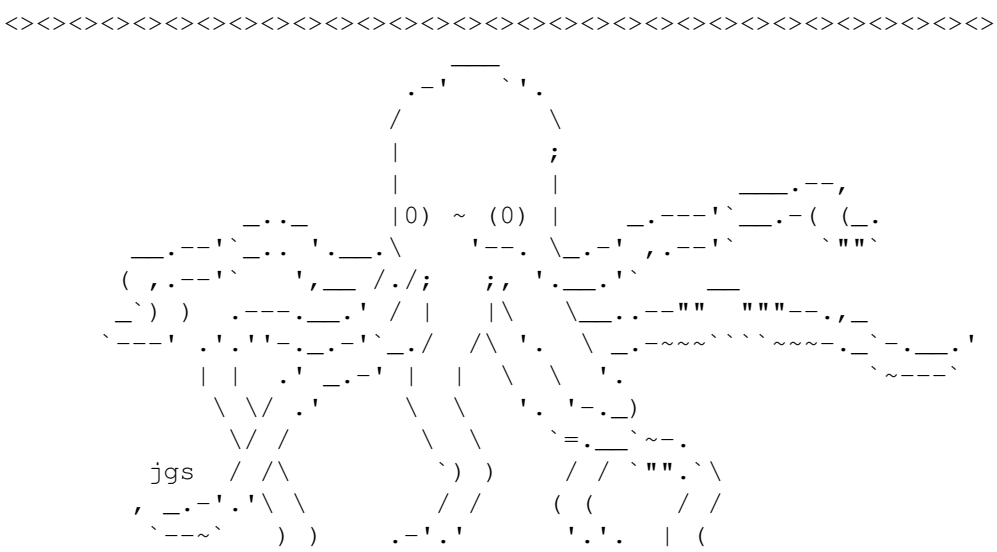
This input file should be essentially self-explanatory.

Note that when a species is not specified in the Species block, octopus reads the information of pseudopotentials from the **defaults** file (located under **PREFIX/share/octopus/PP/**. This file also contains default values for Radius and Spacing.

Then run octopus ? for example, do

```
$ octopus > out
```

so that the output is stored in **out** file. If everything goes OK, **out** should look like:



```
                 (/`     ( (`           ) )  '-;
                  `       '-;          (-'

    This program is free software; you can redistribute it and/or modify
    it under the terms of the GNU General Public License as published by
    the Free Software Foundation; either version 2, or (at your option)
    any later version.

    This program is distributed in the hope that it will be useful,
    but WITHOUT ANY WARRANTY; without even the implied warranty of
    MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
    GNU General Public License for more details.

    You should have received a copy of the GNU General Public License
    along with this program; if not, write to the Free Software
    Foundation, Inc., 51 Franklin Street, Fifth Floor, Boston, MA

    <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>

                           Running octopus

Version                : 5.0.1
Revision               : 15042
Build time             : Tue Jan 12 11:04:57 EST 2016
Configuration options  : max-dim=3 mpi sse2
Optional libraries     : arpack berkeleygw etsf_io gdlib metis mpi2 netcdf newuoa parmetis parpa
Architecture           : x86_64
C compiler             : /opt/local/bin/mpicc-mpich-mp (/usr/bin/clang)
C compiler flags       :  -pipe -O3 -arch x86_64
Fortran compiler       : /opt/local/bin/mpif90-mpich-mp (/opt/local/bin/gfortran-mp-5)
Fortran compiler flags : -pipe -O3

  The octopus is swimming in dhcp-18-189-27-45.dyn.MIT.EDU (Darwin)


            Calculation started on 2016/01/13 at 20:24:58


************************* Calculation Mode *************************
Input: [CalculationMode = gs]
********************************************************************

Reading Coordinates from Coordinates block

***************************** Species ******************************
Reading pseudopotential from file:
      '/opt/local/share/octopus/PP/PSF/Na.psf'
      Calculating atomic pseudo-eigenfunctions for species Na....
Info: l =  0 component used as local potential.
Info: l =  0 is maximum angular momentum considered.
Number of orbitals: total =     16, bound =      4
********************************************************************


**************************** Symmetries ****************************
Symmetry elements : (i) (Cinf) (sigma)
Symmetry group    : Kh
********************************************************************
```

```
Input: [SpinComponents = unpolarized]
Input: [SmearingFunction = semiconducting]
Input: [SymmetrizeDensity = no]

***************************** States *********************************
Total electronic charge  =        1.000
Number of states         =        1
States block-size        =        1
**********************************************************************

Info: Using default spacing(1) [b] =  0.567
Info: Using default spacing(2) [b] =  0.567
Info: Using default spacing(3) [b] =  0.567
Input: [CurvMethod = curv_uniform]
Input: [DerivativesStencil = stencil_star]

************************* Parallelization ****************************
Octopus will run in *serial*
**********************************************************************

Info: Generating weights for finite-difference discretization of x-gradient
Info: Generating weights for finite-difference discretization of y-gradient
Info: Generating weights for finite-difference discretization of z-gradient
Info: Generating weights for finite-difference discretization of Laplacian

******************************** Grid ********************************
Simulation Box:
  Type = minimum
  Species =    Na     Radius =  13.228 b
  Octopus will run in 3 dimension(s).
  Octopus will treat the system as periodic in 0 dimension(s).
Main mesh:
  Spacing [b] = ( 0.567, 0.567, 0.567)    volume/point [b^3] =      0.18221
  # inner mesh =      52971
  # total mesh =      79699
  Grid Cutoff [H] =    15.354165    Grid Cutoff [Ry] =    30.708329
**********************************************************************

Info: states-block size = 0.6 MiB
Input: [StatesOrthogonalization = gram_schmidt]

***************************** Hartree ********************************
The chosen Poisson solver is 'interpolating scaling functions'
**********************************************************************


************************** Theory Level ******************************
Input: [TheoryLevel = dft]

Exchange-correlation:
  Exchange
    Slater exchange (LDA)
    [1] PAM Dirac, Proceedings of the Cambridge Philosophical Society 26, 376 (1930)
    [2] F Bloch, Zeitschrift fuer Physik 57, 545 (1929)
  Correlation
    Perdew & Zunger (Modified) (LDA)
    [1] Perdew and Zunger, Phys. Rev. B 23, 5048 (1981)
    [2] Modified to improve the matching between the low- and high-rs parts
```

```
Input: [SICCorrection = sic_none]
************************************************************************

Input: [FilterPotentials = filter_none]
Info: Pseudopotential for Na
  Radii for localized parts:
    local part     =  3.5 b
    non-local part =  0.0 b
    orbitals       = 19.9 b

Input: [RelativisticCorrection = non_relativistic]
Input: [AbsorbingBoundaries = not_absorbing]

***************** Approximate memory requirements ******************
Mesh
  global  :       1.5 MiB
  local   :       1.8 MiB
  total   :       3.4 MiB

States
  real    :       0.6 MiB (par_kpoints + par_states + par_domains)
  complex :       1.2 MiB (par_kpoints + par_states + par_domains)

************************************************************************

Info: Generating external potential
      done.
Info: Octopus initialization completed.
Info: Starting calculation mode.
Info: Allocating ground state wave-functions
Info: Blocks of states
      Block       1 contains       1 states:       1 -       1
Info: Ground-state allocation done.

** Warning:
**   Could not find 'restart/gs' directory for restart.
**   No restart information will be read.


** Warning:
**   Unable to read wavefunctions.
**   Starting from scratch!

Input: [MixField = density] (what to mix during SCF cycles)
Input: [TypeOfMixing = broyden]

*************************** Eigensolver ****************************
Input: [Eigensolver = cg]
Input: [Preconditioner = pre_filter]
Input: [SubspaceDiagonalization = standard]
************************************************************************

Input: [LCAOStart = lcao_full]
Input: [LCAOScaleFactor = 1.000]
Input: [LCAOMaximumOrbitalRadius = 20.00 b]
Info: Single-precision storage for     1 extra orbitals will be allocated.
Info: Unnormalized total charge =      0.999665
Info: Renormalized total charge =      1.000000
Info: Setting up Hamiltonian.
```

```
Info: Performing initial LCAO calculation with      2 orbitals.
Info: Getting Hamiltonian matrix elements.
ETA: .......1......2.......3......4......5.......6......7.......8......9......0

Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation
   1   --    -0.103066       1.000000
Info: Ground-state restart information will be written to 'restart/gs'.
Info: SCF using real wavefunctions.
Info: Starting SCF iteration.
ETA: .......1......2.......3......4......5.......6......7.......8......9......0


********************** SCF CYCLE ITER #    1 ************************
 etot = -1.84238245E-01 abs_ev   =  3.88E-04 rel_ev   =  3.75E-03
                        abs_dens =  6.54E-03 rel_dens =  6.54E-03
Matrix vector products:     27
Converged eigenvectors:      0
Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation     Error
   1   --    -0.103455       1.000000      (5.5E-05)

Elapsed time for SCF step     1:          0.08
************************************************************************

ETA: .......1......2.......3......4......5.......6......7.......8......9......0


********************** SCF CYCLE ITER #    2 ************************
 etot = -1.84238838E-01 abs_ev   =  1.02E-04 rel_ev   =  9.88E-04
                        abs_dens =  4.55E-03 rel_dens =  4.55E-03
Matrix vector products:     27
Converged eigenvectors:      0
Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation     Error
   1   --    -0.103353       1.000000      (1.3E-06)

Elapsed time for SCF step     2:          0.10
************************************************************************

ETA: .......1......2.......3......4......5.......6......7.......8......9......0


********************** SCF CYCLE ITER #    3 ************************
 etot = -1.84239600E-01 abs_ev   =  2.23E-04 rel_ev   =  2.16E-03
                        abs_dens =  4.35E-04 rel_dens =  4.35E-04
Matrix vector products:     19
Converged eigenvectors:      1
Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation     Error
   1   --    -0.103130       1.000000      (9.3E-07)

Elapsed time for SCF step     3:          0.09
************************************************************************

ETA: .......1......2.......3......4......5.......6......7.......8......9......0


********************** SCF CYCLE ITER #    4 ************************
```

```
 etot = -1.84239592E-01 abs_ev   =  2.81E-07 rel_ev   =  2.73E-06
                        abs_dens =  6.62E-04 rel_dens =  6.62E-04
Matrix vector products:     12
Converged eigenvectors:      1
Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation     Error
   1   --    -0.103130       1.000000      (7.2E-07)

Elapsed time for SCF step     4:          0.07
************************************************************************

ETA: .......1......2.......3......4......5.......6......7.......8......9......0


********************** SCF CYCLE ITER #    5 ************************
 etot = -1.84239609E-01 abs_ev   =  6.42E-06 rel_ev   =  6.23E-05
                        abs_dens =  9.12E-06 rel_dens =  9.12E-06
Matrix vector products:     15
Converged eigenvectors:      1
Eigenvalues [H]
 #st  Spin   Eigenvalue      Occupation     Error
   1   --    -0.103123       1.000000      (8.7E-07)

Elapsed time for SCF step     5:          0.07
************************************************************************


             Info: Writing states. 2016/01/13 at 20:24:59


        Info: Finished writing states. 2016/01/13 at 20:24:59

Info: SCF converged in    5 iterations

Info: Finished writing information to 'restart/gs'.

             Calculation ended on 2016/01/13 at 20:24:59

                          Walltime:  01.  6s

Octopus emitted 2 warnings.
```

Take now a look at the working directory. Besides the initial file (**inp**) and the **out** file, three new directories appear. In **static/**, you will find the file **info**, with information about the static calculation (it should be hopefully self-explanatory, otherwise please complain to the authors...). In **restart/**, you will find the **gs** directory that contains restart information about the ground-state, which is used if, for example, you want to start a time-dependent calculation afterwards. Finally, the **exec** directory has information about the run of octopus; inside the **parser.log** contains all the input variables parsed by octopus.

Exercises

- Study how the total energy and eigenvalue of the sodium atom improve with the mesh spacing.
- Calculate the static polarizability of the sodium atom (CalculationMode = em_resp). A **em_resp/freq_0.0000/alpha** will be created containing the static polarizability tensor.

- Calculate a few unoccupied states (CalculationMode = unocc). The eigenspectrum will be in the file **static/eigenvalues**. Why don't we find a Rydberg series in the eigenspectrum?
- Repeat the previous calculation with different exchange and correlation functionals like PBE, LB94, and exact exchange (see XCFunctional).
- Perform a time-dependent evolution (CalculationMode = td), to calculate the optical spectrum of the Na atom. Use a TDDeltaStrength = 0.05, polarised in the *x*-direction. The multipole moments of the density are output to the file **td.general/multipoles**. You can process this file with the utility *oct-propagation_spectrum* to obtain the optical spectrum. If you have computer time to waste, re-run the time-dependent simulation for some other xc choices.

Previous Manual:Deprecated Utilities - Next Manual:Examples:Benzene

Back to Manual <p class=newpage>

Benzene

Well, the sodium atom is a bit too trivial. Let's try something harder: benzene. you will just need the geometry for benzene to be able to play. Here it is (in Å):

```
C  0.000  1.396  0.000
C  1.209  0.698  0.000
C  1.209 -0.698  0.000
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 you will probably have to use a tighter mesh. It also takes much more time...

Previous Manual:Examples:Hello world - Next Manual:Updating to a new version

Back to Manual <p class=newpage>

Appendix

<p class=newpage>

Appendix: Updating to a new version

This page lists the issues that may appear when updating to a new version of Octopus and how to solve them.

Octopus 6.0

Installation

- A compiler supporting Fortran 2003 iso_c_binding is now required.
- The executable is always called **octopus**, no longer **octopus_mpi** when compiled in parallel.
- This version supports libxc 3.0.0. Although it is still possible to use libxc 2.0.0 or any of the 2.x versions, updating to libxc 3.0.0 is highly recommended.

Variables

- There is a new format for the Species block and the names of the species options have been revised.
- The variable OutputHow has been renamed to OutputFormat.
- The variable ParallelizationStrategy and ParallelizationGroupRanks have been replaced with ParDomains, ParStates, ParKPoints, and ParOther.

Utilities

The **oct-rotatory_strength** utility has been removed. This utility is replaced by a new PropagationSpectrumType in **oct-propagation_spectrum**.

Octopus 5.0

Restart files

This version breaks the backwards compatibility of the restart files. Nevertheless, it is not too difficult to update the restart files generated with a previous version. Here is a summary of the changes and how to update the files:

- Casida restart data now goes to a directory **restart/casida**, and a file **kernel** or **kernel_triplet**. One then needs to create the directory and rename the files.
- The format of the **occs** file changed with the addition of an extra field for the imaginary part of the eigenvalues. To update the file one needs to add a column of zeros by hand after the column of eigenvalues.
- The line starting with *fft_alpha* was removed from the **mesh** file.

Note that the mesh partition restart is also not compatible any more. In this case the partition needs to be recalculated, which is usually not a problem.

Variables

Some variables changed name or changed format. If an obsolete variable is found, Octopus will stop and will tell you the variable that replaces it.

Octopus 4.1

Installation

This version requires libxc 2.0.0 or higher, so it might be necessary to update libxc before installing Octopus.

Restart files

Casida restart file is incompatible with that generated by version 4.0. The new format avoids problems with restarting with a different number of states.

Octopus 4.0

Installation

- Libxc is now an independent library. To compile Octopus 4.0.0 you will have to compile libxc 1.1.0 first. These are the short instructions to compile it (we assume that libxc will be installed in $DIR, this can be the same directory where Octopus is going to be installed):

```
tar -xvzf libxc-1.1.0.tar.gz
cd libxc-1.1.0
./configure --prefix=$DIR
make
make install
```

Now, when configuring Octopus pass the option --with-libxc-prefix=$DIR.

- The configure option for the location of netcdf and etsf_io are --with-netcdf-prefix and --with-etsf-io-prefix.

Variables

- TDEvolutionMethod is now called `TDPropagator`.

Utilities

- **`oct-cross_section`** was renamed to **`oct-propagation_spectrum`**.
- **`oct-broad`** was renamed to **`oct-casida_spectrum`**.
- The format for **`oct-help`** has changed. Now **`-s`** is used instead of **`search`**, **`-p`** instead of **`show`**, and **`-l`** instead of **`list`**.

Octopus 3.0

Input variables

Some variables changed name or changed format. If an obsolete variable is found, Octopus will stop and will tell you the variable that replaces it.

- `Units`, `UnitsInput` and `UnitsOutput` now take a named option as argument instead of a string. So

```
Units = "eVA"
```

should be replaced by

```
Units = eV_Angstrom
```

The code will stop if the old format is encountered.

- XFunctional and CFunctional were replaced by XCFunctional, for example

```
XFunctional = lda_x
CFunctional = lda_c_vwn
```

must be replaced with

```
XCFunctional = lda_x + lda_c_vwn
```

- TDLasers was replaced by TDExternalFields.
- Some options for CalculationMode were renamed.

Output directories

Some directories in Octopus output were renamed, restart files now are stored under **restart/** instead of **tmp/**. Files previously found under **status/** are now located in **exec/**.

Restart file format

Octopus writes restart files in a binary format, this format has been updated and improved. As a result Octopus is no longer able to restart automatically the calculation of a run performed with older versions.

Recovering old restart files

If you really need to recover your old restart files, first you have to generate NetCDF restart files with your old version of Octopus. Then you will have to rename the **tmp/** directory to **restart/** and remove the **restart_** prefix from its subdirectories, for example **tmp/restart_gs/** now should be called **restart/gs/**.

Now you can run Octopus 3.0 and it will find your restart information.

Previous Manual:Examples:Benzene - Next Manual:Building from scratch

Back to Manual <p class=newpage>

Appendix: Building from scratch

Compiling Octopus on some systems might be difficult, this is mainly because some libraries are required and they have to be all compiled with same Fortran compiler. This is a guide on how to compile Octopus and the required libraries starting from scratch (a Fortran compiler is required) in a standard Unix system.

NOTE: This page should be considered a last resort. On most systems you will be able to install many of these dependencies from a package manager or other pre-built binaries, which will save you a lot of effort.

Prerequisites

You will need the following:

- A standard Unix/Linux system, where you want to install Octopus.
- A basic knowledge on how to use the system (manage files, edit text files, extract tar archives, etc.).
- A directory where we will install the created binaries, this can be a specially created directory or even your `$HOME`. From now, we will assume that the directory is **<basedir>**, whenever it appears you should replace it with the actual directory you are using. *Note that the files that you will download and the directories with the sources, including the ones of Octopus, don't need to be placed in this directory.*
- A working C compiler, gcc is the ideal choice for x86/x86_64 systems. For other platforms you might want to choose a compiler that produces more optimized code. We will assume that the command to run the compiler is **<cc>**.
- A working Fortran 95 compiler, if you don't have one you can probably get gfortran or g95. We will assume that the command to run the Fortran compiler is **<fc>**.
- If you are compiling for a dual 32/64 bits architecture, it is a good idea to tell the compilers explicitly what type of binaries you want, many problems are caused by unadvertedly mixing 32 and 64 bits code. For Octopus normally you will want a 64 bits binary (`-m64` flag in most compilers). Since this flag should be passed always we recommend you to include it in the compiler command used in this guide (sometimes optimization flags are left out), so for example **<cc>** could be *`gcc -m64`*.

Compiler flags

Since probably you want Octopus to run fast, you will probably would to set optimization flags for both the C and Fortran compilers on your system (at least -O3). In general Octopus should run fine with aggressive optimization options. We will assume now that you have found a set of flags for **<cc>** and **<fc>**, we will call them **<cflags>** and **<fcflags>**. For example **<cflags>** could be *`-O3 -march=native`*.

*Note: if **<cc>**, **<fc>**, **<cflags>** or **<fcflags>** contain spaces you should not enclose them in "". We will put the "" explicitly when it is necessary.*

Compilation of libraries

First we will compile and install the libraries required by Octopus.

BLAS

The first library we will compile is blas. We will use the generic reference implementation, this version is not highly optimized but it is free software and simple to install. So after you have a working version of Octopus you may want to use a more optimized blas implementation as libgoto, ATLAS, MKL, ACML, ESSL, etc.

- Download the package from the netlib site: http://www.netlib.org/blas/blas.tgz
- Extract the package and enter into the newly created **BLAS** directory.
- Edit the **make.inc** file and modify the definition of the fortran compiler that now should be:

```
FORTRAN  = <fc>
OPTS     = <fcflags>
DRVOPTS  = $(OPTS)
NOOPT    =
LOADER   = <fc>
LOADOPTS =
```

- Now type *`make`* to compile, this will take a while.

- One compilation is finished, create the directory **<basedir>/lib**

```
mkdir <basedir>/lib
```

and copy the file **blas_LINUX.a** to **<basedir>/lib/libblas.a**

```
cp blas_LINUX.a <basedir>/lib/libblas.a
```

*Note: the generated file librrary will be always called **blas_LINUX.a** independently of the operating system you are using, this is just a name.*

LAPACK

We will use the open source reference implementation of Lapack.

- Get the Lapak package from netlib: http://www.netlib.org/lapack/lapack.tgz
- Extract the archive and enter the newly created lapack directory.
- Copy **make.inc.example** to **make.inc**:

```
cp make.inc.example make.inc
```

- Edit **make.inc** to indicate the compiler the will be used. The relevant part of the file should look like:

```
FORTRAN  = <fc>
OPTS     = <fcflags>
DRVOPTS  = $(OPTS)
NOOPT    =
LOADER   = <fc>
LOADOPTS =
```

- Now build the library with

```
make lib
```

- Copy the newly created library **lapack_LINUX.a** to **<basedir>/lib/liblapack.a** .

GSL

- Get the source of the latest version of GSL from ftp://ftp.gnu.org/gnu/gsl/ , currently it is GSL 1.16: ftp://ftp.gnu.org/gnu/gsl/gsl-1.16.tar.gz .
- Extract the archive and enter the newly created directory.
- Run the configure script with:

```
./configure CC="<cc>" --prefix=<basedir> --disable-shared --enable-static
```

- Compile and install:

```
make
make install
```

FFTW 3

- Get the sources for the latest version of FFTW, currently http://www.fftw.org/fftw-3.3.4.tar.gz .
- Extract the archive and enter the newly created directory.
- Configure:

```
./configure  --prefix=<basedir> CC="<cc>" CFLAGS="<cflags>" F77="<fc>" F77FLAGS="<fcflags>"
```

- Compile and install:

```
make
make install
```

LibXC

- Get Libxc, currently http://www.tddft.org/programs/octopus/down.php?file=libxc/libxc-2.2.0.tar.gz .
- Extract the archive and enter the newly created directory.

```
tar -xvzf libxc-2.2.0.tar.gz
cd libxc-2.2.0
```

- Configure:

```
./configure --prefix=<basedir> CC="<cc>" CFLAGS="<cflags>" FC="<fc>" FCFLAGS="<fcflags>"
```

- Compile and install:

```
make
make install
```

Compilation of Octopus

After compiling the libraries, now we are ready to compile Octopus. These are the steps you have to follow:

- Download the last version of Octopus:
  http://www.tddft.org/programs/octopus/down.php?file=6.0/octopus-6.0.tar.gz
- Extract the file and enter the newly created directory.
- Define the following environment variables to be used by the configure script (we assume that you are using bash, if you are using another shell, the commands should be modified accordingly):

```
export LIBS_BLAS=<basedir>/lib/libblas.a
export LIBS_LAPACK=<basedir>/lib/liblapack.a
export LIBS_FFT=<basedir>/lib/libfftw3.a
```

- Now call the configure script:

```
./configure CC="<cc>" CFLAGS="<cflags>" FC="<fc>" FCFLAGS="<fcflags>" --prefix=<basedir> --with-
```

- Compile and install

```
make
```

```
make install
```

- If everything went fine, you should have Octopus installed in the **<basedir>** directory, this means that the executables are in **<basedir>/bin/**. You may want to add this last directory to your path to run octopus commands directly, otherwise you will have to give the full path.
- To test the compilation is correct, you can run the testsuite of Octopus, that compares the results obtained with the created version against reference values. To do it, run

```
make check
```

All tests should be passed if the compilation is correct. If all of them fail, there is probably a problem with your executable, typically missing dynamic libraries. If just some fail, there might be a more serious problem, we recommend you to look for help in the Mailing lists.

Previous Manual:Updating to a new version - Next Tutorial:Running Octopus on Graphical Processing Units (GPUs)

Back to Manual <p class=newpage>

Appendix: Octopus with GPU support

Recent versions of Octopus support execution on graphical processing units (GPUs). In this tutorial we explain how the GPU support works and how it can be used to speed-up calculations.

Consideration before using a GPU

Calculations that will be accelerated by GPUs

A GPU is a massively parallel processor, to work efficiently it need large amounts of data to process. This means that using GPUs to simulate small systems, like molecules of less than 20 atoms or low dimensionality systems, will probably will be slower than using the CPU.

Not all the calculations you can do with Octopus will be effectively accelerated by GPUs. Essentially ground state calculations with the rmmdiis eigensolver (and calculations based on ground state calculations, like geometry optimization) and time propagation with the etrs and aetrs propagators are the simulations that will use the GPU more effectively. For other types of calculations you might see some improvements in perfomance. Moreover, some Octopus features do not support GPUs at all. Currently these are:

- Periodic systems.
- HGH or relativistic pseudopotentials.
- Non-collinear spin.
- Curvilinear coordinates.

In these cases Octopus will be silently executed on the CPU.

Supported GPUs

Octopus GPU support is based on the OpenCL framework, so it is vendor independent, currently it has been tested on GPUs from Nvidia and AMD (ex-ATI).

In order to run Octopus, the GPU must have double precision support. For AMD/ATI cards this is only available in high-end models: Radeon 58xx, 69xx, 78xx, 79xx, and Firepro/Firestream cards. All recent Nvidia cards support double precision (4xx and newer), low- and middle-end cards however have very limited processing power and are probably slower running Octopus than a CPU.

The other important factor is GPU memory, you need a GPU with at least 1.5 GiB of RAM to run Octopus, but 3 GiB or more are recommended.

You can run the OpenCL version of Octopus on CPUs, however this is much slower than running Octopus directly.

Activating GPU support

Octopus has GPU support since version 4.0; to activate it you need a version compiled with OpenCL support enabled (see the manual for details). If your version of Octopus was compiled with OpenCL support you should see that 'opencl' among the configuration options:

```
                        Running octopus

Version                : superciliosus
Revision               :
Build time             : Thu Feb 14 22:19:10 EST 2013
Configuration options  : max-dim=3 openmp opencl sse2 avx
Optional libraries     : netcdf clamdfft clamdblas
```

Ideally your Octopus version should also be compiled with the optional libraries 'clamdfft' and 'clamdblas', that are part of the AMD APPML package (these libraries work on hardware from other vendors too, including Nvidia).

Starting the tutorial: running without OpenCL

If you have a version of Octopus compiled with OpenCL support, by setting the `DisableOpenCL` to `yes` you can tell Octopus not to use OpenCL.

Selecting the OpenCL device

OpenCL is designed to work with multiple devices from different vendors. Most likely you will have a single OpenCL device, but in some cases you need to select the OpenCL device that Octopus should use.

In OpenCL a 'platform' identifies an OpenCL implementation, you can have multiple platforms installed in a system. Octopus will list the available platforms at the beginning of the execution, for example:

```
Info: Available CL platforms: 2
    * Platform 0 : NVIDIA CUDA (OpenCL 1.1 CUDA 4.2.1)
      Platform 1 : AMD Accelerated Parallel Processing (OpenCL 1.2 AMD-APP (1084.4))
```

By default Octopus will use the first platform. You can select a different platform with the OpenCLPlatform variable. You can select the variable by name, for example:

```
OpenCLPlatform = amd
```

or you can use numeric values that select the platform by its index in the list:

```
OpenCLPlatform = 1
```

The first form should be preferred as it is independent of the order of the platforms.

Each OpenCL platform can contain several devices, the available devices on the selected platform are printed by Octopus, like this:

```
Info: Available CL devices: 2
      Device 0 : Tahiti
      Device 1 : Intel(R) Core(TM) i7-3820 CPU @ 3.60GHz
```

Each OpenCL device has a certain type that can be 'cpu', 'gpu', or 'accelerator'. By default Octopus tries to use the first device of type 'gpu', if this fails Octopus tries to use the default device for the system, as defined by OpenCL implementation. To select a different device you can use the OpenCLDevice variable, you can select the device by its index or by its type ('cpu', 'gpu', or 'accelerator').

Note: the Octopus OpenCL implementation is currently designed to execute efficiently on GPUs. Octopus will run on CPUs using OpenCL, but it will be slower than using the CPU directly.

After Octopus has selected an OpenCL device it will print some information about it, for example:

```
Selected CL device:
     Device vendor          : Advanced Micro Devices, Inc.
     Device name            : Tahiti
     Driver version         : 1084.4 (VM)
     Compute units          : 32
     Clock frequency        : 925 GHz
     Device memory          : 2048 MiB
     Max alloc size         : 512 MiB
     Device cache           : 16 KiB
     Local memory           : 32 KiB
     Constant memory        : 64 KiB
     Max. workgroup size    : 256
     Extension cl_khr_fp64  : yes
     Extension cl_amd_fp64  : yes
```

The block-size

To obtain good peformance on the GPU (and CPUs), Octopus uses blocks of states as the basic data object. The size of these blocks is controlled by the StatesBlockSize variable. For GPUs the value must be a power of 2 (the default is 32) and for optimal performance must be as large as possible, the catch is that for large values you might run out of GPU memory.

StatesPack

The Poisson solver

If you want to used a GPU-accelerated Poisson solver, you need to use the 'fft' solver and to have the 'clamdfft' library support compiled. To select the solver, just add

```
PoissonSolver = fft
FFTLibrary = clfft
```

to your input file.

Previous Tutorial:Open boundaries - Next Tutorial:Sternheimer linear response

Back to Tutorial <p class=newpage>

Appendix: Specific architectures

Here the general instructions for building Octopus are supplemented by instructions for some specific large supercomputers. Included also is how to configure the optional ETSF_IO library, and how you can run the testsuite in parallel.

Generic Ubuntu 10.10

Install the following packages:

```
* Required: gfortran, gcc, make, automake, m4, libtool, libgsl0-dev, libblas-dev, liblapack-dev,
* Optional: mpi-default-dev, libgd2-xpm-dev, libsparskit-dev, libnetcdf-dev, libtrilinos-dev
```

[Unfortunately you should not use `libblacs-mpi-dev, libscalapack-mpi-dev` packages because they can give incorrect results. To use BLACS and ScaLAPACK (optional) you must build them yourself.]

First download libxc from Libxc:download, extract with `tar xzf`, enter the resulting directory, and execute:

```
./configure --prefix=`pwd`/.. CC=gcc FC=gfortran FCCPP="/lib/cpp -ansi" FCFLAGS=-O3 CFLAGS=-O3
make install
```

For octopus, download and extract, and execute the following (inserting the path where you put libxc):

```
./configure --prefix=`pwd` CC=gcc FC=gfortran FCCPP="/lib/cpp -ansi" FCFLAGS=-O3 CFLAGS=-O3 --wi
make install
```

If you are using MPI, replace the compilers by `CC=/usr/bin/mpicc FC=/usr/bin/mpif90` and add `--enable-mpi`.

To build ETSF_IO, `libnetcdf-dev` is required.

```
./configure --prefix=`pwd` CC=gcc FC=gfortran FCFLAGS="-O3" CFLAGS="-O3" --with-netcdf-ldflags="
make install
```

Add `--with-etsf-io-prefix="$DIR/etsf_io-1.0.4"` to the Octopus configure line, where `$DIR/etsf_io-1.0.4` is where you installed ETSF_IO.

(2 May 2011)

Generic MacOS

Octopus is now available in MacPorts. For more info, and how to build by hand with MacPorts libraries, see Compiling_octopus_in_OS_X.

United States

Sequoia/Vulcan (IBM Blue Gene/Q)

Supercomputers at Lawrence Livermore National Laboratory based on the IBM Blue Gene/Q architecture. This was tested in Vulcan, but it should work on Sequoia as well.

https://computing.llnl.gov/tutorials/bgq/

```
export LIBS_BLAS="-L/usr/local/tools/essl/5.1/lib/ -lesslsmpbg"
export LIBS_LAPACK="/usr/local/tools/lapack/lib/liblapack.a"
export LIBS_FFT="-L/usr/local/tools/fftw-3.3.3/lib/ -lfftw3_omp"
export FC_INTEGER_SIZE=4
export CC_FORTRAN_INT=int
export CC=mpixlc_r
export FC=mpixlf95_r
export LDFLAGS="-qsmp=omp"
export CFLAGS="-g -O3"
export FCFLAGS=$CFLAGS" -qxlf90=autodealloc -qessl"
./configure --with-libxc-prefix=$HOME --prefix=$HOME --host=powerpc32-unknown-linux-gnu  --build
```

(This build does not use Scalapack)

Stampede

10 PFLOPS (PF) Dell Linux Cluster based on 6,400+ Dell PowerEdge server nodes, each outfitted with 2 Intel Xeon E5 (Sandy Bridge) processors and an Intel Xeon Phi Coprocessor (MIC Architecture). Texas Advanced Computing Center, University of Texas, Austin, USA.

https://portal.tacc.utexas.edu/user-guides/stampede

```
module swap mvapich2 impi
module load fftw3 gsl hdf5 netcdf
MKL_DIR=$MKLROOT
./configure --prefix=`pwd` CC=mpicc FC=mpif90 CFLAGS="-O3" FCFLAGS="-O3" --enable-mpi \
--with-blas="-L$MKL_DIR/lib/intel64 -Wl,--start-group -lmkl_intel_lp64 -lmkl_sequential -lmkl_co
--with-netcdf-prefix="$TACC_NETCDF_DIR" --enable-newuoa --with-libxc-prefix=`pwd`/../libxc-2.2.2
```

```
--with-scalapack="$MKL_DIR/lib/intel64/libmkl_scalapack_lp64.a"
make -j 6 install
```

For libxc:

```
./configure --prefix=`pwd` CC=mpicc FC=mpif90 FCFLAGS="-O3" CFLAGS="-O3"
make -j 6 install
make check
```

testsuite script:

```
#!/usr/bin/env bash

#SBATCH -n 16
#SBATCH -p development
#SBATCH -t 01:00:00
#SBATCH --export=ALL

module load perl
WORKDIR=$PWD
export TEMPDIRPATH=$SCRATCH/tmp
cd $HOME/octopus
export OCT_TEST_NJOBS=8
export MPIEXEC=`which ibrun`
make check &> $WORKDIR/makecheck
```

(13 September 2016)

Edison

Cray XC30 at National Energy Research Scientific Computing Center (NERSC), Lawrence Berkeley National Laboratory, USA

http://www.nersc.gov/nusers/systems/

```
module load fftw gsl cray-netcdf parpack

./configure --prefix=`pwd` --with-libxc-prefix=/usr/common/usg/libxc/2.2.2/intel --enable-mpi --
CC=cc FC=ftn FCFLAGS="-fast -no-ipo" CFLAGS="-fast -no-ipo"  \
FCCPP="/lib/cpp -ffreestanding" --with-fftw-prefix=$FFTW_DIR/..
--with-arpack="$ARPACK" --with-parpack=no \
--with-metis-prefix=/usr/common/usg/metis/5.1.0/intel --with-parmetis-prefix=/usr/common/usg/par
make -j 6 install
```

To run the testsuite in parallel:

```
#!/bin/bash -l
#SBATCH -J pulpo
#SBATCH -n 48
#SBATCH -p regular
#SBATCH -t 02:00:00
#SBATCH --export=ALL

cd $HOME/edison/octopus
```

```
export OMP_NUM_THREADS=2
export MPIEXEC="`which srun` -c $OMP_NUM_THREADS"
export TEMPDIRPATH=$SCRATCH/tmp
export OCT_TEST_NJOBS=12
make check &> $SLURM_SUBMIT_DIR/makecheck
```

To build *ETSF_IO* 1.0.4 (optional): (some tests fail)

```
module load netcdf
./configure --prefix=`pwd` FC=ftn FCFLAGS="-fast -no-ipo" CC=cc CFLAGS="-fast -no-ipo" \
--with-netcdf-module-path="$NETCDF_DIR/include" --with-netcdf-prefix="$NETCDF_DIR"
make -j 6 install
make check
```

(version 6.0, 7 September 2016)

Cori

Cray XC40 at National Energy Research Scientific Computing Center (NERSC), Lawrence Berkeley National Laboratory, USA

http://www.nersc.gov/users/computational-systems/cori/

```
module load fftw gsl cray-netcdf parpack
```

For libxc (you can use the installed version instead)

```
./configure --prefix=`pwd` CC=cc FC=ftn FCFLAGS="-fast -no-ipo" CFLAGS="-fast -no-ipo"
make -j 6 install
make check
```

For octopus (note: parpack here causes scalapack problems):

```
./configure --prefix=`pwd` --with-libxc-prefix=/usr/common/software/libxc/2.1.2-intel --enable-m
CC=cc FC=ftn FCFLAGS="-fast -no-ipo" CFLAGS="-fast -no-ipo" \
--with-arpack="$ARPACK" --with-parpack=no --with-berkeleygw-prefix=/usr/common/software/berkeley
FCCPP="/lib/cpp -ffreestanding" --with-fftw-prefix=$FFTW_DIR/..
make -j 6 install
```

To run the testsuite in parallel:

```
#!/bin/bash -l
#SBATCH -J pulpo
#SBATCH -n 64
#SBATCH -p regular
#SBATCH -t 04:00:00
#SBATCH --export=ALL

cd $HOME/cori/octopus
export OMP_NUM_THREADS=2
export MPIEXEC="`which srun` -c $OMP_NUM_THREADS"
export TEMPDIRPATH=$SCRATCH/tmp
export OCT_TEST_NJOBS=20
make check &> $SLURM_SUBMIT_DIR/makecheck
```

To build *ETSF_IO* 1.0.4 (optional): (some tests fail)

```
module load netcdf
./configure --prefix=`pwd` FC=ftn FCFLAGS="-fast -no-ipo" CC=cc CFLAGS="-fast -no-ipo"
make -j 6 install
make check
```

(6 September 2016)

Lonestar

Dell Linux cluster at Texas Advanced Computing Center (TACC), University of Texas, Austin, USA

Part of National Science Foundation's TeraGrid

http://services.tacc.utexas.edu/index.php/lonestar-user-guide

```
module load gsl
module load mkl
module load netcdf
module load fftw3
cd libxc
./configure --prefix=`pwd`/.. --enable-mpi CC=mpicc FC=mpif90 F77=mpif90 FCFLAGS=-O3 CFLAGS=-O3
make install
cd ..
export SLKPATH=/opt/apps/intel11_1/mvapich2_1_6/scalapack/1.8.0/lib
./configure --prefix=`pwd` --enable-mpi CC=mpicc FC=mpif90 \
--with-blas="-Wl,--start-group $TACC_MKL_LIB/libmkl_intel_lp64.a $TACC_MKL_LIB/libmkl_sequential
--with-fft-lib="-L$TACC_FFTW3_LIB -lfftw3" --with-netcdf-prefix="$TACC_NETCDF_DIR" --disable-gdl
--with-etsf-io-prefix="$HOME/etsf_io-1.0.3" --enable-newuoa --with-libxc-prefix=`pwd` \
--with-blacs="$SLKPATH/libscalapack.a $SLKPATH/blacs_MPI-LINUX-0.a $SLKPATH/blacsF77init_MPI-LIN
make install
```

To build *ETSF_IO*:

```
module load netcdf
./configure --prefix=`pwd` FC=mpif90 --with-netcdf-module-path=$TACC_NETCDF_INC --with-netcdf-ld
make install
make check
```

To run the testsuite in parallel:

```
#!/bin/bash

#$ -N test_pulpo
#$ -cwd
#$ -pe 6way 12
#$ -q development
#$ -l h_rt=00:45:00
#$ -V

cd $HOME/octopus
export TEMPDIRPATH=$SCRATCH/tmp
if [ ! -d $TEMPDIRPATH ]; then
```

```
    mkdir $TEMPDIRPATH
fi

export MPIEXEC=`which ibrun`
export OCT_TEST_NPROCS=1
make check &> makecheck
```

(2 May 2011)

Lawrencium

Dell Linux cluster at Lawrence Berkeley National Laboratory, USA

Cluster available only to Lawrence Berkeley National Laboratory researchers

http://lrc.lbl.gov/html/Lawrencium.html

```
module load icc/10.1.018
module load ifort/10.1.018
module load mkl/2011.1.107
module load openmpi/1.4.3-intel
module load netcdf/4.0-intel
module load fftw/3.1.2-intel
module load autoconf/2.65
module load gsl/1.13-intel
module load gdlib/2.0.35
module load libtool/2.2.6b

./configure --prefix=`pwd` CC=mpicc FC=mpif90 CFLAGS="-O3" FCFLAGS="-O3 -check bounds" --enable-
--with-blas="-L$MKLROOT/lib/intel64 -Wl,--start-group -lmkl_intel_lp64 -lmkl_sequential -lmkl_co
--with-fft-lib="-L/global/software/centos-5.x86_64/modules/fftw/3.1.2-intel/lib -lfftw3" --with-
--with-libxc-prefix=`pwd` --with-blacs="$MKL_DIR/lib/intel64/libmkl_blacs_openmpi_lp64.a" --with
```

To build *ETSF_IO*:

```
module load netcdf/4.2-intel-p
./configure --prefix=`pwd` CC=mpicc FC=mpif90 CFLAGS="-O3" FCFLAGS="-O3" --with-netcdf-module-pa
```

(21 Aug 2012)

Europe

Curie

PFFT 1.0.5 and BigDFT 1.6.0

The Curie supercomputer, owned by GENCI and operated into the TGCC by CEA, is the first French Tier0 system open to scientists through the French participation into the PRACE research infrastructure.

Curie is offering 3 different fractions of x86-64 computing resources for addressing a wide range of scientific challenges and offering an aggregate peak performance of 2 PetaFlops.

General information: http://www-hpc.cea.fr/en/complexe/tgcc-curie.htm

Compilation with PFFT version 1.0.5 and LibISF taken from BigDFT 1.6.0 (previously compiled):

```
#!/bin/bash

module load c/intel
module load fortran/intel
module load bullxmpi
module load mkl
module load gsl/1.14

WPREFIX=$WORKDIR/software
PREFIX=$HOME/software
export ISF_HOME="$WORKDIR/software/libisf"

export CC=mpicc
export CFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$ISF_HOME/include"
export FC=mpif90
export FCFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$PREFIX/fftw/3.3/include -I$I

export LIBS_BLAS="${MKL_LIBS}"
export LIBS_FFT="-Wl,--start-group -L$PREFIX/pfft/1.0.5/lib -L$PREFIX/fftw/3.3/lib -lpfft -lfftw
export LDFLAGS=$LDFLAGS" -L$ISF_HOME/lib -lisfsolver -lrt"

../configure --prefix=$WPREFIX/octopus/superciliosus_pfft \
  --disable-openmp --with-libxc-prefix=$WPREFIX/libxc/2.0.x \
  --disable-gdlib --with-gsl-prefix=/usr/local/gsl-1.14 \
  --enable-mpi --enable-newuoa \
  --with-pfft-prefix=$PREFIX/pfft/1.0.5
```

BigDFT was configured like this:

```
#!/bin/bash

export FC=mpif90

../configure --with-ext-linalg="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lm" \
  --with-ext-linalg-path="-L/usr/local/Intel_compilers/c/composer_xe_2011_sp1.7.256/mkl/lib/inte
  --prefix=$WORKDIR/software/bigdft
```

PFFT 1.0.7 and BigDFT 1.7.0

```
#!/bin/bash

module load c/intel
module load fortran/intel
module load bullxmpi
module load mkl
module load gsl/1.14

WPREFIX=$WORKDIR/poisson/software
WLPREFIX=$WORKDIR/poisson/local
export ISF_HOME="$WLPREFIX/libisf"
```

```
export FFTW_HOME="$WLPREFIX/fftw-3.3.3"
export PFFT_HOME="$WLPREFIX/pfft-1.0.7-alpha"

export CC=mpicc
export CFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$ISF_HOME/include"
export FC=mpif90
export FCFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$FFTW_HOME/include -I$ISF_HOM

export LIBS_BLAS="${MKL_LIBS}"
export LIBS_FFT="-Wl,--start-group -L$PFFT_HOME/lib -L$FFTW_HOME/lib -lpfft -lfftw3 -lfftw3_mpi

export LDFLAGS=" -L/usr/lib64 -L$ISF_HOME/lib -lPSolver-1 -lrt"
export LD_LIBRARY_PATH=$ISF_HOME/lib:$LD_LIBRARY_PATH

../configure --prefix=$WPREFIX/octopus/superciliosus_pfft \
  --disable-openmp --with-libxc-prefix=$WPREFIX/libxc/11066 \
  --disable-gdlib --with-gsl-prefix=/usr/local/gsl-1.14 \
  --enable-mpi --enable-newuoa \
  --with-pfft-prefix=$PFFT_HOME
```

LibISF compilation:

```
#!/bin/bash

module load c/intel
module load fortran/intel
module load bullxmpi
module load mkl
module load gsl/1.14

export FC=mpif90

../configure --with-ext-linalg="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lm" \
   --with-ext-linalg-path="-L/usr/local/Intel_compilers/c/composer_xe_2011_sp1.7.256/mkl/lib/int
   --prefix=$WORKDIR/poisson/local/libisf \
   --disable-libbigdft --disable-binaries --enable-dynamic-libraries
```

FFTW 3.3.3 compilation script is in http://www-user.tu-chemnitz.de/~mpip/software/install_fftw-3.3.3_gcc.sh and it is changed as follow:

```
< myprefix=$HOME/local
---
> module load c/intel
> module load fortran/intel
> module load bullxmpi
> module load mkl
> module load gsl/1.14
>
> myprefix=$WORKDIR/poisson/local
23c29,30
< wget http://www.fftw.org/fftw-$FFTW_VERSION.tar.gz
---
> # wget http://www.fftw.org/fftw-$FFTW_VERSION.tar.gz
> cp ../fftw-$FFTW_VERSION.tar.gz .
876c883
< ./configure --prefix=$INSTALLDIR --enable-mpi --enable-openmp --enable-shared \
---
```

```
> ./configure --prefix=$INSTALLDIR --enable-mpi --enable-openmp --enable-shared --disable-shared
```

PFFTW 1.0.7 compilation script is in
http://www-user.tu-chemnitz.de/~mpip/software/install_pfft-1.0.7-alpha_gcc.sh and it is changed as follow:

```
< myprefix=$HOME/local
---
>
> module load c/intel
> module load fortran/intel
> module load bullxmpi
> module load mkl
> module load gsl/1.14
>
> myprefix=$WORKDIR/poisson/local
24c31,32
< wget http://www.tu-chemnitz.de/~mpip/software/pfft-$PFFT_VERSION.tar.gz
---
> #wget http://www.tu-chemnitz.de/~mpip/software/pfft-$PFFT_VERSION.tar.gz
> cp ../pfft-$PFFT_VERSION.tar.gz .
```

Fermi/Juqueen

IBM Blue Gene/Q, Cineca, Italy

General information: http://www.hpc.cineca.it/content/ibm-fermi-user-guide

The exactly the same script has been tested in the Juqueen, Forschungszentrum Jülich, Jülich Supercomputing Centre (JSC), Jülich, Germany. General information:
http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html

```
#/bin/bash

module load gsl
module load lapack
module load blacs
module load scalapack

export PFFT_HOME="$HOME/local/pfft-threads-1.0.5-alpha"
export FFTW3_HOME="$HOME/local/fftw-threads-3.3.2"
export LD_LIBRARY_PATH=$PFFT_HOME/lib:$FFTW3_HOME/lib:$LD_LIBRARY_PATH

export FC_INTEGER_SIZE=8
export CC_FORTRAN_INT=int
export CC=mpicc
export CFLAGS="-g -Wl,-relax -O3 -I$PFFT_HOME/include -I$FFTW3_HOME/include"
export FC=mpif90
export FCFLAGS=$CFLAGS" -qxlf90=autodealloc -qessl -qsmp=omp "
export LIBS_BLAS="-lesslsmpbg -L/opt/ibmmath/essl/4.4/lib -lesslbg"
export LIBS_LAPACK="-L$LAPACK_LIB -llapack"

export LIBS_FFT="-L$FFTW3_HOME/lib/ -lfftw3_mpi -lfftw3 -lm"
echo "GSL DIR = $GSL_HOME "
echo "PFFT DIR = $PFFT_HOME "
```

```
export LDFLAGS=$LDFLAGS" -R/opt/ibmcmp/lib/bg/bglib \
   -L/bgsys/drivers/V1R4M2_200_2010-100508P/ppc/gnu-linux/powerpc-bgp-linux/lib \
   -L/bgsys/drivers/V1R4M2_200_2010-100508P/ppc/gnu-linux/lib/gcc/powerpc-bgp-linux/4.1.2 \
   -L/opt/ibmcmp/xlf/bg/11.1/bglib \
   -L/opt/ibmcmp/xlmass/bg/4.4/bglib \
   -L/opt/ibmcmp/xlsmp/bg/1.7/bglib \
   -L/bgsys/drivers/V1R4M2_200_2010-100508P/ppc/runtime/SPI \
   -L/bgsys/drivers/V1R4M2_200_2010-100508P/ppc/comm/sys/lib \
   -L/bgsys/drivers/V1R4M2_200_2010-100508P/ppc/comm/default/lib \
   -L/usr/local/zlib/v1.2.3/lib \
   -L/bgsys/drivers/ppcfloor/runtime/SPI \
   -L$PFFT_HOME/lib -L$FFTW3_HOME/lib \
   -lpfft -lfftw3_mpi -lfftw3 -lm \
   -ldl -lxl -lxlopt -lrt -lpthread"

SVN_VERS=$(svn info .. | grep Revision | awk '{print $2}')
echo $SVN_VERS

../configure --prefix=$HOME/software/octopus_omp \
   --with-libxc-prefix=$HOME/software/libxc_new \
   --with-fft-lib="$FFTW3_HOME/lib/libfftw3.a  $FFTW3_HOME/lib/libfftw3_omp.a" \
   --host=powerpc32-unknown-linux-gnu \
   --build=powerpc64-unknown-linux-gnu \
   --disable-gdlib \
   --disable-f90-forall \
   --with-blas="-L/opt/ibmmath/lib64 -lesslbg" \
   --with-lapack="-L$LAPACK_LIB -llapack" \
   --with-gsl-prefix=$GSL_HOME \
   --enable-mpi --enable-openmp
```

To build FFTW3. Small changes are made to the script taken from M. Pippig web site http://www-user.tu-chemnitz.de/~mpip/software.php?lang=en It has a patch and is build with MPI and multithreaded (multithreaded may not work in Juqueen):

```
#!/bin/sh -e

myprefix=$HOME/local
FFTW_VERSION="3.3.2"
INSTALLDIR="$myprefix/fftw-threads-${FFTW_VERSION}"
TMP="tmp-mine-fftw-${FFTW_VERSION}"

# bash check if directory exists
if [ -d $TMP ]; then
        echo "Directory $TMP already exists. Delete it? (y/n)"
        read answer
        if [ ${answer} = "y" ]; then
                rm -rf $TMP
        else
                echo "Program aborted."
                exit 1
        fi
 fi

mkdir $TMP && cd $TMP

wget http://www.fftw.org/fftw-$FFTW_VERSION.tar.gz
gzip -dc fftw-$FFTW_VERSION.tar.gz | tar xvf -
cd fftw-$FFTW_VERSION
```

```
# fix bug in fftw alltoall routine that causes deadlocks
patch -b -p0 <<\EOF
--- mpi/transpose-alltoall.c
+++ mpi/transpose-alltoall.c
@@ -223,8 +223,8 @@
          sbo[pe] = (int) (pe * (b * p->tblock) * vn);
          rbs[pe] = (int) (db * bt * vn);
          rbo[pe] = (int) (pe * (p->block * bt) * vn);
-         if (sbs[pe] != (b * p->tblock) * vn
-             || rbs[pe] != (p->block * bt) * vn)
+         if (dbt != p->tblock
+             || db != p->block)
               equal_blocks = 0;
     }
     pln->send_block_sizes = sbs;
EOF

./configure --build=powerpc64-bgq-linux-gnu --host=powerpc64-bgq-linux \
--prefix=$INSTALLDIR --enable-mpi --enable-openmp --enable-threads --disable-shared \
CC=mpixlc_r F77=mpixlf90_r MPICC=mpixlc_r MPICXX=mpixlcxx_r MPIFC=mpixlf90_r MPILIBS=" " \
CFLAGS='-O3 -g' \
FCFLAGS='-O3 -g' \

make -j 4
make install
```

To build PFFT, also taken from http://www-user.tu-chemnitz.de/~mpip/software.php?lang=en

```
#!/bin/sh -e

myprefix=$HOME/local
PFFT_VERSION=1.0.5-alpha
FFTW_VERSION=3.3.2
INSTDIR=$myprefix/pfft-threads-$PFFT_VERSION
FFTWDIR=$myprefix/fftw-threads-$FFTW_VERSION
TMP="tmp-mine-pfft-$PFFT_VERSION"

# bash check if directory exists
if [ -d $TMP ]; then
        echo "Directory $TMP already exists. Delete it? (y/n)"
        read answer
        if [ ${answer} = "y" ]; then
                rm -rf $TMP
        else
                echo "Program aborted."
                exit 1
        fi
fi

mkdir $TMP && cd $TMP

wget http://www.tu-chemnitz.de/~mpip/software/pfft-$PFFT_VERSION.tar.gz
gzip -dc pfft-$PFFT_VERSION.tar.gz | tar xvf -
cd pfft-$PFFT_VERSION
./configure --build=powerpc64-bgq-linux-gnu --host=powerpc64-bgq-linux \
--prefix=$INSTDIR --with-fftw3=$FFTWDIR \
MPICC=mpif90 MPICXX=mpicxx MPIFC=mpif90 CC=mpicc FC=mpif90 \
```

```
CFLAGS='-O3 -g -qmaxmem=-1' \
FCFLAGS='-O3 -g -qmaxmem=-1' \
--disable-shared

make -j 4
make install
```

Hydra

Hydra is a supercomputer located at the RZG/MPG. More information:
http://www.rzg.mpg.de/services/computing/hydra/about-the-system

Instruction that work with version 13307

```
#!/bin/bash

. /etc/profile.d/modules.sh

module purge
module load intel/14.0
module load mkl/11.1
module load mpi.ibm/1.3.0
module load gsl
module load fftw
module load netcdf-serial

export MKL="-L$MKL_HOME/lib/intel64 -lmkl_intel_lp64 -lmkl_core -lmkl_intel_thread -lpthread -lm

export NFF_HOME="/hydra/u/system/SLES11/soft/nfft/3.2.3/intel-14.0/mpi.ibm-1.3"
export ISF_HOME=$HOME/local/PSolver/1.7.6

export CC=mpiicc
export CFLAGS="-g -O3 -xHost -openmp -I$FFTW_HOME/include"
export FC=mpiifort
export FCFLAGS="-g -O3 -xHost -openmp -I$FFTW_HOME/include"

export LDFLAGS="-I$FFTW_HOME/include -L$MKL_HOME/lib/intel64 -lmkl_intel_lp64 -lmkl_core -lmkl_i

export LD_LIBRARY_PATH=$ISF_HOME/lib:$LD_LIBRARY_PATH

../configure --enable-mpi  --disable-gdlib --enable-openmp \
   --prefix=$HOME/software/octopus/repository \
   --with-gsl-prefix=$GSL_HOME \
   --with-nfft=$NFF_HOME  \
   --with-libxc-prefix=/hydra/u/system/SLES11/soft/libxc/2.0.3/intel-14.0/mpi.ibm-1.3 \
   --with-blas="$MKL" \
   --with-lapack="$MKL" \
   --with-isf-prefix=$ISF_HOME \
   --with-isf-include=$ISF_HOME/include \
   --with-metis-prefix=$HOME/local/parmetis \
   --with-parmetis-prefix=$HOME/local/parmetis \
   --with-netcdf-prefix=$NETCDF_HOME
```

Jugene

FZJ-JSC IBM Blue Gene/P, JÜLICH SUPERCOMPUTING CENTRE (JSC), Germany

May also work on other Blue Gene/P computers

General information: http://www.fz-juelich.de/jsc/jugene

Usage information: http://www.fz-juelich.de/jsc/jugene/usage/

```
module load gsl;
module load lapack;
autoreconf -i;
export FC_INTEGER_SIZE=4;
export CC_FORTRAN_INT=int;
export CC=mpixlc_r;
export CFLAGS='-g -O3 -qarch=450d';
export FC=mpixlf90_r;
export FCFLAGS='-g -O3 -qarch=450d -qxlf90=autodealloc -qessl -qsmp=omp';
export LIBS_BLAS="-lesslsmpbg -L/opt/ibmmath/essl/4.4/lib -lesslbg";
export LIBS_LAPACK="-L$LAPACK_LIB -llapack";
export LIBS_FFT="-L/bgsys/local/fftw3/lib/ -lfftw3 -lm";
./configure --prefix=$outdir \
     --host=powerpc32-unknown-linux-gnu \
     --build=powerpc64-unknown-linux-gnu \
     --disable-gdlib \
     --with-gsl-prefix=$GSL_DIR \
     --enable-mpi --enable-openmp;
```

To run you have to change to $WORK directory and run LoadLeveler. Below is an example of the tutorial (http://www.tddft.org/programs/octopus/wiki/index.php/Tutorial:Benzene_molecule) executing in 32 nodes in the SMP mode (4 threads per chip). The execution mode is hybrid; OpenMP/MPI.

Here is a example job input script:

```
# @ job_name = Octopus_Sample_1
# @ comment = "BGP Job by Size"
# @ error = $(job_name).$(jobid).out
# @ output = $(job_name).$(jobid).out
# @ environment = COPY_ALL;
# @ wall_clock_limit = 00:30:00
# @ notification = error
# @ notify_user = foo@gmail.com
# @ job_type = bluegene
# @ bg_size = 32
# @ queue
mpirun  -exe $OCTOPUS_HOME/bin/octopus_mpi -mode SMP -verbose 1
```

To execute the above script:

```
llsubmit executing_script
```

MareNostrum II

MareNostrum is a supercomputer in Europe, the most powerful in Spain. This is one of the seven supercomputers of the Spanish Supercomputing Network. The supercomputer consists of 2,560 JS21 blade computing nodes, each with 2 dual-core IBM 64-bit PowerPC 970MP processors running at 2.3 GHz for 10,240 CPUs in total. The computing nodes of MareNostrum communicate primarily through Myrinet.

You may need to compile GSL and FFTW libraries before starting then installation.

Here is a script to build Octopus:

```
#!/bin/bash

export LD_LIBRARY_PATH=/usr/lib
export CC=mpicc
export FC=mpif90

export CFLAGS="-q64 -O3 -qtune=ppc970 -qarch=ppc970 -qcache=auto -qnostrict -qignerrno -qinlglue
export FCFLAGS=$CFLAGS" -qessl -qxlf90=autodealloc"

export LIBS_BLAS="-L/usr/lib64 -lessl"

./configure   \
   --with-lapack=/gpfs/apps/LAPACK/lib64/liblapack.a \
   --disable-gsltest \
   --disable-gdlib \
   --with-gsl-prefix=$outdirGSL \
   --with-fft-lib=$outdirFFT/lib/libfftw3.a  \
   --prefix=$outdir --enable-mpi --disable-f90-forall
```

As you can see in the script the --with-gsl-prefix has to point to your GSL and --with-fft-lib to your FFTW. You should compile those with the same CFLAGS and FCFLAGS. Here is an example of configuring GSL (we use GSL-1.11):

```
./configure --prefix=$outdirGSL CC=gcc -m64 --enable-static --disable-shared
```

We use FFTW-3.1.3. To configure FFTW3 just write:

```
./configure --prefix=$outdirFFT
```

Recently Marenostrum has changed to the SLURM manager. To execute a job you have to submit it with jobsubmit (more details in the User's Guide).

MareNostrum III

MareNostrum III is a supercomputer based on Intel SandyBridge processors, iDataPlex Compute Racks, a Linux Operating System and an Infiniband interconnection. More information:
http://www.bsc.es/marenostrum-support-services/mn3

```
module load MKL
module load GSL
```

```
export PREFIX=$HOME/Software
export FFTW3_HOME=$HOME/local/fftw-3.3.2
export PFFT_HOME=$HOME/local/pfft-1.0.5-alpha

export MKL_LIBS=$MKL_HOME/lib/intel64
export MKLROOT=$MKL_HOME
export MKL_LIBS="-L$MKLROOT/lib/intel64 -lmkl_scalapack_lp64 -lmkl_intel_lp64 -lmkl_intel_thread
export CC=mpicc
export CFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$ISF_HOME/include  -openmp -I$
export FC=mpif90
export FCFLAGS="-xHost -O3 -m64 -ip -prec-div -static-intel -sox -I$FFTW3_HOME/include  -openmp

export LIBS_BLAS="${MKL_LIBS}"
export LIBS_FFT="-Wl,--start-group -L$PFFT_HOME/lib -L$FFTW3_HOME/lib -lpfft -lfftw3 -lfftw3_mpi


../configure --prefix=$PREFIX/octopus/ \
 --enable-openmp --with-libxc-prefix=$PREFIX/libxc \
 --disable-gdlib --with-gsl-prefix=/apps/GSL/1.15 \
 --enable-mpi --enable-newuoa \
 --with-pfft-prefix=$PFFT_HOME
```

Corvo

Corvo is the computational cluster of the Nano-bio Spectroscopy Group. It consists of 1504 processor cores and 5284 GiB of RAM connected by an Infiniband network.

Script to build LIBFM library included in the Scafacos library (modified Scafacos svn version 1920, this is valid since version 9887 of Octopus):

```
./configure --enable-fcs-solvers=fmm,direct --enable-fcs-fmm-comm=armci \
  --enable-fcs-fmm-unrolled --enable-fcs-fmm-max-mpol=40 \
  CFLAGS=-O3 CXXFLAGS=-O3 FCFLAGS=-O3 --disable-doc CXX=mpic++ CC=mpicc \
  FC=mpif90 --prefix=$HOME/Software/scafacos \
  LDFLAGS=-L/opt/scalapack/1.8.0/lib -L/opt/blacs/1.1/lib \
  -L/opt/gotoblas2/1.08/lib -L/opt/netcdf/4.0.1/lib -L/opt/lapack/3.2/lib \
  -L/opt/etsf_io/1.0.2/lib --enable-fcs-int=int --enable-fcs-float=double \
  --enable-fcs-integer=integer --enable-fcs-real=real*8

make
make install
```

The scripts to compile FFTW 3.3.2 and PFFT 1.0.5

```
#!/bin/sh -e

myprefix=$HOME/local
FFTW_VERSION="3.3.2"
INSTALLDIR="$myprefix/fftw/${FFTW_VERSION}"
TMP="tmp-fftw-${FFTW_VERSION}"

# bash check if directory exists
if [ -d $TMP ]; then
       echo "Directory $TMP already exists. Delete it? (y/n)"
       read answer
       if [ ${answer} = "y" ]; then
```

```
                rm -rf $TMP
        else
                echo "Program aborted."
                exit 1
        fi
fi

mkdir $TMP && cd $TMP

wget http://www.fftw.org/fftw-$FFTW_VERSION.tar.gz
gzip -dc fftw-$FFTW_VERSION.tar.gz | tar xvf -
cd fftw-$FFTW_VERSION

# fix bug in fftw alltoall routine that causes deadlocks
patch -b -p0 <<\EOF
--- mpi/transpose-alltoall.c
+++ mpi/transpose-alltoall.c
@@ -223,8 +223,8 @@
          sbo[pe] = (int) (pe * (b * p->tblock) * vn);
          rbs[pe] = (int) (db * bt * vn);
          rbo[pe] = (int) (pe * (p->block * bt) * vn);
-         if (sbs[pe] != (b * p->tblock) * vn
-             || rbs[pe] != (p->block * bt) * vn)
+         if (dbt != p->tblock
+             || db != p->block)
              equal_blocks = 0;
     }
     pln->send_block_sizes = sbs;
EOF

./configure --prefix=$INSTALLDIR --enable-mpi --enable-openmp --enable-threads --disable-shared
CC="mpicc" F77="mpif90" MPICC="mpicc" \
CFLAGS="-O3" FFLAGS="-O3" \
MPILIBS=" "

make -j 4
make install



#!/bin/sh -e

myprefix=/home/local
PFFT_VERSION=1.0.5-alpha
FFTW_VERSION=3.3.2
INSTDIR=$myprefix/pfft/$PFFT_VERSION
FFTWDIR=$myprefix/fftw/$FFTW_VERSION
TMP="tmp-pfft-$PFFT_VERSION"
module unload fftw/3.2.2

# bash check if directory exists
if [ -d $TMP ]; then
        echo "Directory $TMP already exists. Delete it? (y/n)"
        read answer
        if [ ${answer} = "y" ]; then
                rm -rf $TMP
        else
                echo "Program aborted."
```

```
                exit 1
        fi
fi

mkdir $TMP && cd $TMP
export CC=mpicc
export FC=mpif90

wget http://www.tu-chemnitz.de/~mpip/software/pfft-$PFFT_VERSION.tar.gz
gzip -dc pfft-$PFFT_VERSION.tar.gz | tar xvf -
cd pfft-$PFFT_VERSION
./configure --prefix=$INSTDIR --with-fftw3=$FFTWDIR --disable-shared

make install
```

This is the scrip to compile Octopus with PFFT and FMM support (through Scafacos library):

```
module add gcc
module add ifort
module add gsl
module add etsf_io
module add lapack
module add netcdf
module add gotoblas2
module add mpibull2
module add blacs
module add scalapack

export CC=mpicc
export FC="mpif90"

# It is important that "/opt/intel/Compiler//11.1/038/bin/intel64/" not to be in the PATH
export PATH=/opt/mpi/mpibull2-1.3.9-14.s/bin:/opt/netcdf/4.0.1/bin:/opt/etsf_io/1.0.2/bin:/opt/g

export LIBFM_HOME="$HOME/Software/scafacos"
export PFFT_HOME="$HOME/local/pfft-1.0.5-alpha"
export FFTW3_HOME="$HOME/local/fftw-3.3.2"
export LIBS_PFFT="-L$PFFT_HOME/lib -L$FFTW3_HOME/lib -lpfft -lfftw3_mpi -lfftw3"
export CFLAGS=" -I$PFFT_HOME/include -I$FFTW3_HOME/include -I$LIBFM_HOME/include"
export LDFLAGS=$LDFLAGS" -L$LIBFM_HOME/lib -L$PFFT_HOME/lib -L$FFTW3_HOME/lib -lpfft -lfftw3_mpi
export FCFLAGS=$CFLAGS
export CPPFLAGS=" -I$LIBFM_HOME/include "
export LD_LIBRARY_PATH=$LIBFM_HOME/lib:$LD_LIBRARY_PATH

../configure --enable-mpi --with-libxc-prefix=$HOME/Software/libxc_9882 \
   --prefix=$HOME/Software/octopus \
   --with-blacs=/opt/blacs/1.1/lib/libblacs.a --with-scalapack \
   --with-libfm="-L$LIBFM_HOME/lib -lfcs4fortran -lfcs -lfcs_direct -lfcs_fmm -lfcs_near -lfcs_g
   --disable-openmp
```

LaPalma

LaPalma is a supercomputer of the IAC. It is a part of the old MareNostrum II computer. It was not possible to compile with XL compilers, so GNU 4.6.1 version is used.

Previously to Octopus, Libxc (2.2), FFTW (3.3.4), GSL (1.16) and OpenBLAS (0.2.13) were required to compile.

GSL

```
export LD_LIBRARY_PATH=/usr/lib:/gpfs/apps/MPICH2/slurm-2.5.6/64/lib/:/gpfs/apps/GCC/4.9.2/lib64
export CC="/gpfs/apps/MPICH2/mx/default/64/bin/mpicc -cc=/gpfs/apps/GCC/4.9.2/bin/gcc"
export FC="/gpfs/apps/MPICH2/mx/default/64/bin/mpif90 -fc=/gpfs/apps/GCC/4.9.2/bin/gfortran"

./configure --prefix=$HOME/local/gsl/gnu --enable-static --disable-shared
```

OpenBLAS

```
make PREFIX=$HOME/local/openblas/4.6.1 BINARY=64 CC=/gpfs/apps/GCC/4.6.1/bin/gcc FC=/gpfs/apps/G
```

Libxc

```
export PATH=/gpfs/apps/MPICH2/mx/default/64/bin:$PATH
export LD_LIBRARY_PATH=/gpfs/apps/MPICH2/mx/default/64/lib:/gpfs/apps/MPICH2/slurm/64/lib

export LD_LIBRARY_PATH=/gpfs/apps/GCC/4.6.1/lib64/:$HOME/local/openblas/lib:$LD_LIBRARY_PATH
export CC="/gpfs/apps/MPICH2/mx/default/64/bin/mpicc -cc=/gpfs/apps/GCC/4.6.1/bin/gcc"
export FC="/gpfs/apps/MPICH2/mx/default/64/bin/mpif90 -fc=/gpfs/apps/GCC/4.6.1/bin/gfortran"

export CFLAGS="-m64 -O3"
export FCFLAGS=$CFLAGS

./configure --prefix=$HOME/local/libxc/gnu/4.6.1/2.2
```

Octopus

```
export PATH=/gpfs/apps/MPICH2/mx/default/64/bin:$PATH
export LD_LIBRARY_PATH=/gpfs/apps/MPICH2/mx/default/64/lib:/gpfs/apps/MPICH2/slurm/64/lib

export LD_LIBRARY_PATH=/gpfs/apps/GCC/4.6.1/lib64/:$HOME/local/openblas/4.6.1/lib:$LD_LIBRARY_PA
export CC="/gpfs/apps/MPICH2/mx/default/64/bin/mpicc -cc=/gpfs/apps/GCC/4.6.1/bin/gcc"
export FC="/gpfs/apps/MPICH2/mx/default/64/bin/mpif90 -fc=/gpfs/apps/GCC/4.6.1/bin/gfortran"

export CFLAGS="-m64 -O2 -I $PWD/external_libs/isf/wrappers "
export FCFLAGS=$CFLAGS

../configure   \
   --with-blas=$HOME/local/openblas/4.6.1/lib/libopenblas.so.0 \
   --with-lapack=/gpfs/apps/LAPACK/lib64/liblapack.a \
   --disable-gdlib \
   --with-gsl-prefix=$HOME/local/gsl/gnu \
   --with-fft-lib=$HOME/local/fftw/3.3.4/lib/libfftw3.a  \
   --with-libxc-prefix=$HOME/local/libxc/gnu/4.6.1/2.2 \
   --prefix=/gpfs/projects/ehu31/software/octopus/gnu/4.6.1 \
   --enable-mpi --disable-f90-forall
```

XBES

Located at the University of Hamburg in Hamburg. It has a login node and a 24 nodes with Intel Xeon. Here a basic configuration script:

```
./configure \
PATH="$PATH:/home/common/lib/gsl-1.16-intel/bin" \
```

```
CC="mpiicc -m64" CFLAGS=" -O3 -march=native  -I${MKLROOT}/include/intel64/lp64 -I${MKLROOT}/incl
FC="mpiifort -m64" FCFLAGS="-O3  -I${MKLROOT}/include/intel64/lp64 -I${MKLROOT}/include" \
GSL_CONFIG=/home/common/lib/gsl-1.16-intel/bin/gsl-config --with-gsl-prefix="/home/common/lib/gs
--with-libxc-prefix=$LIBXC_PREFIX   \
--with-blas="${MKLROOT}/lib/intel64/libmkl_blas95_lp64.a ${MKLROOT}/lib/intel64/libmkl_lapack95_
--with-lapack="${MKLROOT}/lib/intel64/libmkl_blas95_lp64.a ${MKLROOT}/lib/intel64/libmkl_lapack9
--with-fft-lib=/home/common/lib/fftw-3.3.4-intel/lib/libfftw3.a
```

Previous Tutorial:Running Octopus on Graphical Processing Units (GPUs) - Next Manual:Appendix:Porting Octopus and Platform Specific Instructions

Back to Manual <p class=newpage>

Appendix: Porting Octopus and Platform Specific Instructions

This page contains information about Octopus portability, with specific information to compile and run octopus for many architectures. If you managed to compile octopus for a different system, please contribute. Warning: this information is quite out of date and may no longer be valid.

General information and tips about compilers

- Octopus is developed in the GNU environment and sometimes we depend on system features that are GNU extensions without knowing it. These are bugs and we will try to fix them; please report any problem that you find.

- If you have problems with the C compiler, try to use gcc. It normally works better than vendor compilers and it's available on most systems. However, be careful with locally installed versions of gcc: sometimes they don't work.

- The Fortran / / concatenation operator is sometimes recognized as a C++-style comment and the preprocessor gives erroneous results: sometimes it doesn't expand macros after it or simply eliminates what comes after. To solve this problem, use the preprocessor with the -C (keep comments) and -ansi or equivalent options (in ANSI C / / is not a comment).

- If you are compiling in dual 32/64-bit architectures like PowerPC, UltraSparc or AMD64 systems here are some tips:
    - A 64-bit version of Octopus is only needed if you are going to use more than 2-3 Gb of physical RAM.
    - Some operating systems have 64 bits kernels and 32 bits userspace (Solaris, OS X); if you want a 64-bit Octopus there, you have to compile all required libraries in 64-bit (normally a 64-bit libc is available).
    - Typically Linux distributions *for* AMD64 have a 64-bit userspace, so you will get a 64-bit executable there.

SSE2 support

- We have some SSE2 code written using compiler primitives that can give an important increase in perfomance. For this you need hardware support (AMD Opteron/Athlon 64/Sempron/Turion or Intel Pentium 4 or newer) and compiler support, supported compilers are GCC and pathcc. For gcc you need to

put the correct `-march` flags (for example `-march=opteron` or `-march=pentium4`).

- Besides this, for x86 (32 bits) you have to link dynamically because we have to use a tweaked malloc function that doesn't work with static linking. For x86_64 (64 bits) this is not needed.

Operating systems

Linux

The main development operating system for Octopus.

Solaris

Octopus compiles correctly either with sun compilers or gcc/gfortran. By default Solaris doesn't have GNU coreutils, so some test won't run.

Tru 64

It works.

Mac OS X

It works. Don't try to compile static binaries, they are not supported by the OS.

Windows

Toy operating systems are not supported for the moment, sorry.

Compilers

Intel Compiler for x86/x86_64

- status: ok
- Version 9 and version 7.1 Build 20040901Z are ok. Versions 8 and 8.1 can be problematic.
- Recommended flags: FCFLAGS="-u -zero -fpp1 -nbs -pc80 -pad -align -unroll -O3 -ip -tpp7 -xW"
- Intel artificially blocks their compilers from using certain optimization in non-Intel processors.
- With Octopus 3.2.0, use of the flags `-check all -traceback` with `ifort` 10.1.018 will cause an internal compiler segmentation fault while compiling `src/grid/mesh_init.F90`.

Intel Compiler for Itanium

- status: ok
- Version: 8.1.033 (older 8 releases and version 9 are reported to cause problems), version 10 works but it is much slower than 8.1.
- Recommended flags:
    - FCFLAGS="-O3 -tpp2 -ip -IPF_fp_relaxed -ftz -align all -pad"
    - CFLAGS="-O3 -tpp2 -ip -IPF_fp_relaxed -ftz"

Open64

This is an open source compiler based on the liberated code of SGI MIPSpro compiler. It is available for x86, x86_64 and Itanium architectures.

Pathscale Fortran Compiler

- Versions tested: 2.2, 2.3 and 2.5
- Architecure: x86, AMD64
- Recommended flags:

```
FCFLAGS="-Wall -O3 -march=auto -mcpu=auto -OPT:Ofast -fno-math-errno"
```

- Issues:
  - Everything works.
  - It's necessary to compile blas/lapack with the same compiler.

NAG compiler

AMD64:

```
FCFLAGS="-colour -kind=byte -mismatch_all -abi=64 -ieee=full -O4 -Ounroll=4"
```

GNU C Compiler (gcc)

GNU Fortran (gfortran)

- Status: ok.
- Version: gcc version 4.1.1 or newer. (4.1.0 *does not* work) For the parallel version you need at least gfortran 4.3.
- You may also need to compile blas, lapack and fftw3 using that specific gfortran version.
- Some recommended flags: `-march=athlon64 -msse2 -mfpmath=sse -malign-double -funroll-loops -O3`

g95

- Status: works
- Tested architectures: x86/Linux, PowerPC/Darwin
- Version: version 4.0.3 (g95 0.91!) May 24 2007
- G95 doesn't recognize the linemarkers created by the preprocessor, so it's necessary to pass the -P flag to cpp.
- Flags:

```
FC=g95
FCFLAGS="-O3 -funroll-loops -ffast-math"
FCCPP="cpp -ansi-P"
```

There may be problems with versions 0.92 or 0.93, depending on the underlying version of gcc. See G95 for info on building version 0.94 with gcc 4.2.4.

Portland 6

Flags:

```
FCFLAGS="-fast -mcmodel=medium -O4"
```

Known problems:

The following problem with the PGI compiler version 6.0 and MPICH version 1.2.6 on x86_64 has been reported:

The MPI detection during the *configure* step does not work properly. This may lead to compilation failures on e. g. the file **par_vec.F90**. This problem is considered a bug in either the PGI compiler or the MPICH implementation. Please apply the following change by hand after running *configure*:

In the file **config.h**, replace the line

```
/* #undef MPI_H */
```

by

```
#define MPI_H 1
```

and remove the line

```
#define MPI_MOD 1
```

Portland 7, 8, 9

Flags (tested on Cray XT4):

```
FCFLAGS="-O2 -Munroll=c:1 -Mnoframe -Mlre -Mscalarsse -Mcache_align -Mflushz"
```

The configure script may fail in the part `checking for Fortran libraries of mpif90` for `autoconf` version 2.59 or earlier. The solution is to update `autoconf` to 2.60 or later, or manually set `FCLIBS` in the `configure` command line to remove a spurious apostrophe.

Portland 10

For Octopus 3.2.0, the file `src/basic/lookup.F90` is incorrectly optimized yielding many segmentation faults in the testsuite. With PGI 10.5 the optimization flag should be `-O2` or less; with PGI 10.8 the optimization flag should be `-O1` or less. Note that `-fast` and `-fastsse` are between `-O2` and `-O3`. For later versions of Octopus, a PGI pragma compels this file to be `-O0` regardless of what is specified in `FCFLAGS`, so you may safely set `FCFLAGS` to `-fast`.

Portland 11

11.4 does not work and will crash with glibc memory corruption errors. 11.7 is fine.

Portland 12

12.5 and 12.6 cannot compile due to an internal compiler errors of this form:

```
PGF90-S-0000-Internal compiler error. sym_of_ast: unexpected ast    6034 (simul_box.F90: 1103)
```

12.4 and 12.9 are ok.

Absoft

Flags x86:

```
FCFLAGS="-O3 -YEXT_NAMES=LCS -YEXT_SFX=_"
```

Flags amd64/em64t:

```
FCFLAGS="-O3 -mcmodel=medium -m64 -cpu:host -YEXT_NAMES=LCS -YEXT_SFX=_"
```

Compaq compiler

```
FCFLAGS="-align dcommons -fast -tune host -arch host -noautomatic"
```

Xlf

- Status: works

-bmaxdata:0x80000000 -qmaxmem=-1 -qsuffix=f=f90 -Q -O5 -qstrict -qtune=auto -qarch=auto -qhot -qipa

- Because of the exotic mixture of MAC OS and BSD, this system is not very standard. Compiling Octopus can be problematic.
- OS X doesn't support static linking of binaries, so don't try.

SGI MIPS

-O3 -INLINE -n32 -LANG:recursive=on

Sun Studio

You can download this compiler for free, it supports Linux and Solaris over x86, amd64 and sparc. A very fast compiler but quite buggy.

- Flags:
  - CFLAGS="-fast -xprefetch -xvector=simd -D__SSE2__"
  - FCFLAGS=$FLAGS

MPI Implementations

OpenMPI

MPICH2

SGI MPT

Intel MPI

Sun HPC ClusterTools

MVAPICH

NetCDF

Octopus uses the Fortran 90 interface of netCDF, this means that it's likely that you will have to compile it using the same compiler you will use to compile Octopus. You can get the sources and follow installation instructions from the NetCDF site.

BLAS and LAPACK

These are standard libraries that provide a series of common vector and matrix operations. Octopus uses as much as possible this libraries. There are several version available depending on your hardware. Around 40% of Octopus execution time is spend in BLAS level 1 routines, so getting a fast implementation for your hardware might be important. On the other hand, Lapack performance is not very important.

AMD ACML

This is the AMD Mathematical Library optimized to run in Athlon and Opteron processors. You can get a free copy from http://developer.amd.com/acml.jsp .

ATLAS

Compaq CXML

[GOTO BLAS]

Probably the fastest implementation of blas, source code is available and it can be compiled in many architectures.

Intel MKL

See https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor for MKL's advice on the proper way to link. Here is an example, in which `--with-lapack` is left blank because it is included in `--with-blas`.

```
MKL_DIR=/opt/intel/mkl/lib/intel64
--with-blas="-L$MKL_DIR -Wl,--start-group -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -Wl,--end
--with-blacs="$MKL_DIR/libmkl_blacs_intelmpi_lp64.a" --with-scalapack="$MKL_DIR/libmkl_scalapack
```

Netlib

The reference implementation of BLAS and Lapack. It is available in most linux distributions. You can get the source code from http://www.netlib.org/blas http://www.netlib.org/lapack .

Previous Manual:Specific architectures - Next Manual:Appendix:Reference Manual

Back to Manual <p class=newpage>

Appendix: Reference Manual

Previous Manual:Appendix:Porting Octopus and Platform Specific Instructions - Next Manual:Appendix:Copying

Back to Manual <p class=newpage>

Appendix: Copying

INTRODUCTION

The real-space TDDFT code octopus ("octopus") is provided under the GNU General Public License ("GPL"), Version 2, with exceptions for external libraries that are contained solely for convenience in this distribution.

You can find a copy of the GPL license here.

A copy of the exceptions and licenses follow this introduction.

LICENSE EXCEPTIONS

Octopus provides several external libraries, which are located in the "external_libs" subdirectory of the octopus source distribution. The GNU General Public License does not apply to these libraries. Separate copyright notices can be found for each library in the respective subdirectories of "external_libs". Copyright notices are also contained in this document.

Currently the following external libraries are provided:

Expokit

- Roger B. Sidje
- Department of Mathematics, University of Queensland
- Brisbane, QLD-4072, Australia
- Email: rbs@maths.uq.edu.au
- WWW: http://www.maths.uq.edu.au/expokit/
- Copyright: http://www.maths.uq.edu.au/expokit/copyright

Metis 4.0

- George Karypis
- Department of Computer Science & Engineering
- Twin Cities Campus
- University of Minnesota, Minneapolis, MN, USA
- Email: karypis@cs.umn.edu
- WWW: http://www-users.cs.umn.edu/~karypis/metis/index.html

METIS COPYRIGHT NOTICE

qshep

- Robert Renka
- University of North Texas
- (817) 565-2767

QSHEP COPYRIGHT NOTICE

The ACM grants to you (hereafter, User) a royalty-free, nonexclusive right to execute, copy, modify and distribute both the binary and source code solely for academic, research and other similar noncommercial uses, subject to the following conditions:

1. User acknowledges that the Software is still in the development stage and that it is being supplied "as is," without any support services from ACM. Neither ACM nor the author makes any representations or warranties, express or implied, including, without limitation, any representations or warranties of the merchantability or fitness for any particular purpose, or that the application of the software, will not infringe on any patents or other proprietary rights of others.

2. ACM shall not be held liable for direct, indirect, incidental or consequential damages arising from any claim by User or any third party with respect to uses allowed under this Agreement, or from any use of the Software.

3. User agrees to fully indemnify and hold harmless ACM and/or the author(s) of the original work from and against any and all claims, demands, suits, losses, damages, costs and expenses arising out of the User's use of the Software, including, without limitation, arising out of the User's modification of the Software.

4. User may modify the Software and distribute that modified work to third parties provided that: (a) if posted separately, it clearly acknowledges that it contains material copyrighted by ACM (b) no charge is associated with such copies, (c) User agrees to notify ACM and the Author(s) of the distribution, and (d) User clearly notifies secondary users that such modified work is not the original Software.

5. User agrees that ACM, the authors of the original work and others may enjoy a royalty-free, non-exclusive license to use, copy, modify and redistribute these modifications to the Software made by the User and distributed to third parties as a derivative work under this agreement.

6. This agreement will terminate immediately upon User's breach of, or non-compliance with, any of its terms. User may be held liable for any copyright infringement or the infringement of any other proprietary rights in the Software that is caused or facilitated by the User's failure to abide by the terms of this agreement.

7. This agreement will be construed and enforced in accordance with the law of the state of New York applicable to contracts performed entirely within the State. The parties irrevocably consent to the exclusive jurisdiction of the state or federal courts located in the City of New York for all disputes concerning this agreement.

Commercial Use

Any User wishing to make a commercial use of the Software must contact ACM at permissions@acm.org to arrange an appropriate license. Commercial use includes (1) integrating or incorporating all or part of the source code into a product for sale or license by, or on behalf of, User to third parties, or (2) distribution of the binary or source code to third parties for use with a commercial product sold or licensed by, or on behalf of, User.

Revised 6/98

Previous Manual:Appendix:Reference Manual - Next Manual

Back to Manual

Back to Documentation