

## **Preface**

Rayleigh\_link is small fortran programs to access output data from Rayleigh. This program is written to make a programs to read Rayleigh data.

# 1 Introduction

Calypso is a program package for magnetohydrodynamics (MHD) simulations in a rotating spherical shell for geodynamo problems. This package consists of the simulation program, preprocessing program, post processing program to generate field data for visualization programs, and several small utilities. The simulation program runs on parallel computing systems using MPI and OpenMP parallelization.

Calypso solves the equations that govern convection and magnetic-field generation in a rotating spherical shell. Flow is driven by thermal or compositional buoyancy in a Boussinesq fluid. Calypso also support various boundary conditions (e.g. fixed temperature, heat flux, composition, and compositional flux), and permits a conductive and rotatable inner core. Results are written as spherical harmonics coefficients, Gauss coefficients for the region outside of the fluid shell, and field data in Cartesian coordinate for easily visualization with a number of visualization programs.

This user guide describes the essentials of the magnetohydrodynamics theory and equations behind Calypso, and provides instructions for the configuration and execution of Calypso.

# 2 History

Calypso has its origins in two earlier projects. One is a dynamo simulation code written by Hiroaki Matsui in 1990's using a spectral method. This code solves for the poloidal and toroidal spectral coefficients, like Calypso, but it calculates the nonlinear terms in the spectral domain using a parallelization for SMP architectures. The other project is the thermal convection version of GeoFEM, which is Finite Element Method (FEM) platform for massively parallel computational environment, originally written by Hiroshi Okuda in 2000. Under GeoFEM Project, Lee Chen developed cross sectioning, iso-surfacing, and volume rendering modules for data visualization for parallel computations..

Hiroaki Matsui was responsible for adding routines to GeoFEM to perform magnetohydrodynamics simulation in a rotating frame. In 2002 this code successfully performed dynamo simulations in a rotating spherical shell using insulating magnetic boundary conditions. The following year Matsui implemented a subgrid scale (SGS) model in the FEM dynamo model in collaboration with Bruce Buffett. A module to solve for double diffusive convection was added to the FEM dynamo model by Hiroaki Matsui in 2009.

Progress in understanding the role of subgrid scale models in magnetohydrodynamic simulations relies on quantitative estimates for the transfer of energy between spatial scales. This information is most easily obtained from a spherical harmonic expansion of the simulation results, even when the simulation is performed by FEM. Hiroaki Matsui

implemented the spherical harmonic transform in 2007 using a combination of MPI and OpenMP, and later included the spherical harmonic transform routines into his old dynamo code to create Calypso. Additional software in the program package for visualization is based on data formats from the FEM model. In addition, the control parameter file format is adapted from the input formats used in GeoFEM.

Calypso Ver. 1.0 supports the following features and capabilities

- Magnetohydrodynamics simulation for a Boussinesq fluid in a rotating spherical shell.
- Convection driven by thermal and compositional buoyancy.
- Temperature or heat flux is fixed at boundaries
- Composition or compositional flux is fixed at boundaries
- Non-slip or free-slip boundary conditions
- Outside of the fluid shell is electrically insulated or pseudo vacuum boundary.
- A conductive inner core with the same conductivity as the surrounding fluid
- A rotating inner core driven by the magnetic and viscous torques.

## 2.1 Updates for Ver 1.1

In Version 1.1, a number of bug fixes and additional comments for Doxygen are completed. The following large bugs are fixed:

- `configure` command is updated to find appropriate GNU make command. (see Section ??)
- Label for radial grid type in the file `ctl_sph_shell radial_grid_type_ctl` is changed to `radial_grid_type_ctl`. If the old name is used in the control file, program `gen_sph_grid` will crash.

And, the following features are implemented

- New ordering is used for spherical harmonics data to reduce communication time. The old version of spectrum indexing data, which is generated by `gen_sph_grids` in Ver. 1.0 is also supported in Ver. 1.1.

- Evaluation of Coriolis term is updated. Now, Adams-Gaunt integrals are evaluated in the initialization process in the simulation program `sph_mhd`, so the data file for Adams-Gaunt integrals which is made by `gen_sph_grids` is not required.
- Add a program `sph_add_initial_field`. to modify existed initial field data. This program is used to modify or add new fields in spectrum data. (See Section ??.)
- Heat and composition source terms are implemented. These source terms are fixed with time, and defined as spectrum data. The source terms are defined by using initial field generation program `sph_initial_field` or `sph_add_initial_field`. (See section ?? and ??.)
- The boundary conditions for temperature and composition can be defined by using spherical harmonics coefficients. (i.e. inhomogeneous boundary conditions can be applied.) These boundary conditions are defined by using single external data file. (See Section ??)

## 2.2 Updates for Ver 1.2

In Version 1.2, the following features are implemented:

- To reduce the number of calculation, Legendre transform is calculated with taking account to the symmetry with respect to the equator. Time for Legendre transform is approximately half of that in Ver 1.1.
- BLAS library can be used for the Legendre transform optionally.
- Cross sectioning and isosurfacing module are newly implemented. These modules are re-written by Fortran90 from the parallel sectioning modules in GeoFEM by Lee Chen in C, and some features are added for visualizations of geodynamo simulations. See section ?? and ??.
- Initial data assemble program `assemble_mhd` is parallelized. This program can perform with any number of MPI processes, but we recommend to run the program with **one** process or the same number of processes as the number of subdomains for the target configuration which is defined by `num_new_domain_ctl`. See section ??.
- The time and time step information in the restart data can be modified by `assemble_mhd`. See section ??

### 3 Acknowledgements

Calypso was primarily developed by Dr. Hiroaki Matsui in collaboration with Prof. Bruce Buffett at the University of California, Berkeley. The following NSF grants supported the development of Calypso,

- B.A. Buffett, NSF EAR-0509893; Models of sub-grid scale turbulence in the Earth's core and the geodynamo; 2005 - 2007.
- B.A. Buffett and D. Lathrop, NSF EAR-0652882; CSEDI Collaborative Research: Integrating numerical and experimental geodynamo models, 2007 - 2009
- B.A. Buffett, NSF EAR-1045277; Development and application of turbulence models in numerical geodynamo simulations ; 2010 - 2012

### 4 Citation

Computational Infrastructure for Geodynamics (CIG) and the Calypso developers are making the source code to Calypso available to researchers in the hope that it will aid their research and teaching. A number of individuals have contributed a significant amount of time and energy into the development of Calypso. We request that you cite the appropriate papers and make acknowledgements as necessary. The Calypso development team asks that you cite the following papers:

Matsui, H., E. King, and B.A. Buffett, Multi-scale convection in a geodynamo simulation with uniform heat flux along the outer boundary, *Geochemistry, Geophysics, Geosystems*, **15**, 3212 – 3225, 2014.

## 5 Installation

### 5.1 Library Requirements

Calypso requires the following libraries.

- GNU make
- MPI libraries (OpenMPI, MPICH, etc)
- FFTPACK Ver 5.1D ([http://people.sc.fsu.edu/~jburkardt/f\\_src/fftpack5.1d/fftpack5.1d.html](http://people.sc.fsu.edu/~jburkardt/f_src/fftpack5.1d/fftpack5.1d.html)). The source files for FFTPACK are included in `src/EXTERNAL_libs` directory.

Linux and Max OS X use GNU make as a default 'make' command, but some system (e.g. BSD or SOLARIS) does not use GNU make as default. `configure` command searches and set correct GNU make command.

In addition, the following environment and libraries can be used (optional).

- OpenMP
- BLAS
- FFTW version 3 (<http://www.fftw.org>) including Fortran wrapper
- zlib (<http://www.zlib.net>)
- PARALLEL HDF5 (<https://support.hdfgroup.org/HDF5/PHDF5>) including Fortran wrapper.

Note: Calypso does NOT use MPI and OpenMP features in FFTW3.

In the most of platforms, the Fourier transform by FFTW is faster than that by FFTPACK.

zlib is used for compressed data IO. Zlib is installed in most of UNIX platforms.

HDF5 is used for field data output with XDMF format instead of VTK format. The comparison of field data format is described in section `refsec:VTK`.

OpenMP is used for the parallelization under the shared memory. Better choice to use both MPI and OpenMP parallelization (so-called Hybrid parallelization) or only using MPI (so-called flat MPI) is depends on the computational platform and compiler. For example, flat MPI has much better performance on Linux cluster with Intel Xeon processors and with Intel fortran compiler, but Hybrid model has better performance on Hitachi SR16000 with Power 6 processors.

## 5.2 Known problems

### FFTPACK and Intel compiler

FFTPACK fails to compile with Intel fortran using the `'-warn all'` option. Currently the `'-warn all'` option is excluded by Makefile when FFTPACk is compiled.

### Homebrew's FFTW3 on Mac OS X

Calypso uses Fortran wrappers in FFTW3. If FFTW3 is installed using Homebrew for Mac OS X (<http://mxcl.github.com/homebrew/>), the required fortran wrappers are not installed. In this case, please install FFTW3 with Fortran wrappers with another package manager (Macports (<http://www.macports.org>, for example), build FFTW3 by yourself including the Fortran wrapper, or turn off FFTW3 features in Calypso.

### XL fortran

In XL fortran, preprocessor options is not specified by `-D...`, but `-Wf, '-D...'`. Please edit preprocessor macro option `F90CPPFLAGS` in `work/Makefile` by an editor.

### Cross compiler support

`configure` command in Calypso does not support cross compilation. If you want to compile with a cross compiler, please set the variables in Makefile manually (see section ??)

## 5.3 Directories

The top directory of Calypso (ex. `[CALYPSO_HOME]`) contains the following directories.

```
% cd [CALYPSO_HOME]
% ls
CMakeLists.txt Makefile.in configure.in examples
INSTALL bin doc src
LICENSE configure doxygen work
```

`bin`: directory for executable files

`cmake`: directory for cmake configurations

`cmake`: directory for document generated by doxygen  
`doc`: documentations  
`examples`: examples  
`src`: source files  
`work`: work directory. Compile is done in this directory.

## 5.4 Doxygen

Doxygen (<http://www.doxygen.org>) is an powerful document generation tool from source files. We only save a configuration file in this directory because thousands of html files generated by doxygen. The documents for source codes are generated by the following command:

```
% cd [CALYPSO_HOME]/doxygen
% doxygen ./Doxyfile_CALYPSO
```

The html documents can see by opening `[CALYPSO_HOME]/doxygen/html/index.html`. Automatically generated documentation is also available on the CIG website at <http://www.geodynamics.org/cig/software/calypso/>.

## 5.5 Install using `configure` command

### 5.5.1 Configuration using `configure` command

Calypso uses the `configure` script for configuration to install. The simplest way to install programs is the following process in the top directory of Calypso.

```
%pwd
[CALYPSO_HOME]
% ./configure
...
% make
...
% make install
```

After the installation, object modules can be deleted by the following command;

```
% make clean
```



`./configure` generates a Makefile in the current directory. Available options for `configure` can be checked using the `./configure --help` command. The following options are available in the `configure` command.

Optional Features:

```
--disable-option-checking  ignore unrecognized --enable/--with options
--disable-FEATURE          do not include FEATURE (same as --enable-FEATURE=no)
--enable-FEATURE[=ARG]    include FEATURE [ARG=yes]
--enable-fftw3             Use fftw3 library
```

Optional Packages:

```
--with-PACKAGE[=ARG]      use PACKAGE [ARG=yes]
--without-PACKAGE         do not use PACKAGE (same as --with-PACKAGE=no)
--with-hdf5=yes/no/PATH  full path of h5pcc for parallel HDF5 configuration
--with-blas=<lib>         use BLAS library <lib>
--with-zlib=DIR           root directory path of zlib installation defaults to
                          /usr/local or /usr if not found in /usr/local
--without-zlib            to disable zlib usage completely
```

Some influential environment variables:

```
CC          C compiler command
CFLAGS      C compiler flags
LDFLAGS     linker flags, e.g. -L<lib dir> if you have libraries in a
            nonstandard directory <lib dir>
LIBS        libraries to pass to the linker, e.g. -l<library>
CPPFLAGS    (Objective) C/C++ preprocessor flags, e.g. -I<include dir> if
            you have headers in a nonstandard directory <include dir>
FC          Fortran compiler command
FCFLAGS     Fortran compiler flags
MPICC       MPI C compiler command
MPIFC       MPI Fortran compiler command
PKG_CONFIG  path to pkg-config utility
CPP         C preprocessor
FFTW3_CFLAGS C compiler flags for FFTW3, overriding pkg-config
FFTW3_LIBS  linker flags for FFTW3, overriding pkg-config
```

An example of usage of the `configure` command is the following;

```
% ./configure --prefix='/Users/matsui/local' \
? CFLAGS='-O -Wall -g' FCFLAGS='-O -Wall -g' \
? PKG_CONFIG_PATH='/Users/matsui/local/lib/pkgconfig' \
```

```
? --with-blas=yes --enable-fftw3 --with-zlib=/usr/local \
? --with-hdf5='/Users/matsui/local/bin/h5pcc'
```

### 5.5.2 Compile

Compile is performed using the `make` command. The Makefile in the top directory is used to generate another Makefile in the `work` directory, which is automatically used to complete the compilation. The object file and libraries are compiled in the `work` directory. Finally, the executive files are assembled in `bin` directory. You should find the following programs in the `bin` directory.

```
gen_sph_grids: Preprocessing program for data transfer for spherical transform
sph_mhd: Simulation program
sph_initial_field: Example program to generate initial field
sph_add_initial_field: Example program to add initial field in existing spectrum data
sph_snapshot: Data transfer from spectrum data to field data
sph_dynamobench: Data processing for dynamo benchmark test by Christensen et al. (2002)
sph_zm_snapshot: Generate zonal mean field
assemble_sph: Data transfer program to change number of subdomains.
t_ave_sph_mean_square: Time averaging program for the mean square data.
t_ave_picked_sph_coefs: Time averaging program for the picked spectrum data.
t_ave_nusselt: Time averaging program for the Nusselt number data.
check_sph_grids: Check program for tests.
make_f90depends: Program to generate dependency of the source code (make command uses to generate work/Makefile)
```

The following library files are also made in `work` directory.

`libcalypso.a`: Calypso library

`libfftpack.5d.a`: FFTPACK 5.1 library

### 5.5.3 Clean

The object and fortran module files in `work` directory is deleted by typing

```
% make clean
```

This command deletes files with the extension `.o`, `.mod`, `.par`, `.diag`, and `.`

### 5.5.4 Distclean

To revert the files and directory to the original package, use `make distclean` as

```
% make distclean
```

### 5.5.5 Install

The executive files are copied to the install directory `$(INSTDIR)/bin`. The install directory `$(INSTDIR)` is defined in `Makefile`, and can also set by `${--prefix}` option for `configure` command. Alternatively, you can use the programs in `$(SRCDIR)/bin` directory without running `make install`. If directory `$(PREFIX)` does not exist, `make install` creates `$(PREFIX)`, `$(PREFIX)/lib`, `$(PREFIX)/bin`, and `$(PREFIX)/include` directories. No files are installed in `$(PREFIX)/lib` and `$(PREFIX)/include`.

## 5.6 Install without using configure

It is possible to compile Calypso without using the `configure` command. To do this, you need to edit the `Makefile`. First, copy `Makefile` from `template Makefile.in` as

```
% cp Makefile.in Makefile
```

In `Makefile`, the following variables should be defined.

`SHELL` Name of shell command.

`SRCDIR` Directory of this `Makefile`.

`INSTDIR` Install directory.

`MPICHDIR` Directory names for MPI implementation. If you set `fortran90` compiler name for MPI programs in `MPIF90`, you do not need to define this valuable.

`MPICHINCDIR` Directory names for include files for MPI implementation. If you set `fortran90` compiler name for MPI programs in `MPIF90`, you do not need to define this valuable.

`MPILIBS` Library names for MPI implementation. If you set `fortran90` compiler name for MPI programs in `MPIF90`, you do not need to define this valuable.

`F90_LOCAL` Command name of local Fortran 90 compiler to compile module dependency listing program.

`MPIF90` Command name of Fortran90 compiler and linker for MPI programs. If command does not have MPI implementation, you need to define the definition of MPI libraries `MPICHDIR`, `MPICHINCDIR`, and `MPILIBS`.

`AR` Command name for archive program (ex. `ar`) to generate libraries. If you need some options for archive command, options are also included in this valuable.

`RANLIB` Command name for `ranlib` to generate index to the contents of an archive. If system does not have `ranlib`, set `true` in this valuable. `true` command does not do anything for libraries.

`F90OPTFLAGS` Optimization flags for Fortran90 compiler (including OpenMP flags)

`BLAS_LIBS` Library lists for BLAS (ex. `-lblas`)

`ZLIB_CFLAGS` Option flags for FFTW3 (ex. `-I/usr/include`)

`ZLIB_LIB` Library lists for FFTW3 (ex. `-L/usr/lib -lz`)

`FFTW3_CFLAGS` Option flags for FFTW3 (ex. `-I/usr/local/include`)

`FFTW3_LIBS` Library lists for FFTW3 (ex. `-L/usr/local/lib -lfftw3 -lm`)

`HDF5_FFLAGS` Option flags to compile with HDF5. This setting can be found by using `hfd5` command `h5pfc -show`.

**HDF5\_LDFLAGS** Option flags to link with HDF5. This setting can be found by using `hfd5 command h5pfc -show`.

**HDF5\_FLIBS** Library lists for HDF5. This setting can be found by using `hfd5 command h5pfc -show`.

## 5.7 Install using cmake

CMake is a cross-platform, open-source build system. CMake can be downloaded from <http://www.cmake.org>. The following procedure is required to install.

1. Create working directory (you can also use `[CALYPSO_HOME]/work`).
2. Generate Makefile and working directories by `cmake` command.
3. Compile programs by `make` command.

In this section, `[CALYPSO\_HOME]/work` is used as the working directory. Options for CMake can be checked by `cmake -i [CALYPSO_HOME]` command at `[CALYPSO_HOME]/work`. There are a number of options can be found, but the following valuables are important settings for installation:

**CMAKE\_INSTALL\_PREFIX** Install directory

**CMAKE\_Fortran\_COMPILER** Fortran90 compiler.

**CMAKE\_DISABLE\_FIND\_PACKAGE\_OpenMP\_Fortran** OpenMP is not used if 'yes' is set in this valuable.

**CMAKE\_DISABLE\_FIND\_PACKAGE\_FFTW** FFTW3 library does not linked if 'yes' is set in this valuable.

**CMAKE\_LIBRARY\_PATH** CMake library search paths. This directory is used to search FFTW3 library.

**CMAKE\_INCLUDE\_PATH** CMake include search paths. This directory is used to search include file for FFTW3.

**CMAKE\_DISABLE\_FIND\_PACKAGE\_FFTW** FFTW3 library does not linked if 'yes' is set in this valuable.

**HDF5\_INCLUDE\_DIRS** Include file directories to compile with HDF5. This setting can be found by using `hfd5 command h5pfc -show`.

**HDF5\_LIBRARY\_DIRS** Location of HDF5 library. This setting can be found by using **hfd5** command **h5pfc -show**.

**HDF5\_LIBRARIES** Library lists for HDF5. This setting can be found by using **hfd5** command **h5pfc -show**.

**CMAKE\_DISABLE\_FIND\_PACKAGE\_HDF5** HDF5 library does not linked if 'yes' is set in this valuable.

An example of using CMake on Mac OS X is the following:

```
% cd work
% h5pfc -show
mpif90 -I/home/matsui/local/include -L/home/matsui/local/lib
/home/matsui/local/lib/libhdf5hl_fortran.a
/home/matsui/local/lib/libhdf5_hl.a
/home/matsui/local/lib/libhdf5_fortran.a
/home/matsui/local/lib/libhdf5.a
-L/home/matsui/local/lib -lmpi -lz -ldl -lm
% cmake .. -DCMAKE_LIBRARY_PATH='/home/matsui/local/lib' \
? -DCMAKE_INCLUDE_PATH='/home/matsui/local/include' \
? -DHDF5_INCLUDE_DIRS='/home/matsui/local/include' \
? -DHDF5_LIBRARY_DIRS='/home/matsui/local/lib' \
? -DHDF5_LIBRARIES='/home/matsui/local/lib/libhdf5hl_fortran.a \
? /home/matsui/local/lib/libhdf5_hl.a \
? /home/matsui/local/lib/libhdf5_fortran.a \
? /home/matsui/local/lib/libhdf5.a'
```

After configuration, compile and install are started by

```
% make
...
% make install
```

After running make command, execute files are built in [CALYPSO\_HOME]/work/bin directory.

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