BOUT++ Users Manual

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Contents

1 Introduction

BOUT++ is a C++ framework for writing plasma fluid simulations with an arbitrary number of equations in 3D curvilinear coordinates [1, 2]. It has been developed from the original **BOU**ndary **T**urbulence 3D 2-fluid edge simulation code [3, 4, 5] written by X.Xu and M.Umansky at LLNL.

Though designed to simulate tokamak edge plasmas, the methods used are very general and almost any metric tensor can be specified, allowing the code to be used to simulate (for example) plasmas in slab, sheared slab, and cylindrical coordinates. The restrictions on the simulation domain are that the equilibrium must be axisymmetric (in the z coordinate), and that the parallelisation is done in the x and y (parallel to $\mathbf{B}$) directions.

The aim of BOUT++ is to automate the common tasks needed for simulation codes, and to separate the complicated (and error-prone) details such as differential geometry, parallel

communication, and file input/output from the user-specified equations to be solved. Thus the equations being solved are made clear, and can be easily changed with only minimal knowledge of the inner workings of the code. As far as possible, this allows the user to concentrate on the physics, rather than worrying about the numerics. This doesn't mean that users don't have to think about numerical methods, and so selecting differencing schemes and boundary conditions is discussed in this manual. The generality of the BOUT++ of course also comes with a limitation: although there is a large class of problems which can be tackled by this code, there are many more problems which require a more specialised solver and which BOUT++ will not be able to handle. Hopefully this manual will enable you to test whether BOUT++ is suitable for your problem as quickly and painlessly as possible.

This manual is written for the user who wants to run (or modify) existing plasma models, or specify a new problem (grid and equations) to be solved. In either case, it's assumed that the user isn't all that interested in the details of the code. For a more detailed descriptions of the code internals, see the developer and reference guides. After describing how to install BOUT++ (section 2), run the test suite (section 2.6) and a few examples (section 4, more detail in section 20), increasingly sophisticated ways to modify the problem being solved are introduced. The simplest way to modify a simulation case is by altering the input options, described in section 6. Checking that the options are doing what you think they should be by looking at the output logs is described in section 4, and an overview of the IDL analysis routines for data post-processing and visualisation is given in section 5. Generating new grid files, particularly for tokamak equilibria, is described in section 11.

Up to this point, little programming experience has been assumed, but performing more drastic alterations to the physics model requires modifying C++ code. Section 12 describes how to write a new physics model specifying the equations to be solved, using ideal MHD as an example. The remaining sections describe in more detail aspects of using BOUT++: section 15 describes the differential operators and methods available; section 16 covers the experimental staggered grid system.

Various sources of documentation are:

- Most directories in the BOUT++ distribution contain a README file. This should describe briefly what the contents of the directory are and how to use them.
- This user's manual, which goes through BOUT++ from a user's point of view
- The developer's manual, which gives details of the internal working of the code.
- The reference guide, which summarises functions, settings etc. Intended more for quick reference rather than a guide.
- Most of the code contains Doxygen comment tags (which are slowly getting better). Running doxygen (`www.doxygen.org`) on these files should therefore generate an HTML reference. This is probably going to be the most up-to-date documentation.

1.1 License and terms of use

BOUT++ is free software, but since it is a scientific code we also ask that you show professional courtesy when using this code:

1. Since you are benefiting from work on BOUT++, we ask that you submit any improvements you make to the code to us by emailing Ben Dudson at bd512@york.ac.uk

2. If you use BOUT++ results in a paper or professional publication, we ask that you send your results to one of the BOUT++ authors first so that we can check them. It is understood that in most cases if one or more of the BOUT++ team are involved in preparing results then they should appear as co-authors.

3. Publications or figures made with the BOUT++ code should acknowledge the BOUT++ code by citing B.Dudson et. al. Comp.Phys.Comm 2009 [1] and/or other BOUT++ papers. See the file CITATION for details.

2 Getting started

This section goes through the process of getting, installing, and starting to run BOUT++. Only the basic functionality needed to use BOUT++ is described here; the next section (3) goes through more advanced options, and how to fix some common problems.

On large facilities (e.g NERSC or Archer), the compilers and libraries needed should already be installed. It is common to organise libraries using the `modules` system, so try typing "`module avail`" to get a list of available modules. Some instructions for specific machines can be found in appendix A. If you are installing on your own machine, you may need to install an MPI compiler and the libraries yourself.

This section will go through the following steps:

1. Obtaining a copy of BOUT++
2. Installing an MPI compiler (2.2)
3. Installing libraries (2.3)
4. Configuring BOUT++ analysis codes (2.4)
5. Compiling BOUT++ (2.5)
6. Running the test suite (2.6)

Note: In this manual commands to run in a BASH shell will begin with '$', and commands specific to CSH with a '%'.

2.1 Obtaining BOUT++

BOUT++ is now hosted publicly on github (`http://github.com/bendudson/BOUT`), and includes instructions on downloading and installing BOUT++ in wiki pages. This website also has a list of current issues and history of changes. To obtain a copy of the latest version, run

```
$ git clone git://github.com/bendudson/BOUT.git
```

which will create a directory `BOUT` containing the code. To get the latest changes later, go into the `BOUT` directory and run

```
$ git pull
```

For more details on using git to work with BOUT++, see the developer's manual.

2.2 Installing an MPI compiler

To compile and run the examples BOUT++ needs an MPI compiler. If you are installing on a cluster or supercomputer then the MPI C++ compilers will already be installed, and on Cray or IBM machines will probably be called 'CC' and 'xlC' respectively. If you're installing on a smaller server or your own machine then you need to check that you have an MPI compiler by running

```
$ mpicc
```

This should produce an error message along the lines of "no input files", but if you see something like "command not found" then you need to install MPI first. There are several free MPI distributions available, the main ones currently being MPICH2 (`www.mcs.anl.gov/mpi/mpich2`), OpenMPI (`www.open-mpi.org/`), and LAM (`www.lam-mpi.org/`). On Ubuntu or Debian distributions if you have administrator rights then you can install MPICH2 by running

```
$ sudo apt-get install mpich2 libmpich2-dev
```

If this works, and you now have a working `mpicc` command, skip to the next section on installing libraries. If not, and particularly if you don't have administrator rights, you should install MPI in your home directory by compiling it from source. In your home directory, create two subdirectories: One called "install" where we'll put the source code, and one called "local" where we'll install the MPI compiler:

```
$ cd
$ mkdir install
$ mkdir local
```

Download the latest stable version of MPICH2 from `http://www.mcs.anl.gov/research/projects/mpich2/downloads/` and put the file in the "install" subdirectory created above. At the time of writing (June 2012), the file was called `mpich2-1.4.1p1.tar.gz`. Untar the file:

```
$ tar -xzvf mpich2-1.4.1p1.tar.gz
```

which will create a directory containing the source code. 'cd' into this directory and run

```
$ ./configure --prefix=$HOME/local
$ make
$ make install
```

Each of which might take a while. This is the standard way of installing software from source, and will also be used for installing libraries later. The `--prefix=` option specifies where the software should be installed. Since we don't have permission to write in the system directories (e.g. `/usr/bin`), we just use a subdirectory of our home directory. The `configure` command configures the install, finding the libraries and commands it needs. `make` compiles everything using the options found by `configure`. The final `make install` step copies the compiled code into the correct places under `$HOME/local`.

To be able to use the MPI compiler, you need to modify the `PATH` environment variable. To do this, run

```
$ export PATH=$PATH:$HOME/local/bin
```

and add this to the end of your startup file `$HOME/.bashrc`. If you're using CSH rather than BASH, the command is

```
% setenv PATH ${PATH}:${HOME}/local/bin
```

and the startup file is `$HOME/.cshrc`. You should now be able to run `mpicc` and so have a working MPI compiler.

2.3 Installing libraries

After getting an MPI compiler, the next step is to make sure the libraries BOUT++ needs are installed. At minimum BOUT++ needs the FFTW-3 library, and to run any of the examples you'll also need NetCDF-4 (prior to 4.2) or HDF5 installed.

> **NOTE**: There are currently issues with support for NetCDF's new C++ API, which appeared in 4.2. For now use NetCDF 4.1.x

Most large machines (e.g. NERSC Hopper, HECToR, HPC-FF etc.) will have these libraries and many more already installed, but you may need to load a module to use them. To see a list of the available modules, try running

```
modules avail
```

which works on many systems, but not all. See your system's documentation on modules and which ones to load. If you don't know, or modules don't work, you can still install libraries in your home directory by following the instructions below.

If you're installing on your own machine, then install the packages for your distribution. On Ubuntu or Debian, the necessary packages can be installed by running

```
$ sudo apt-get install libfftw3-dev libnetcdf-dev
```

The easiest way to test if the libraries are installed correctly is try configuring BOUT++. In the `BOUT` directory obtained previously, run

```
$ ./configure
```

If this finishes by printing a summary, and paths for IDL, Python, and Octave, then the libraries are set up and you can skip to the next section. If you see a message "`ERROR: FFTW not found. Required by BOUT++`" then you need to install FFTW-3. If you haven't already, create directories "install" and "local" in your home directory:

```
$ cd
$ mkdir install
$ mkdir local
```

Download the latest stable version from `http://www.fftw.org/download.html` into the "install" directory. At the time of writing, this was called `fftw-3.3.2.tar.gz`. Untar this file, and 'cd' into the resulting directory. As with the MPI compiler, configure and install the FFTW library into `$HOME/local` by running:

```
$ ./configure --prefix=$HOME/local
$ make
$ make install
```

Go back to the `BOUT` directory and re-run the configure script. If you used `$HOME/local` as the prefix, BOUT++ configure should find the FFTW library now. If you installed somewhere else, you can specify the directory with the `--with-fftw=` option:

```
$ ./configure --with-fftw=$HOME/local
```

Configure should now find FFTW, and search for the NetCDF library. If configure finishes successfully, then skip to the next section, but if you see a message `NetCDF support disabled` then configure couldn't find the NetCDF library. Unless you have PACT or pnetcdf installed, this will be followed by a message `ERROR: At least one file format must be supported`.

Download the 4.1.3 **bundled**[1] release of NetCDF from `http://www.unidata.ucar.edu/downloads/netcdf/netcdf-4_1_3/` and put the `netcdf-4.1.3.tar.gz` file into your "install" directory. Untar the file and 'cd' into the resulting directory:

```
$ tar -xzvf netcdf-4.1.3.tar.gz
$ cd netcdf-4.1.3
```

As with MPI compilers and FFTW, configure, then make and make install:

```
$ ./configure --prefix=$HOME/local
$ make
$ make install
```

[1] Support for the more recent unbundled versions is coming soon

Sometimes configure can fail, in which case try disabling Fortran and the HDF5 interface:

```
$ ./configure --prefix=$HOME/local --disable-fortran --disable-netcdf-4
$ make
$ make install
```

Download the latest stable release of NetCDF-4 C++ from

Go back to the BOUT directory and run the configure script again, this time specifying both the location of FFTW (if you installed it from source above), and the NetCDF library:

```
$ ./configure --with-fftw=$HOME/local --with-netcdf=$HOME/local
```

which should now finish successfully, printing a summary of the configuration:

```
Configuration summary
  FACETS support: no
  PETSc support: no
  IDA support: no
  CVODE support: no
  NetCDF support: yes
  Parallel-NetCDF support: no
  PDB support: no
  Hypre support: no
  MUMPS support: no
```

If not, see section 3 for some things you can try to resolve common problems.

2.4 Configuring analysis routines

The BOUT++ installation comes with a set of useful routines which can be used to prepare inputs and analyse outputs. Most of this code is in IDL, but an increasing amount is in Python. In particular all the test suite scripts use Python, so to run these you'll need this configured. If you just want to compile BOUT++ then you can skip to the next section, but make a note of what configure printed out.

When the configure script finishes, it prints out the paths you need to get IDL, Python, and Octave analysis routines working. After running the command which looks like

```
$ export IDL_PATH=...
```

check that `idl` can find the analysis routines by running:

```
$ idl
IDL> .r collect
IDL> help, /source
```

You should see the function `COLLECT` in the `BOUT/tools/idllib` directory. If not, something is wrong with your `IDL_PATH` variable. On some machines, modifying `IDL_PATH` causes problems, in which case you can try modifying the path inside IDL by running

```
IDL> !path = !path + ":/path/to/BOUT/tools/idllib"
```

where you should use the full path. You can get this by going to the `tools/idllib` directory and typing '`pwd`'. Once this is done you should be able to use `collect` and other routines.

To use Python, you will need the NumPy and SciPy libraries. On Debian or Ubuntu these can be installed with

```
$ sudo apt-get install python-scipy
```

which should then add all the other dependencies like NumPy. To test if everything is installed, run

```
$ python
>>> import scipy
```

If not, see the SciPy website `http://www.scipy.org` for instructions on installing.

To do this, the path to `tools/pylib` should be added to the `PYTHONPATH` environment variable. Instructions for doing this are printed at the end of the configure script, for example:

```
Make sure that the tools/pylib directory is in your PYTHONPATH
e.g. by adding to your ~/.bashrc file

   export PYTHONPATH=/home/ben/BOUT/tools/pylib/:$PYTHONPATH
```

To test if this command has worked, try running

```
$ python
>>> import boutdata
```

If this doesn't produce any error messages then Python is configured correctly.

2.5 Compiling BOUT++

Once BOUT++ has been configured, you can compile the bulk of the code by going to the `BOUT` directory (same as `configure`) and running

```
$ make
```

(on OS-X, FreeBSD, and AIX this should be `gmake`). This should print something like:

```
----- Compiling BOUT++ -----
CXX      =  mpicxx
CFLAGS   =  -O -DCHECK=2 -DSIGHANDLE \
 -DREVISION=13571f760cec446d907e1bbeb1d7a3b1c6e0212a \
 -DNCDF -DBOUT_HAS_PVODE
CHECKSUM =  ff3fb702b13acc092613cfce3869b875
INCLUDE  =  -I../include
  Compiling  field.cxx
  Compiling  field2d.cxx
```

At the end of this, you should see a file `libbout++.a` in the `lib/` subdirectory of the BOUT++ distribution. If you get an error, please send an error report to a BOUT++ developer such as `mailto:benjamin.dudson@york.ac.uk` containing

- Which machine you're compiling on
- The output from make, including full error message
- The `make.config` file in the BOUT++ root directory

2.6 Running the test suite

In the `examples/` subdirectory there are a set of short test cases which are intended to test portions of the BOUT++ code and catch any bugs which could be introduced. To run the test cases, the Python libraries must first be set up by following the instructions in section 2.4. Go into the `examples` subdirectory and run

```
$ ./test_suite
```

This will go through a set of tests, each on a variety of different processors. **Note:** currently this uses the `mpirun` command to launch the runs, so won't work on machines which use a job submission system like PBS or SGE.

These tests should all pass, but if not please send an error report to `mailto:benjamin.dudson@york.ac.uk` containing

- Which machine you're running on
- The `make.config` file in the BOUT++ root directory
- The run.log.* files in the directory of the test which failed

If the tests pass, congratulations! You have now got a working installation of BOUT++. Unless you want to use some experimental features of BOUT++, skip to section 4 to start running the code.

3 Advanced installation options

This section describes some common issues encountered when configuring and compiling BOUT++, and how to configure optional libraries like SUNDIALS and PETSc.

3.1 File formats

BOUT++ can currently use four different file formats: Portable Data Binary (PDB) which is part of PACT[2], NetCDF-4[3], HDF5[4] and experimental support for Parallel NetCDF. PDB was developed at LLNL, was used in the UEDGE and BOUT codes, and was the original format used by BOUT++. NetCDF is a more widely used format and so has many more tools for viewing and manipulating files. In particular, the NetCDF-4 library can produce files in either NetCDF3 "classic" format, which is backwards-compatible with NetCDF libraries since 1994 (version 2.3), or in the newer NetCDF4 format, which is based on (and compatible with) HDF5. HDF5 is another widely used format. If you have multiple libraries installed then BOUT++ can use them simultaneously, for example reading in grid files in PDB format, but writing output data in NetCDF format.

To enable NetCDF support, you will need to install NetCDF version 4.0.1 or later. Note that although the NetCDF-4 library is used for the C++ interface, by default BOUT++ writes the "classic" format. Because of this, you don't need to install zlib or HDF5 for BOUT++ NetCDF support to work. If you want to output to HDF5 then you need to first install the zlib and HDF5 libraries, and then compile NetCDF with HDF5 support. When NetCDF is installed, a script `nc-config` should be put into somewhere on the path. If this is found then configure should have all the settings it needs. If this isn't found then configure will search for the NetCDF include and library files.

PACT `http://pact.llnl.gov/` is needed for reading and writing Portable Data Binary (PDB) format files. This is mainly for backwards compatibility with BOUT and UEDGE, and NetCDF-4 is recommended. If you need to be able to read or write PDB files, details on installing PACT are given in Appendix B.

3.2 SUNDIALS

The BOUT++ distribution includes a 1998 version of CVODE (then called PVODE) by Scott D. Cohen and Alan C. Hindmarsh, which is the default time integration solver. Whilst no serious bugs have been found in this code (as far as the authors are aware of), several features such as user-supplied preconditioners and constraints cannot be used with this solver.

[2] `http://pact.llnl.gov`

[3] `http://www.unidata.ucar.edu/software/netcdf/`

[4] `https://www.hdfgroup.org/HDF5/`

Currently, BOUT++ also supports the SUNDIALS solvers CVODE, IDA and ARKODE which are available from `https://computation.llnl.gov/casc/sundials/main.html`.

SUNDIALS is only downloadable from the home page, as submitting your name and e-mail is required for the download. As for the date of this typing, SUNDIALS version 2.6.2 is the newest. In order for a smooth install it is recommended to install SUNDIALS from an install directory. The full installation guide is found in the downloaded `.tar.gz`, but we will provide a step-by-step guide to install it and make it comatible with BOUT++ here.

NOTE: It is important to note that if you do configure PETSc with SUNDIALS then BOUT must use/link the same version of SUNDIALS

```
cd ~
mkdir local
cd local
mkdir examples
cd ..
mkdir install
cd install
mkdir sundials-install
cd sundials-install
# Move the downloaded sundials-2.6.2.tar.gz to sundials-install
tar -xzvf sundials-2.6.2.tar.gz
mkdir build
cd build

cmake \
-DCMAKE_INSTALL_PREFIX=$HOME/local \
-DEXAMPLES_INSTALL_PATH=$HOME/local/examples \
-DCMAKE_LINKER=$HOME/local/lib \
-DLAPACK_ENABLE=ON \
-DOPENMP_ENABLE=ON \
-DMPI_ENABLE=ON \
../sundials-2.6.2

make
make install
```

The SUNDIALS IDA solver is a Differential-Algebraic Equation (DAE) solver, which evolves a system of the form $\mathbf{f}(\mathbf{u}, \dot{\mathbf{u}}, t) = 0$. This allows algebraic constraints on variables to be specified.

To configure BOUT++ with SUNDIALS only (see section 3.3 on how to build PETSc with SUNDIALS), go to the root directory of BOUT++ and type

```
./configure --with-sundials
```

SUNDIALS will allow you to select at run-time which solver to use. See section 9.1 for more details on how to do this.

3.3 PETSc

BOUT++ can use PETSc `http://www.mcs.anl.gov/petsc/` for time-integration and for solving elliptic problems, such as inverting Poisson and Helmholtz equations.

Currently, BOUT++ supports PETSc version 3.1, 3.2, 3.3 and 3.4 (support for newer versions are planned for the future). To install PETSc version 3.4.5, use the following steps

```
cd ~
wget http://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-3.4.5.tar.gz
tar -xzvf petsc-3.4.5.tar.gz
# Optional
# rm petsc-3.4.5.tar.gz
cd petsc-3.4.5
```

To build PETSc without SUNDIALS, configure with

```
./configure \
--with-clanguage=cxx \
--with-mpi=yes \
--with-precision=double \
--with-scalar-type=real \
--with-shared-libraries=0
```

Add `--with-debugging=yes` to `./configure` in order to allow debugging.

To build PETSc with SUNDIALS, install SUNDIALS as explained in section 3.2, and append `./configure` with `--with-sundials-dir=$HOME/local`

> **NOTE**: It is important to note that if you do configure PETSc with SUNDIALS then BOUT must use/link the same version of SUNDIALS

It is also possible to get PETSc to download and install MUMPS (see section 3.5), by adding

```
--download-mumps \
--download-scalapack \
--download-blacs \
--download-f-blas-lapack=1 \
--download-parmetis \
--download-ptscotch \
--download-metis
```

to `./configure` To make PETSc, type

```
make PETSC_DIR=$HOME/petsc-3.4.5 PETSC_ARCH=arch-linux2-cxx-debug all
```

Should blas, lapack or any other packages be missing, you will get an error, and a suggestion that you can append `--download-name-of-package` to the `./configure` line. You may want to test that everything is configured properly. To do this, type

```
make PETSC_DIR=$HOME/petsc-3.4.5 PETSC_ARCH=arch-linux2-cxx-debug test
```

To configure BOUT++ with PETSc, go to the BOUT++ root directory, and type

```
./configure --with-petsc=$HOME/petsc-3.4.5
```

To configure BOUT++ with PETSc and sundials, type instead

```
./configure --with-petsc=$HOME/petsc-3.4.5 --with-sundials
```

Finally compile PETSc:

```
make
```

To use PETSc, you have to define the variable `PETSC_DIR` to point to the petsc directory, type

```
export PETSC_DIR=$HOME/petsc-3.4.5
```

and add to your startup file `$HOME/.bashrc`

```
export PETSC_DIR=$HOME/petsc-3.4.5
```

3.4 LAPACK

BOUT++ comes with linear solvers for tridiagonal and band-diagonal systems, but these are not particularly optimised and are in any case descended from Numerical Recipes code (hence NOT covered by LGPL license).

To replace these routines, BOUT++ can use the LAPACK library. This is however written in FORTRAN 77, which can cause linking headaches. To enable these routines use

```
./configure --with-lapack
```

and to specify a non-standard path

```
./configure --with-lapack=/path/to/lapack
```

3.5 MUMPS

This is still experimental, but does work on at least some systems at York. The PETSc library can be used to call MUMPS for directly solving matrices (e.g. for Laplacian inversions), or MUMPS can be used directly. To enable MUMPS, configure with

```
./configure --with-mumps
```

MUMPS has many dependencies, including ScaLapack and ParMetis, which the configuration script assumes are in the same place as MUMPS. The easiest way to get MUMPS installed is to install PETSc with MUMPS, as the configuration script will check the PETSc directory.

3.6 MPI compilers

These are usually called something like mpicc and mpiCC (or mpicxx), and the configure script will look for several common names. If your compilers aren't recognised then set them using

```
$ ./configure MPICC=<your C compiler> MPICXX=<your C++ compiler>
```

NOTES:

- On LLNL's Grendel, mpicxx is broken. Use mpiCC instead by passing "MPICXX=mpiCC" to configure. Also need to specify this to NetCDF library by passing "CXX=mpiCC" to NetCDF configure.

3.7 Issues

3.7.1 Wrong install script

Before installing, make sure the correct version of `install` is being used by running

```
~/ $ which install
```

This should point to a system directory like `/usr/bin/install`. Sometimes when IDL has been installed, this points to the IDL install (e.g. something like `/usr/common/usg/idl/idl70/bin/instal` on Franklin). A quick way to fix this is to create a link from your local bin to the system install:

```
~/ $ ln -s /usr/bin/install $HOME/local/bin/
```

"which install" should now print the install in your local bin directory.

3.7.2 Compiling cvode.cxx fails

Occasionally compiling the CVODE solver interface will fail with an error similar to:

```
cvode.cxx: In member function ‘virtual int CvodeSolver::init(rhsfunc, bool, int, BoutR..
cvode.cxx:234:56: error: invalid conversion from ‘int (*)(CVINT...
...
```

This is caused by different sizes of ints used in different versions of the CVODE library. The configure script tries to determine the correct type to use, but may fail in unusual circumstances. To fix, edit **src/solver/impls/cvode/cvode.cxx**, and change line 48 from

```
typedef int CVODEINT;
```

to

```
typedef long CVODEINT;
```

4 Running BOUT++

The `examples/` directory contains some test cases for a variety of fluid models. The ones starting **test-** are short tests, which often just run a part of the code rather than a complete simulation. The simplest example to start with is **examples/conduction/**. This solves a single equation for a 3D scalar field T:

$$\frac{\partial T}{\partial t} = \nabla_{||}\left(\chi \partial_{||} T\right) \tag{1}$$

There are several files involved:

- **conduction.cxx** contains the source code which specifies the equation to solve
- **conduct_grid.nc** is the grid file, which in this case just specifies the number of grid points in X and Y (`nx` & `ny`) with everything else being left as the default (e.g. grid spacings dx and dy are 1, the metric tensor is the identity matrix). For details of the grid file format, see section 11.
- **generate.py** is a Python script to create the grid file. In this case it just writes nx and ny
- **data/BOUT.inp** is the settings file, specifying how many output timesteps to take, differencing schemes to use, and many other things. In this case it's mostly empty so the defaults are used.

First you need to compile the example:

```
$ gmake
```

which should print out something along the lines of

```
Compiling  conduction.cxx
Linking conduction
```

If you get an error, most likely during the linking stage, you may need to go back and make sure the libraries are all set up correctly. A common problem is mixing MPI implementations, for example compiling NetCDF using Open MPI and then BOUT++ with MPICH2. Unfortunately the solution is to recompile everything with the same compiler.

Then try running the example. If you're running on a standalone server, desktop or laptop then try:

```
$ mpirun -np 2 ./conduction
```

If you're running on a cluster or supercomputer, you should find out how to submit jobs. This varies, but usually on these bigger machines there will be a queueing system and you'll need to use `qsub`, `msub`, `llsubmit` or similar to submit jobs.

When the example runs, it should print a lot of output. This is recording all the settings being used by the code, and is also written to log files for future reference. The test should take a few seconds to run, and produce a bunch of files in the **data/** subdirectory.

- **BOUT.log.*** contains a log from each process, so because we ran with "-np 2" there should be 2 logs. The one from processor 0 will be the same as what was printed to the screen. This is mainly useful because if one process crashes it may only put an error message into its own log.
- **BOUT.restart.*.nc** are the restart files for the last time point. Currently each processor saves its own state in a separate file, but there is experimental support for parallel I/O. For the settings, see section 6.3.
- **BOUT.dmp.*.nc** contain the output data, including time history. As with the restart files, each processor currently outputs a separate file.

Restart files allow the run to be restarted from where they left off:

```
$ mpirun -np 2 ./conduction restart
```

This will delete the output data **BOUT.dmp.*.nc** files, and start again. If you want to keep the output from the first run, add "append"

```
$ mpirun -np 2 ./conduction restart append
```

which will then append any new outputs to the end of the old data files. For more information on restarting, see section 4.4.

To analyse the output of the simulation, cd into the **data** subdirectory and start IDL. If you don't have IDL, don't panic as all this is also possible in Python and discussed in section 5.5. First, list the variables in one of the data files:

```
IDL> print, file_list("BOUT.dmp.0.nc")
iteration MXSUB MYSUB MXG MYG MZ NXPE NYPE BOUT_VERSION t_array ZMAX ZMIN T
```

All of these except 'T' are in all output files, and they contain information about the layout of the mesh so that the data can be put in the correct place. The most useful variable is 't_array' which is a 1D array of simulation output times. To read this, we can use the `collect` function:

```
IDL> time = collect(var="t_array")
IDL> print, time
      1.10000      1.20000      1.30000      1.40000      1.50000 ...
```

The number of variables in an output file depends on the model being solved, which in this case consists of a single scalar field 'T'. To read this into IDL, again use `collect`:

```
IDL> T = collect(var="T")
IDL> help, T
T               FLOAT     = Array[5, 64, 1, 20]
```

This is a 4D variable, arranged as `[x, y, z, t]`. The x direction has 5 points, consisting of 2 points either side for the boundaries and one point in the middle which is evolving. This case is only solving a 1D problem in y with 64 points so to display an animation of this

```
IDL> showdata, T[2,*,0,*]
```

which selects the only evolving x point, all y, the only z point, and all time points. If given 3D variables, showdata will display an animated surface

```
IDL> showdata, T[*,*,0,*]
```

and to make this a coloured contour plot

```
IDL> showdata, T[*,*,0,*], /cont
```

The equivalent commands in Python are as follows. To print a list of variables in a file:

```
>>> from boututils.datafile import DataFile
>>> DataFile("BOUT.dmp.0.nc").list()
```

To collect a variable,

```
>>> from boutdata.collect import collect
>>> T = collect("T")
>>> T.shape
```

Note that the order of the indices is different in Python and IDL: In Python, 4D variables are arranged as `[t, x, y, z]`. To show an animation

```
>>> from boututils.showdata import showdata
>>> showdata(T[:,:,:,0])
```

The next example to look at is **test-wave**, which is solving a wave equation using

$$\frac{\partial f}{\partial t} = \partial_{||} g \qquad \frac{\partial g}{\partial t} = \partial_{||} f \tag{2}$$

using two different methods. Other examples contain two scripts: One for running the example and then an IDL script to plot the results:

```
./runcase.sh
idl runidl.pro
```

Assuming these examples work (which they should), looking through the scripts and code may give you an idea of how BOUT++ works. More information on setting up and running BOUT++ is given in section 4, and details of analysing the results using IDL are given in section 5.

Alternatively, one can run BOUT++ with the python wrapper `bout_runners` , as explained in section F.3. Examples of using `bout_runners` can be found in **examples/bout_runners_examp**

4.1 When things go wrong

BOUT++ is still under development, and so occasionally you may be lucky enough to discover a new bug. This is particularly likely if you're modifying the physics module source code (see section 12) when you need a way to debug your code too.

- Check the end of each processor's log file (tail data/BOUT.log.*). When BOUT++ exits before it should, what is printed to screen is just the output from processor 0. If an error occurred on another processor then the error message will be written to it's log file instead.

- By default when an error occurs a kind of stack trace is printed which shows which functions were being run (most recent first). This should give a good indication of where an error occurred. If this stack isn't printed, make sure checking is set to level 2 or higher (`./configure --with-checks=2`)
- If the error is a segmentation fault, you can try a debugger such as totalview
- If the error is due to non-finite numbers, increase the checking level (`./configure --with-checks=3`) to perform more checking of values and (hopefully) find an error as soon as possible after it occurs.

4.2 Startup output

When BOUT++ is run, it produces a lot of output initially, mainly listing the options which have been used so you can check that it's doing what you think it should be. It's generally a good idea to scan over this see if there are any important warnings or errors. Each processor outputs its own log file `BOUT.log.#` and the log from processor 0 is also sent to the screen. This output may look a little different if it's out of date, but the general layout will probably be the same.

First comes the introductory blurb:

```
BOUT++ version 1.0
Revision: c8794400adc256480f72c651dcf186fb6ea1da49
MD5 checksum: 8419adb752f9c23b90eb50ea2261963c
Code compiled on May 11 2011 at 18:22:37

B.Dudson (University of York), M.Umansky (LLNL) 2007
Based on BOUT by Xueqiao Xu, 1999
```

The version number (1.0 here) gets increased occasionally after some major feature has been added. To help match simulations to code versions, the Git revision of the core BOUT++ code and the date and time it was compiled is recorded. Because code could be modified from the revision, an MD5 checksum of all the code is also calculated. This information makes it possible to verify precisely which version of the code was used for any given run.

Next comes the compile-time options, which depend on how BOUT++ was configured (see section 2.5)

```
Compile-time options:
        Checking enabled, level 2
        Signal handling enabled
        PDB support disabled
        netCDF support enabled
```

Thins says that some run-time checking of values is enabled, that the code will try to catch segmentation faults to print a useful error, that PDB files aren't supported, but that NetCDF files are.

The processor number comes next:

```
Processor number: 0 of 1
```

This will always be processor number '0' on screen as only the output from processor '0' is sent to the terminal. After this the core BOUT++ code reads some options:

```
Option /nout = 50 (data/BOUT.inp)
Option /timestep = 100 (data/BOUT.inp)
Option /grid = slab.6b5.r1.cdl (data/BOUT.inp)
Option /dump_float = true   (default)
Option /non_uniform = false (data/BOUT.inp)
Option /restart = false  (default)
Option /append = false  (default)
Option /dump_format = nc (data/BOUT.inp)
Option /StaggerGrids = false  (default)
```

This lists each option and the value it has been assigned. For every option the source of the value being used is also given. If a value had been given on the command line then `(command line)` would appear after the option.

```
Setting X differencing methods
        First       :  Second order central (C2)
        Second      :  Second order central (C2)
        Upwind      :  Third order WENO (W3)
        Flux        :  Split into upwind and central (SPLIT)
Setting Y differencing methods
        First       :  Fourth order central (C4)
        Second      :  Fourth order central (C4)
        Upwind      :  Third order WENO (W3)
        Flux        :  Split into upwind and central (SPLIT)
Setting Z differencing methods
        First       :  FFT (FFT)
        Second      :  FFT (FFT)
        Upwind      :  Third order WENO (W3)
        Flux        :  Split into upwind and central (SPLIT)
```

This is a list of the differential methods for each direction. These are set in the BOUT.inp file (`[ddx]`, `[ddy]` and `[ddz]` sections), but can be overridden for individual operators. For

each direction, numerical methods can be specified for first and second central difference terms, upwinding terms of the form $\frac{\partial f}{\partial t} = \boldsymbol{v} \cdot \nabla f$, and flux terms of the form $\frac{\partial f}{\partial t} = \nabla \cdot (\boldsymbol{v} f)$. By default the flux terms are just split into a central and an upwinding term.

In brackets are the code used to specify the method in BOUT.inp. A list of available methods is given in section 15.1 on page 109.

```
Setting grid format
        Option /grid_format =  (default)
        Using NetCDF format for file 'slab.6b5.r1.cdl'
Loading mesh
        Grid size: 10 by 64
        Option /mxg = 2 (data/BOUT.inp)
        Option /myg = 2 (data/BOUT.inp)
        Option /NXPE = 1 (default)
        Option /mz = 65 (data/BOUT.inp)
        Option /twistshift = false (data/BOUT.inp)
        Option /TwistOrder = 0 (default)
        Option /ShiftOrder = 0 (default)
        Option /shiftxderivs = false (data/BOUT.inp)
        Option /IncIntShear = false  (default)
        Option /BoundaryOnCell = false  (default)
        Option /StaggerGrids = false  (default)
        Option /periodicX = false  (default)
        Option /async_send = false  (default)
        Option /zmin = 0 (data/BOUT.inp)
        Option /zmax = 0.0028505 (data/BOUT.inp)

WARNING: Number of inner y points 'ny_inner' not found. Setting to 32
```

Optional quantities (such as `ny_inner` in this case) which are not specified are given a default (best-guess) value, and a warning is printed.

```
        EQUILIBRIUM IS SINGLE NULL (SND)
        MYPE_IN_CORE = 0
        DXS = 0, DIN = -1. DOUT = -1
        UXS = 0, UIN = -1. UOUT = -1
        XIN = -1, XOUT = -1
        Twist-shift:
```

At this point, BOUT++ reads the grid file, and works out the topology of the grid, and connections between processors. BOUT++ then tries to read the metric coefficients from the grid file:

```
        WARNING: Could not read 'g11' from grid. Setting to 1.000000e+00
        WARNING: Could not read 'g22' from grid. Setting to 1.000000e+00
        WARNING: Could not read 'g33' from grid. Setting to 1.000000e+00
        WARNING: Could not read 'g12' from grid. Setting to 0.000000e+00
        WARNING: Could not read 'g13' from grid. Setting to 0.000000e+00
        WARNING: Could not read 'g23' from grid. Setting to 0.000000e+00
```

These warnings are printed because the coefficients have not been specified in the grid file, and so the metric tensor is set to the default identity matrix.

```
        WARNING: Could not read 'zShift' from grid. Setting to 0.000000e+00
        WARNING: Z shift for radial derivatives not found
```

To get radial derivatives, the quasi-ballooning coordinate method is used . The upshot of this is that to get radial derivatives, interpolation in Z is needed. This should also always be set to FFT.

```
        WARNING: Twist-shift angle 'ShiftAngle' not found. Setting from zShift
        Option /twistshift_pf = false  (default)

        Maximum error in diagonal inversion is 0.000000e+00
        Maximum error in off-diagonal inversion is 0.000000e+00
```

If only the contravariant components (`g11` etc.) of the metric tensor are specified, the covariant components (`g_11` etc.) are calculated by inverting the metric tensor matrix. Error estimates are then calculated by calculating $g_{ij}g^{jk}$ as a check. Since no metrics were specified in the input, the metric tensor was set to the identity matrix, making inversion easy and the error tiny.

```
        WARNING: Could not read 'J' from grid. Setting to 0.000000e+00
        WARNING: Jacobian 'J' not found. Calculating from metric tensor

        Maximum difference in Bxy is 1.444077e-02
Calculating differential geometry terms
        Communicating connection terms
Boundary regions in this processor: core, sol, target, target,
        done

Setting file formats
        Using NetCDF format for file 'data/BOUT.dmp.0.nc'
```

The laplacian inversion code is initialised, and prints out the options used.

```
Initialising Laplacian inversion routines
        Option comms/async = true   (default)
        Option laplace/filter = 0.2 (default)
        Option laplace/low_mem = false  (default)
        Option laplace/use_pdd = false  (default)
        Option laplace/all_terms = false  (default)
        Option laplace/laplace_nonuniform = false  (default)
        Using serial algorithm
        Option laplace/max_mode = 26 (default)
```

After this comes the physics module-specific output:

```
Initialising physics module
        Option solver/type =  (default)
        .
        .
        .
```

This typically lists the options used, and useful/important normalisation factors etc.

Finally, once the physics module has been initialised, and the current values loaded, the solver can be started

```
Initialising solver
        Option /archive = -1 (default)
        Option /dump_format = nc (data/BOUT.inp)
        Option /restart_format = nc (default)
        Using NetCDF format for file 'nc'

Initialising PVODE solver
        Boundary region inner X
        Boundary region outer X
        3d fields = 2, 2d fields = 0 neq=84992, local_N=84992
```

This last line gives the number of equations being evolved (in this case 84992), and the number of these on this processor (here 84992).

```
        Option solver/mudq = 16 (default)
        Option solver/mldq = 16 (default)
        Option solver/mukeep = 0 (default)
        Option solver/mlkeep = 0 (default)
```

The absolute and relative tolerances come next:

```
        Option solver/atol = 1e-10 (data/BOUT.inp)
        Option solver/rtol = 1e-05 (data/BOUT.inp)

        Option solver/use_precon = false  (default)
        Option solver/precon_dimens = 50 (default)
        Option solver/precon_tol = 0.0001 (default)
        Option solver/mxstep = 500 (default)

        Option fft/fft_measure = false  (default)
```

This next option specifies the maximum number of internal timesteps which CVODE will take between outputs.

```
        Option fft/fft_measure = false  (default)
Running simulation

Run started at  : Wed May 11 18:23:20 2011

        Option /wall_limit = -1 (default)
```

4.3 Per-timestep output

At the beginning of a run, just after the last line in the previous section, a header is printed out as a guide

```
Sim Time  |  RHS evals  | Wall Time |  Calc    Inv   Comm    I/O   SOLVER
```

Each timestep (the one specified in BOUT.inp, not the internal timestep), BOUT++ prints out something like

```
1.001e+02         76       2.27e+02    87.1    5.3    1.0    0.0    6.6
```

This gives the simulation time; the number of times the time-derivatives (RHS) were evaluated; the wall-time this took to run, and percentages for the time spent in different parts of the code.

- `Calc` is the time spent doing calculations such as multiplications, derivatives etc
- `Inv` is the time spent in inversion code (i.e. inverting Laplacians), including any communication which may be needed to do the inversion.
- `Comm` is the time spent communicating variables (outside the inversion routine)

- `I/O` is the time spent writing dump and restart files to disk. Most of the time this should not be an issue
- `SOLVER` is the time spent in the implicit solver code.

The output sent to the terminal (not the log files) also includes a run time, and estimated remaining time.

4.4 Restarting runs

Every output timestep, BOUT++ writes a set of files named "BOUT.restart.#.nc" where '#' is the processor number (for parallel output, a single file "BOUT.restart.nc" is used). To restart from where the previous run finished, just add the keyword **restart** to the end of the command, for example:

```
$ mpirun -np 2 ./conduction restart
```

Equivalently, put "restart=true" near the top of the BOUT.inp input file. Note that this will overwrite the existing data in the "BOUT.dmp.*.nc" files. If you want to append to them instead then add the keyword append to the command, for example:

```
$ mpirun -np 2 ./conduction restart append
```

or also put "append=true" near the top of the BOUT.inp input file.

When restarting simulations BOUT++ will by default output the initial state, unless appending to existing data files when it will not output until the first timestep is completed. To override this behaviour, you can specify the option dump_on_restart manully. If dump_on_restart is true then the initial state will always be written out, if false then it never will be (regardless of the values of restart and append).

If you need to restart from a different point in your simulation, or the BOUT.restart files become corrupted, you can either use archived restart files, or create new restart files. Archived restart files have names like "BOUT.restart_0020.#.nc", and are written every 20 outputs by default. To change this, set "archive" in the BOUT.inp file. To use these files, they must be renamed to "BOUT.restart.#.nc". A useful tool to do this is "rename":

```
$ rename 's/_0020//' *.nc
```

will strip out "_0020" from any file names ending in ".nc".

If you don't have archived restarts, or want to start from a different time-point, there are Python routines for creating new restart files. If your PYTHONPATH environment variable is set up (see section 2.4) then you can use the `boutdata.restart.create` function in **tools/pylib/boutdata/restart.py**:

```
>>> from boutdata.restart import create
>>> create(final=10, path='data', output='.')
```

The above will take time point 10 from the BOUT.dmp.* files in the "data" directory. For each one, it will output a BOUT.restart file in the output directory ".".

4.5 Makefiles in BOUT++

BOUT++ has its own makefile system. These can be used to

1. Writing an example or executable (see section 4.5.1)
2. Adding a feature to BOUT++ (see section 4.5.2)

In all makefiles, `BOUT_TOP` is required!

4.5.1 Executables example

If writing an example (or physics module that executes) then the makefile is very simple:

```
BOUT_TOP        = ../..

SOURCEC         = <filename>.cpp

include $(BOUT_TOP)/make.config
```

where `BOUT_TOP` - refers to the relative (or absolute) location of the BOUT directory (the one that includes `/lib` and `/src`) and `SOURCEC` is the name of your file, e.g. `gas_compress.cxx`.

Optionally, it is possible to specify `TARGET` which defines what the executable should be called (e.g. if you have multiple source files). That's it!

4.5.2 Modules example

If you are writing a new module (or concrete implementation), then it is again pretty simple

```
BOUT_TOP = ../..

SOURCEC         = communicator.cpp difops.cpp geometry.cpp grid.cpp
interpolation.cpp topology.cpp
SOURCEH         = $(SOURCEC:%.cpp=%.h)
INCLUDE         = -I../sys -I../field -I../fileio -I../invert
TARGET          = lib

include $(BOUT_TOP)/make.config
```

`TARGET` - must be `lib` to signify you are adding to `libbout++.a`.

The other variables should be pretty self explanatory.

4.5.3 Adding a new subdirectory to 'src'

No worries, just make sure to edit `src/makefile` to add it to the `DIRS` variable.

4.6 BOUT.inp settings

WARNING: THE FOLLOWING LIST IS OUT OF DATE AND SHOULD NOT BE FOLLOWED

```
# This file lists all BOUT++ settings (with default values)
#
# File is divided into sections which can be in any order.
# Comments start with either a ';' or a '#'

NOUT = 1            # Number of outputs
TIMESTEP = 1.0      # Time between outputs
WALL_LIMIT = -1.0   # Wall clock limit in hours. -ve means no limit
archive = -1        # Number of outputs between restart archiving
                    # -ve means no archiving

grid = "data/bout.grd.pdb" # Grid file to use

ShiftXderivs = false    # Use shifted X derivatives
IncIntShear = false     #
ShiftInitial = ShiftXderivs # Shift the initial condition
TwistShift = false      # Use Twist-Shift condition?
ShiftOrder = 0          # X shift order (1,4 or 0 = FFT)
TwistOrder = 0          # Twist-shift order (1,4 or 0 = FFT)

non_uniform = false     # Use corrections for non-uniform meshes

MZ = 65                 # Number of points in Z (2^n + 1)
zperiod = 1             # How many periods in 2pi
                        # NOTE: Instead of zperiod, ZMIN and ZMAX
                        # can be specified in units of 2pi

MXG = 2                 # # of X guard cells (change with care!)
MYG = 2                 # # of Y guard cells (change with care!)
```

```
BoundaryOnCell = false # Location of boundary

StaggerGrids = false   # Use staggered grids

NXPE = 1               # Number of processors in X

dump_float = true      # Output floats to dump file
                       # (false -> doubles)

dump_format = "pdb"    # Data format for the dump files.
                       # for NetCDF, set to "cdl", "nc" or "ncdf"
restart_format = dump_format  # Format for restart files

[comms]

async = true           # Use asyncronous sends
group_nonblock = true  # Use non-blocking group communications

[fft]

fft_measure = true     # If using FFTW, perform tests to determine
                       # fastest method

[solver]

# NOTE: Some of these options only apply to some solvers

mudq = n3d*(MXSUB+2)
mldq = n3d*(MXSUB+2)
mukeep = 0
mlkeep = 0
ATOL = 1.0e-12
RTOL = 1.0e-5

use_precon = false   # If the physics solver specifies a ↩
   preconditioner
                     # then use that, otherwise BBD is used

use_jacobian = false # If the physics solver specifies a Jacobian
                     # then use that. Otherwise a difference quotient
                     # method is used internally
```

```
precon_dimens = 50   # For BBD preconditioner
precon_tol = 1.0e-4  # For BBD

adams_moulton = false # Use Adams-Moulton method (default is BDF)
func_iter = false     # Functional iteration (default is Newton)

[laplace]

filter = 0.2    # Fraction of toroidal modes to filter out
low_mem = false # For parallel algorithm, use less memory
                # This is at the expense of communication overlap

use_pdd = false # Use the approximate Parallel Diagonally Dominant ↩
   solver

all_terms = false # Include all the extra terms in Delp2 and ↩
   inversion

[ddx]

first = C4
second = C4
upwind = W3

[ddy]

first = C4
second = C4
upwind = W3

[ddz]

first = C4
second = C4
upwind = W3
```

5 Output and post-processing

The majority of the existing analysis and post-processing code is written in IDL. The directory `idllib` contains many useful routines for reading PDB files and analysing data. A summary of available IDL routines is given in Appendix E.

Post-processing using Python is also possible, and there are some modules in the `pylib` directory, and a list of routines in Appendix F. This is a more recent addition, and so is not yet as developed as the IDL support.

5.1 Note on reading PDB files

You should never need to use PDB files with BOUT++, as all input and output routines have now been changed to use NetCDF. For backwards compatibility with BOUT, PDB files can still be used if needed. IDL comes with routines to manipulate NetCDF files, but to read PDB files you will need the PDB2IDL library supplied with BOUT++:

```
cd PDB2IDL
make
```

To use the `PDB2IDL` library and IDL analysis codes, set the following environment variables

```
IDL_PATH=$IDL_PATH:<bout>/idllib/
LD_LIBRARY_PATH=$LD_LIBRARY_PATH:<bout>/lib/
```

Before any of the PDB2IDL functions can be used, you first need to run

```
IDL> .r pdb2idl
```

This can be added to your IDL startup file (which is specified by the `IDL_STARTUP` environment variable).

5.2 Reading BOUT++ output into IDL

There are several routines provided for reading data from BOUT++ output into IDL. In the directory containing the BOUT++ output files (usually `data/`), you can list the variables available using

```
IDL> print, file_list("BOUT.dmp.0.nc")
Ajpar Apar BOUT_VERSION MXG MXSUB MYG MYSUB MZ NXPE NYPE Ni Ni0 Ni_x Te0 Te_x
Ti0 Ti_x ZMAX ZMIN iteration jpar phi rho rho_s t_array wci
```

The `file_list` procedure just returns an array, listing all the variables in a given file. This method (and all the file_ methods) works for both NetCDF and PDB files.

One thing new users can find confusing is that different simulations may have very different outputs. This is because **BOUT++ is not a single physics model**: the variables evolved and written to file are determined by the model, and will be very different between (for example) full MHD and reduced Braginskii models. There are however some variables which all BOUT++ output files contain:

- `BOUT_VERSION`, which gives the version number of BOUT++ which produced the file. This is mainly to help output processing codes handle changes to the output file format. For example, BOUT++ version 0.30 introduced 2D domain decomposition which needs to be handled when collecting data.
- `MXG`,`MYG`. These are the sizes of the X and Y guard cells
- `MXSUB`, the number of X grid points in each processor. This does not include the guard cells, so the total X size of each field will be `MXSUB + 2*MXG`.
- `MYSUB`, the number of Y grid points per processor (like MXSUB)
- `MZ`, the number of Z points
- `NXPE, NYPE`, the number of processors in the X and Y directions. `NXPE * MXSUB + 2*MXG= NX`, `NYPE * MYSUB = NY`
- `ZMIN`, `ZMAX`, the range of Z in fractions of 2π.
- `iteration`, the last timestep in the file
- `t_array`, an array of times

Most of these - particularly those concerned with grid size and processor layout - are used by post-processing routines such as `collect`, and are seldom needed directly. To read a single variable from a file, there is the `file_read` function:

```
IDL> wci = file_read("BOUT.dmp.0.nc", "wci")
IDL> print, wci
  9.58000e+06
```

NOTE: The `file_read` command (and NetCDF/PDB access generally) is case-sensitive: variable `Wci` is different to `wci`

To read in all the variables in a file into a structure, use the `file_import` function:

```
IDL> d = file_import("BOUT.dmp.0.nc")
IDL> print, d.wci
  9.58000e+06
```

This is often used to read in the entire grid file at once. Doing this for output data files can take a long time and use a lot of memory.

Reading from individual files is fine for scalar quantities and time arrays, but reading arrays which are spread across processors (i.e. evolving variables) is tedious to do manually. Instead, there is the `collect` function to automate this:

```
IDL> ni = collect(var="ni")
Variable 'ni' not found
-> Variables are case-sensitive: Using 'Ni'
Reading from .//BOUT.dmp.0.nc: [0-35][2-6] -> [0-35][0-4]
```

This function takes care of the case, so that reading "ni" is automatically corrected to "Ni". The result is a 4D variable:

```
IDL> help, ni
NI              FLOAT     = Array[36, 5, 64, 400]
```

with the indices `[X, Y, Z, T]`. Note that in the output files, these variables are stored in `[T, X, Y, Z]` format instead but this is changed by `collect`. Sometimes you don't want to read in the entire array (which may be very large). To read in only a subset, there are several optional keywords with `[min,max]` ranges:

```
IDL> ni = collect(var="Ni", xind=[10,20], yind=[2,2], zind=[0,31],
tind=[300,399])
Reading from .//BOUT.dmp.0.nc: [10-20][4-4] -> [10-20][2-2]
IDL> help, ni
NI              FLOAT     = Array[11, 1, 32, 100]
```

5.3 Summary of IDL file routines

Functions file_* can read/write either PDB or NetCDF files, depending on the file extension. Hence same analysis / pre-processing codes can use PDB and/or NetCDF files. Any file ending ".nc", ".cdl", ".cdf" is assumed to be NetCDF, otherwise PDB.

Open a PDB or NetCDF file:

```
handle = file_open("filename", /write, /create)
```

Array of variable names:

```
list = file_list(handle)
list = file_list("filename")
```

Number of dimensions:

```
nd = file_ndims(handle, "variable")
nd = file_ndims("filename", "variable")
```

Read a variable from file. Inds = [xmin, xmax, ymin, ymax, ...]

```
data = file_read(handle, "variable", inds=inds)
data = file_read("filename", "variable", inds=inds)
```

Write a variable to file. For NetCDF it tries to match up dimensions, and defines new dimensions when needed

```
status = file_write(handle, "variable", data)
```

Close a file after use

```
file_close, handle
```

To read in all the data in a file into a structure:

```
data = file_import("filename")
```

and to write a structure to file:

```
status = file_export("filename", data)
```

Converting file types can now be done using

```
d = file_import("somefile.pdb")
s = file_export("somefile.nc", d)
```

Note that this will mess up the case of the variable names, and names may be changed to become valid IDL variable names. To convert PDB files to NetCDF there is also a code **pdb2cdf** in **BOUT/tools/archiving/pdb2cdf**.

5.4 IDL analysis routines

Now that the BOUT++ results have been read into IDL, all the usual analysis and plotting routines can be used. In addition, there are many useful routines included in the `idllib` subdirectory. There is a `README` file which describes what each of these routines, but some of the most useful ones are listed here. All these examples assume there is a variable `P` which has been read into IDL as a 4D [x,y,z,t] variable:

- `fft_deriv` and `fft_integrate` which differentiate and integrate periodic functions.
- `get_integer`, `get_float`, and `get_yesno` request integers, floats and a yes/no answer from the user respectively.
- `showdata` animates 1 or 2-dimensional variables. Useful for quickly displaying results in different ways. This is useful for taking a quick look at the data, but can also produce bitmap outputs for turning into a movie for presentation. To show an animated surface plot at a particular poloidal location (32 here):

```
IDL> showdata, p[*,32,*,*]
```

To turn this into a contour plot,

```
IDL> showdata, p[*,32,*,*], /cont
```

To show a slice through this at a particular toroidal location (0 here):

```
IDL> showdata, p[*,32,0,*]
```

There are a few other options, and ways to show data using this code; see the README file, or comments in `showdata.pro`. Instead of plotting to screen, showdata can produce a series of numbered bitmap images by using the `bmp` option

```
IDL> showdata, p[*,32,*,*], /cont, bmp="result_"
```

which will produce images called `result_0000.bmp`, `result_0001.bmp` and so on. Note that the plotting should not be obscured or minimised, since this works by plotting to screen, then grabbing an image of the resulting plot.

- `moment_xyzt` takes a 4D variable (such as those from `collect`), and calculates RMS, DC and AC components in the Z direction.
- `safe_colors` A general routine for IDL which arranges the color table so that colors are numbered 1 (black), 2 (red), 3 (green), 4 (blue). Useful for plotting, and used by many other routines in this library.

There are many other useful routines in the `idllib` directory. See the `idllib/README` file for a short description of each one.

5.5 Python routines

There are several modules available for reading NetCDF files, so to provide a consistent interface, file access is wrapped into a class DataFile. This provides a simple interface for reading and writing files from any of the following modules: `netCDF4`; `Scientific.IO.NetCDF`; and `scipy.io.netcdf`. The DataFile class also provides allows access to HDF5 files through the same interface, using the h5py module. To open a file using DataFile:

```
from boututils.datafile import DataFile

f = DataFile("file.nc")  # Open the file
var = f.read("variable") # Read a variable from the file
f.close()                # Close the file
```

or similarly for an HDF5 file

```
from boututils.datafile import DataFile

f = DataFile("file.hdf5")  # Open the file
var = f.read("variable")   # Read a variable from the file
f.close()                  # Close the file
```

To list the variables in a file e.g.

```
>>> f = DataFile("test_io.grd.nc")
>>> print f.list()
['f3d', 'f2d', 'nx', 'ny', 'rvar', 'ivar']
```

and to list the names of the dimensions

```
>>> print d.dimensions("f3d")
('x', 'y', 'z')
```

or to get the sizes of the dimensions

```
>>> print d.size("f3d")
[12, 12, 5]
```

To read in all variables in a file into a dictionary there is the `file_import` function

```
1 from boututils.file_import import file_import
2
3 grid = file_import("grid.nc")
```

As for IDL, there is a `collect` routine which reads gathers together the data from multiple processors

```
1 from boutdata.collect import collect
2
3 Ni = collect("Ni")  # Collect the variable "Ni"
```

5.6 Matlab routines

These are Matlab routines for collecting data, showing animation and performing some basic analysis. To use these routines, either you may copy these routines (from **tools/matlablib**) directly to your present working directory or a path to **tools/matlablib** should be added before analysis.

```
>> addpath <full_path_BOUT_directory>/tools/matlablib/
```

Now, the first routine to collect data and import it to Matlab for further analysis is

```
>> var = import_dmp(path,var_name);
```

Here, *path* is the path where the output data in netcdf format has been dumped. *var_name* is the name of variable which user want to load for further analysis. For example, to load "P" variable from present working directory:

```
>> P = import_dmp('.','P');
```

Variable "P" can be any of [X,Y,Z,T]/[X,Y,Z]/[X,Y]/Constant formats. If we are going to Import a large data set with [X,Y,Z,T] format. Normally such data files are of very big size and Matlab goes out of memory/ or may take too much time to load data for all time steps. To resolve this limitation of above routine *import_dmp*, another routine *import_data_netcdf* is being provided. It serves all purposes the routine *import_dmp* does but also gives user freedom to import data at only few/specific time steps.

```
>> var = import_data_netcdf(path,var_name,nt,ntsp);
```

Here, *path* and *var_name* are same variables as described before. *nt* is the number of time steps user wish to load data. *ntsp* is the steps at which one wish to write data of of total simulation times the data written.

```
>> P = import_data_netcdf('.','P',5,100);
```

Variable "P" has been imported from present working directory for 5 time steps. As the original netcdf data contains time information of 500 steps (assume NT=500 in BOUT++ simulations), user will pick only 5 time steps at steps of *ntsp* i.e. 100 here. Details of other Matlab routines provided with BOUT++ package can be looked in to README.txt of **tools/matlablib** directory. The Matlab users can develop their own routines using *ncread, ncinfo, ncwrite, ncdisp, netcdf etc.* functions provided in Matlab package.

5.7 Mathematica routines

A package to read BOUT++ output data into Mathematica is in **tools/mathematicalib**. To read data into Mathematica, first add this directory to Mathematica's path by putting

```
AppendTo[$Path,"<full_path_to_BOUT>/tools/mathematicalib"]
```

in your Mathematica startup file (usually \$HOME/.Mathematica/Kernel/init.m). To use the package, call

```
Import["BoutCollect.m"]
```

from inside Mathematica. Then you can use e.g.

```
f=BoutCollect[variable,path->"data"]
```

or

```
f=BoutCollect[variable,path->"data"]
```

' bc' is a shorthand for 'BoutCollect'. All options supported by the Python collect() function are included, though Info does nothing yet.

5.8 Octave routines

There is minimal support for reading data into Octave, which has been tested on Octave 3.2. It requires the octcdf library to access NetCDF files.

```
f = bcollect()  # optional path argument is "." by default

f = bsetxrange(f, 1, 10) # Set ranges
# Same for y, z, and t (NOTE: indexing from 1!)

u = bread(f, "U")  # Finally read the variable
```

6 BOUT++ options

The inputs to BOUT++ are a text file containing options, and for complex grids a binary grid file in NetCDF or PDB format. Generating input grids for tokamaks is described in section 11. The grid file describes the size and topology of the X-Y domain, metric tensor components and usually some initial profiles. The option file specifies the size of the domain in the symmetric direction (Z), and controls how the equations are evolved e.g. differencing schemes to use, and boundary conditions. In most situations, the grid file will be used in many different simulations, but the options may be changed frequently.

The text input file BOUT.inp is always in a subdirectory called data for all examples. The files include comments (starting with either ';' or '#') and should be fairly self-explanatory. The format is the same as a windows INI file, consisting of name = value pairs. Comments are started with a hash (#) or semi-colon, which comments out the rest of the line. values can be:

- Integers
- Real values
- Booleans

- Strings

Options are also divided into sections, which start with the section name in square brackets.

```
[section1]

something = 132          # an integer
another = 5.131          # a real value
yetanother = true        # a boolean
finally = "some text"    # a string
```

NOTE: Options are NOT case-sensitive: `TwistShift` and `twistshift` are the same variable

Subsections can also be used, separated by colons ':', e.g.

```
[section:subsection]
```

Have a look through the examples to see how the options are used.

6.1 Command line options

All options can be set on the command line, and will override those set in BOUT.inp. The most commonly used are "restart" and "append", described in section 4. If values are not given for command-line arguments, then the value is set to `true` , so putting `restart` is equivalent to `restart=true` .

Values can be specified on the command line for other settings, such as the fraction of a torus to simulate (ZPERIOD):

```
./command zperiod=10
```

Remember **no** spaces around the '=' sign. Like the BOUT.inp file, setting names are not case sensitive.

Sections are separated by colons ':', so to set the solver type (section 9.1) you can either put this in BOUT.inp:

```
[solver]
type = rk4
```

or put `solver:type=rk4` on the command line. This capability is used in many test suite cases to change the parameters for each run.

6.2 General options

At the top of the BOUT.inp file (before any section headers), options which affect the core code are listed. These are common to all physics models, and the most useful of them are:

```
NOUT = 100        # number of time-points output
TIMESTEP = 1.0    # time between outputs
```

which set the number of outputs, and the time step between them. Note that this has nothing to do with the internal timestep used to advance the equations, which is adjusted automatically. What time-step to use depends on many factors, but for high-β reduced MHD ELM simulations reasonable choices are `1.0` for the first part of a run (to handle initial transients), then around `10.0` for the linear phase. Once non-linear effects become important, you will have to reduce the timestep to around `0.1`.

Most large clusters or supercomputers have a limit on how long a job can run for called "wall time", because it's the time taken according to a clock on the wall, as opposed to the CPU time actually used. If this is the case, you can use the option

```
wall_limit = 10 # wall clock limit (in hours)
```

BOUT++ will then try to quit cleanly before this time runs out. Setting a negative value (default is -1) means no limit.

Often it's useful to be able to restart a simulation from a chosen point, either to reproduce a previous run, or to modify the settings and re-run. A restart file is output every timestep, but this is overwritten each time, and so the simulation can only be continued from the end of the last simulation. Whilst it is possible to create a restart file from the output data afterwards, it's much easier if you have the restart files. Using the option

```
archive = 20
```

saves a copy of the restart files every 20 timesteps, which can then be used as a starting point.

The X and Y size of the computational grid is set by the grid file, but the number of points in the Z (axisymmetric) direction is specified in the options file:

```
MZ = 33
```

This must be $\texttt{MZ} = 2^n + 1$, and can be $2, 3, 5, 9, \ldots$. The power of 2 is so that FFTs can be used in this direction; the +1 is for historical reasons (inherited from BOUT) and is going to be removed at some point.

Since the Z dimension is periodic, the domain size is specified as multiples or fractions of 2π. To specify a fraction of 2π, use

```
ZPERIOD = 10
```

This specifies a Z range from 0 to 2π/`ZPERIOD`, and is useful for simulation of tokamaks to make sure that the domain is an integer fraction of a torus. If instead you want to specify the Z range directly (for example if Z is not an angle), there are the options

```
ZMIN = 0.0
ZMAX = 0.1
```

which specify the range in multiples of 2π.

> **NOTE**: For users of BOUT, the definition of `ZMIN` and `ZMAX` has been changed. These are now fractions of 2π radians i.e. `dz` = 2π(`ZMAX - ZMIN`)/(`MZ-1`)

In BOUT++, grids can be split between processors in both X and Y directions. By default only Y decomposition is used, and to use X decomposition you must specify the number of processors in the X direction:

```
NXPE = 1  # Set number of X processors
```

The grid file to use is specified relative to the root directory where the simulation is run (i.e. running "`ls ./data/BOUT.inp`" gives the options file)

```
grid = "data/cbm18_8_y064_x260.pdb"
```

6.3 Input and Output

The format of the output (dump) files can be controlled, if support for more than one output format has been configured, by setting the top-level option **dump_format** to one of the recognised file extensions: 'nc' for NetCDF; 'hdf5', 'hdf' or 'h5' for HDF5; 'pdb' for PDB. For example to select HDF5 instead of the default NetCDF format put

```
1 dump_format = hdf5
```

before any section headers. The output (dump) files with time-history are controlled by settings in a section called "output". Restart files contain a single time-slice, and are controlled by a section called "restart". The options available are listed in table 1.

enabled is useful mainly for doing performance or scaling tests, where you want to exclude I/O from the timings. **floats** is used to reduce the size of the output files: restart files are stored as double by default (since these will be used to restart a simulation), but output dump files are set to floats by default.

To enable parallel I/O for either output or restart files, set

```
1 parallel = true
```

in the output or restart section. If you have compiled BOUT++ with a parallel I/O library such as pnetcdf (see section 3), then rather than outputting one file per processor, all processors will output to the same file. For restart files this is particularly useful, as it

Table 1: Output file options

Option	Description	Default value
enabled	Writing is enabled	true
floats	Write floats rather than doubles	true (dmp)
flush	Flush the file to disk after each write	true
guards	Output guard cells	true
openclose	Re-open the file for each write, and close after	true
parallel	Use parallel I/O	false

means that you can restart a job with a different number of processors. Note that this feature is still experimental, and incomplete: output dump files are not yet supported by the collect routines.

6.4 Laplacian inversion

A common problem in plasma models is to solve an equation of the form

$$d\nabla_\perp^2 x + \frac{1}{c_1}\left(\nabla_\perp c_2\right)\cdot\nabla_\perp x + ax = b \tag{3}$$

For example,

$$\nabla_\perp^2 x + ax = b \tag{4}$$

appears in reduced MHD for the vorticity inversion and $j_{||}$.

In BOUT++, these equations can be solved in two ways. Currently, both ways neglects the parallel derivatives.

NOTE: Current implementations neglects derivatives in the parallel direction

By neglecting the y-derivatives, one can solve equation (6.4) y point by y point.

The first approach utilizes that it is possible fourier transform the equation in z (using some assumptions, see the `coordinates` manual for details), and solve a tridiagonal system for each mode. These inversion problems are band-diagonal (tri-diagonal in the case of 2nd-order differencing) and so inversions can be very efficient: $O\left(n_z \log n_z\right)$ for the FFTs, $O\left(n_x\right)$ for tridiagonal inversion using the Thomas algorithm [6], where n_x and n_z are the number of grid-points in the x and z directions respectively.

In the second approach, the full 2-D system is being solved. This requires PETSc to be built with BOUT++

The `Laplacian` class is defined in `invert_laplace.hxx` and solves problems formulated like equation () To use this class, first create an instance of it:

```
Laplacian *lap = Laplacian::create();
```

By default, this will use the options in a section called "laplace", but can be given a different section as an argument. By default $d = 1$, $a = 0$, and the $c = 1$. To set the values of these coefficients, there are the `setCoefA`(), `setCoefC`(), and `setCoefD`() methods:

```
Field2D a = ...;
lap->setCoefA(a);
lap->setCoefC(0.5);
```

arguments can be `Field2D`, `Field3D` , or real values.

Settings for the inversion can be set in the input file under the section `laplace` (default) or whichever settings section name was specified when the `Laplacian` class was created. Commonly used settings are listed in tables 2 to 5.

In particular boundary conditions on the x boundaries can be set using the `inner_boundary_flags` and `outer_boundary_flags` variables, as detailed in table 4. Note that DC ('direct-current') refers to $k = 0$ Fourier component, AC ('alternating-current') refers to $k \neq 0$ Fourier components. Non-Fourier solvers use AC options (and ignore DC ones). Multiple boundary conditions can be selected by adding together the required boundary condition flag values together. For example, `inner_boundary_flags` = 3 will set a Neumann boundary condition on both AC and DC components.

It is pertinent to note here that the boundary in BOUT++ is defined by default to be located half way between the first guard point and first point inside the domain. For example, when a Dirichlet boundary condition is set, using `inner_boundary_flags` = 0 , `16`, or `32`, then the first guard point, f_- will be set to $f_- = 2v - f_+$, where f_+ is the first grid point inside the domain, and v is the value to which the boundary is being set to.

NOTE: The current implementation of the tridiagonal solvers are using 2 points to set the boundaries for the cases where we are not using `dirichlet` or `neumann` condition with a non-zero value. In order to just have one point setting the boundary, the `global_flags = 4` should be used.

The `global_flags`, `inner_boundary_flags`, `outer_boundary_flags` and `flags` values can also be set from within the physics module using `setGlobalFlags`, `setInnerBoundaryFlags`, `setOuterBoundaryFlags` and `setFlags` .

```
lap->setGlobalFlags(Global_Flags_Value);
lap->setInnerBoundaryFlags(Inner_Flags_Value);
lap->setOuterBoundaryFlags(Outer_Flags_Value);
lap->setFlags(Flags_Value);
```

Table 2: Laplacian inversion options

Name	Meaning	Default value
`type`	Which implementation to use	`tri` (serial), `spt` (parallel)
`filter`	Filter out modes above (1−`filter`) × k_{max}, if using Fourier solver	0
`maxmode`	Filter modes with $n >$`maxmode`	`MZ`/2
`all_terms`	Include first derivative terms	`true`
`global_flags`	Sets global inversion options See table 3	`0`
`inner_boundary_flags`	Sets boundary conditions on inner boundary. See table 4	`0`
`outer_boundary_flags`	Sets boundary conditions on outer boundary. See table 4	`0`
`flags`	DEPRECATED. Sets global solver options and boundary conditions. See table 5 or `invert_laplace.hxx`	`0`
`include_yguards`	Perform inversion in y-boundary guard cells	`true`

Table 3: Laplacian inversion `global_flags` values: add the required quantities together.

Flag	Meaning	Code variable
0	No global option set	–
1	zero DC component (Fourier solvers)	`INVERT_ZERO_DC`
2	set initial guess to 0 (iterative solvers)	`INVERT_START_NEW`
4	equivalent to `outer_boundary_flags = 128`, `inner_boundary_flags = 128`	`INVERT_BOTH_BNDRY_ONE`
8	Use 4th order differencing (Apparently not actually implemented anywhere!!!)	`INVERT_4TH_ORDER`
16	Set constant component ($k_x = k_z = 0$) to zero	`INVERT_KX_ZERO`

Table 4: Laplacian inversion `outer_boundary_flags` or `inner_boundary_flags` values: add the required quantities together.

Flag	Meaning	Code variable
0	Dirichlet (Set boundary to 0)	–
1	Neumann on DC component (set gradient to 0)	`INVERT_DC_GRAD`
2	Neumann on AC component (set gradient to 0)	`INVERT_AC_GRAD`
4	Zero or decaying Laplacian on AC components ($\frac{\partial^2}{\partial x^2} + k_z^2$ vanishes/decays)	`INVERT_AC_LAP`
8	Use symmetry to enforce zero value or gradient (redundant for 2nd order now)	`INVERT_SYM`
16	Set boundary condition to values in boundary guard cells of second argument, `x0`, of `Laplacian::solve(`↩ `const Field3D &b, const Field3D &x0)` . May be combined with any combination of 0, 1 and 2, i.e. a Dirichlet or Neumann boundary condition set to values which are $\neq 0$ or $f(y)$	`INVERT_SET`
32	Set boundary condition to values in boundary guard cells of RHS, `b` in `Laplacian::solve(const Field3D` ↩ `&b, const Field3D &x0)` . May be combined with any combination of 0, 1 and 2, i.e. a Dirichlet or Neumann boundary condition set to values which are $\neq 0$ or $f(y)$	`INVERT_RHS`
64	Zero or decaying Laplacian on DC components ($\frac{\partial^2}{\partial x^2}$ vanishes/decays)	`INVERT_DC_LAP`
128	Assert that there is only one guard cell in the x-boundary	`INVERT_BNDRY_ONE`
256	DC value is set to parallel gradient, $\nabla_\parallel f$	`INVERT_DC_GRADPAR`
512	DC value is set to inverse of parallel gradient $1/\nabla_\parallel f$	`INVERT_DC_GRADPARINV`
1024	Boundary condition for inner 'boundary' of cylinder	`INVERT_IN_CYLINDER`

Table 5: Laplacian inversion `flags` values (DEPRECATED!): add the required quantities together.

Flag	Meaning
1	Zero-gradient DC on inner (X) boundary. Default is zero-value
2	Zero-gradient AC on inner boundary
4	Zero-gradient DC on outer boundary
8	Zero-gradient AC on outer boundary
16	Zero DC component everywhere
32	Not used currently
64	Set width of boundary to 1 (default is `MXG`)
128	Use 4^{th}-order band solver (default is 2^{nd} order tridiagonal)
256	Attempt to set zero laplacian AC component on inner boundary by combining 2nd and 4th-order differencing at the boundary. Ignored if tridiagonal solver used.
512	Zero laplacian AC on outer boundary
1024	Symmetric boundary condition on inner boundary
2048	Symmetric outer boundary condition

To perform the inversion, there's the `solve` method

```
x = lap->solve(b);
```

If you prefer, there are functions compatible with older versions of the BOUT++ code:

```
Field2D a, c, d;
invert_laplace(b, x, flags, &a, &c, &d);
```

and

```
x = invert_laplace(b, flags, &a, &c, &d);
```

The input `b` and output `x` are 3D fields, and the coefficients `a`, `c`, and `d` are pointers to 2D fields. To omit any of the three coefficients, set them to NULL.

6.5 Communications

The communication system has a section `[comms]`, with a true/false option `async`. This determines whether asynchronous MPI sends are used; which method is faster varies (though not by much) with machine and problem.

6.6 Differencing methods

Differencing methods are specified in three section (`[ddx]`, `[ddy]` and `[ddz]`), one for each dimension.

- `first`, the method used for first derivatives
- `second`, method for second derivatives
- `upwind`, method for upwinding terms
- `flux`, for conservation law terms

The methods which can be specified are U1, U4, C2, C4, W2, W3, FFT Apart from FFT, the first letter gives the type of method (U = upwind, C = central, W = WENO), and the number gives the order.

6.7 Model-specific options

The options which affect a specific physics model vary, since they are defined in the physics module itself (see section 12.3). They should have a separate section, for example the high-β reduced MHD code uses options in a section called `[highbeta]`.

There are three places to look for these options: the BOUT.inp file; the physics model C++ code, and the output logs. The physics module author should ideally have an example input file, with commented options explaining what they do; alternately they may have put comments in the C++ code for the module. Another way is to look at the output logs: when BOUT++ is run, (nearly) all options used are printed out with their default values. This won't provide much explanation of what they do, but may be useful anyway. See section 5 for more details.

7 Variable initialisation

Each variable being evolved has its own section, with the same name as the output data. For example, the high-β model has variables "P", "jpar", and "U", and so has sections `[P]`, `[jpar]`, `[U]` (not case sensitive).

There are two ways to specify the initial conditions for a variable: the original method (similar to that used by BOUT-06) which covers the most commonly needed functions. If more flexibility is needed then a more general analytical expression can be given.

7.0.1 Original method

The shape of the initial value is specified for each dimension separately using the options `xs_opt`, `ys_opt`, and `zs_opt`. These are set to an integer:

0. Constant (this is the default)
1. Gaussian, with a peak location given by `xs_s0`, `ys_s0`, `zs_s0` as a fraction of the domain (i.e. $0 \rightarrow 1$. The width is given by `*s_wd`, also as a fraction of the domain size.
2. Sinusoidal, with the number of periods given by `*s_mode`.
3. Mix of mode numbers, with pseudo-random phases.

The magnitude of the initial value is given by the variable `scale`.

Defaults for all variables can be set in a section called `[All]`, so for example the options below:

```
[All]
scale = 0.0 # By default set variables to zero

xs_opt = 1  # Gaussian in X
ys_opt = 1  # Gaussian in Y
zs_opt = 2  # Sinusoidal in Z (axisymmetric direction)

xs_s0 = 0.5 # Peak in the middle of the X direction
xs_wd = 0.1 # Width is 10% of the domain

ys_s0 = 0.5 # Peak in the middle of the Y direction
ys_wd = 0.3 # Width is 30% of the Y domain

zs_mode = 3 # 3 periods in the Z direction

[U]
scale = 1.0e-5  # Amplitude for the U variable, overrides default
```

For field-aligned tokamak simulations, the Y direction is along the field and in the core this will have a discontinuity at the twist-shift location where field-lines are matched onto each other. To handle this, a truncated Ballooning transformation can be used to construct a smooth initial perturbation:

$$U_0^{balloon} = \sum_{i=-N}^{N} F\left(x\right) G\left(y + 2\pi i\right) H\left(z + q2\pi i\right) \tag{5}$$

NOTE: The initial profiles code currently doesn't work very well for grids with branch-cuts (e.g. divertor tokamak), and will often have jumps which then make timesteps smaller

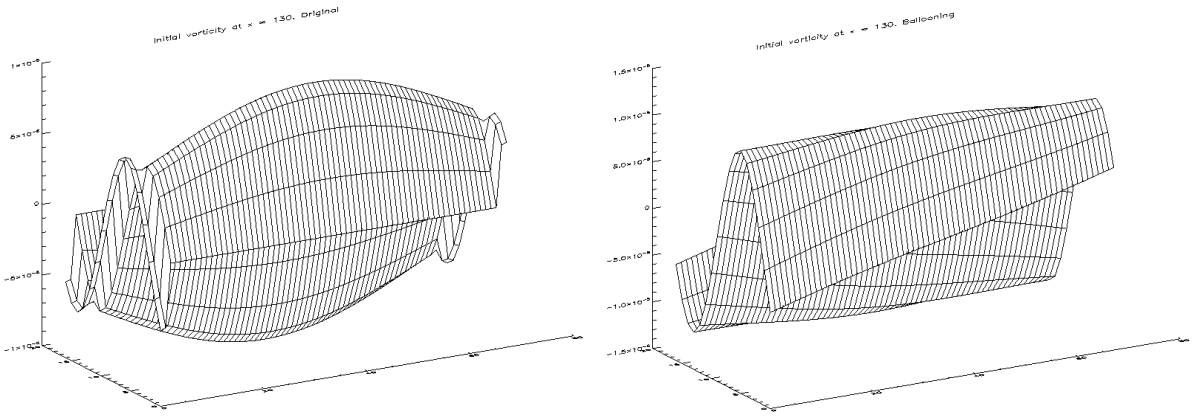


Figure 1: Initial profiles in twist-shifted grid. **Left**: Without ballooning transform, showing discontinuity at the matching location **Right**: with ballooning transform

7.0.2 Expressions

If a more general function is needed, a variable can be initialised using the `function` option for each variable. This overrides the original method for that variable. e.g.

```
[all]

xs_opt = 1  # Gaussian in X
ys_opt = 1  # Gaussian in Y
zs_opt = 2  # Sinusoidal in Z (axisymmetric direction)

[U]
scale = 1.0e-5

[p]
function = 1 + gauss(x-0.5)*gauss(y)*sin(z)
```

will use the original method to set U, but use the given expression to set p.

Expressions can include the usual operators (`+`,`-`,`*`,`/`), including `^` for exponents. The following values are also already defined: By default, x is defined as `i / (nx - 2*MXG)`, where `MXG` is the width of the boundary region, by default 2. Hence x actually goes from 0 on the leftmost point to `(nx-1)/(nx-4)` on the rightmost point. This is not a particularly

Table 6: Initialisation expression values

Name	Description
x	x position between 0 and 1
y	y position between 0 and 2π (excluding the last point)
z	z position between 0 and 2π (excluding the last point)
pi	3.1415...

good definition, but for most cases its sufficient to create some initial profiles. For some problems like island reconnection simulations, it's useful to define x in a particular way which is more symmetric than the default. To do this, set in BOUT.inp

```
[mesh]
symmetricGlobalX = true
```

This will change the definition of x to `i / (nx - 1)`, so x is then between 0 and 1 everywhere.

The functions in table 7 are also available in expressions. Note that to apply a ballooning transform in analytic expressions the `ballooning` function should be used, and the global flag "ballooning" has no effect. There is an example code `test-ballooning` which compares methods of setting initial conditions with ballooning transform.

The `mixmode(x)` function is a mixture of Fourier modes of the form:

$$\text{mixmode}(x) = \sum_{i=1}^{14} \frac{1}{(1+|i-4|)^2} \cos\left[ix + \phi(i, \text{seed})\right] \tag{6}$$

where ϕ is a random phase between $-\pi$ and $+\pi$, which depends on the seed. The factor in front of each term is chosen so that the 4th harmonic ($i = 4$) has the highest amplitude. This is useful mainly for initialising turbulence simulations, where a mixture of mode numbers is desired.

7.1 FieldFactory class

This class provides a way to generate a field with a specified form. It implements a recursive descent parser to turn a string containing something like `"gauss(x-0.5,0.2)*gauss(y)*sin(3*z)"` into values in a `Field3D` or `Field2D` object. Examples are given in the `test-fieldfactory` example:

```
1 FieldFactory f;
2 Field2D b = f.create2D("1 - x");
3 Field3D d = f.create3D("gauss(x-0.5,0.2)*gauss(y)*sin(z)");
```

Table 7: Initialisation expression functions

Name	Description
abs(x)	Absolute value $\|x\|$
asin(x), acos(x), atan(x), atan(y,x)	Inverse trigonometric functions
ballooning(x)	Ballooning transform (eq 5, fig 1)
ballooning(x,n)	Ballooning transform, using n terms (default 3)
cos(x)	Cosine
cosh(x)	Hyperbolic cosine
exp(x)	Exponential
tanh(x)	Hyperbolic tangent
gauss(x)	Gaussian $\exp\left(-x^2/2\right)/\sqrt{2\pi}$
gauss(x, w)	Gaussian $\exp\left[-x^2/\left(2w^2\right)\right]/\left(w\sqrt{2\pi}\right)$
H(x)	Heaviside function: 1 if $x > 0$ otherwise 0
log(x)	Natural logarithm
max(x,y,...)	Maximum (variable arguments)
min(x,y,...)	Minimum (variable arguments)
mixmode(x)	A mixture of Fourier modes
mixmode(x, seed)	seed determines random phase (default 0.5)
power(x,y)	Exponent x^y
sin(x)	Sine
sinh(x)	Hyperbolic sine
sqrt(x)	$\sqrt{x}$
tan(x)	Tangent
erf(x)	The error function
TanhHat(x, width, center, steepness)	The hat function
	$\frac{1}{2}\left(\tanh\left[s\left(x-\left[c-\frac{w}{2}\right]\right)\right]+\tanh\left[s\left(x-\left[c+\frac{w}{2}\right]\right)\right]\right)$

This is done by creating a tree of `FieldGenerator` objects which then generate the field values:

```
49 class FieldGenerator {
50  public:
51   virtual ~FieldGenerator() { }
52   virtual FieldGenerator* clone(const list<FieldGenerator*> args) {↩
        return NULL;}
53   virtual BoutReal generate(int x, int y, int z) = 0;
54 };
```

All classes inheriting from `FieldGenerator` must implement a `generate` function, which returns the value at the given (`x`,`y`,`z`) position. Classes should also implement a `clone`↩

function, which takes a list of arguments and creates a new instance of its class. This takes as input a list of other `FieldGenerator` objects, allowing a variable number of arguments.

The simplest generator is a fixed numerical value, which is represented by a `FieldValue` object:

```
59 class FieldValue : public FieldGenerator {
60  public:
61   FieldValue(BoutReal val) : value(val) {}
62   BoutReal generate(int x, int y, int z) { return value; }
63  private:
64   BoutReal value;
65 };
```

7.2 Adding a new function

To add a new function to the FieldFactory, a new `FieldGenerator` class must be defined. Here we will use the example of the `sinh` function, implemented using a class `FieldSinh` . This takes a single argument as input, but `FieldPI` takes no arguments, and `FieldGaussian` takes either one or two. Study these after reading this to see how these are handled.

First, edit **src/field/fieldgenerators.hxx** and add a class definition:

```
114 class FieldSinh : public FieldGenerator {
115  public:
116   FieldSinh(FieldGenerator* g) : gen(g) {}
117   ~FieldSinh() {if(gen) delete gen;}
118
119   FieldGenerator* clone(const list<FieldGenerator*> args);
120   BoutReal generate(int x, int y, int z);
121  private:
122   FieldGenerator *gen;
123 };
```

The `gen` member is used to store the input argument, and to make sure it's deleted properly we add some code to the destructor. The constructor takes a single input, the `FieldGenerator` argument to the `sinh` function, which is stored in the member `gen` .

Next edit **src/field/fieldgenerators.cxx** and add the implementation of the `clone` and `generate` functions:

```
33 FieldGenerator* FieldSinh::clone(const list<FieldGenerator*> args) {
34   if(args.size() != 1) {
35     throw ParseException("Incorrect number of arguments to sinh ↩
         function. Expecting 1, got %d", args.size());
```

```
36   }
37
38   return new FieldSinh(args.front());
39 }
40
41 BoutReal FieldSinh::generate(double x, double y, double z, double t) ↩
     {
42   return sinh(gen->generate(x,y,z,t));
43 }
```

The `clone` function first checks the number of arguments using `args.size()` . This is used in `FieldGaussian` to handle different numbers of input, but in this case we throw a `ParseException` if the number of inputs isn't one. `clone` then creates a new `FieldSinh` object, passing the first argument (`args.front()`) to the constructor (which then gets stored in the `gen` member variable).

The `generate` function for `sinh` just gets the value of the input by calling `gen->generate(x,y,z)`, calculates `sinh` of it and returns the result.

The `clone` function means that the parsing code can make copies of any `FieldGenerator` class if it's given a single instance to start with. The final step is therefore to give the `FieldFactory` class an instance of this new generator. Edit the `FieldFactory` constructor `FieldFactory::FieldFactory()` in **src/field/field_factory.cxx** and add the line:

```
64 addGenerator("sinh", new FieldSinh(NULL));
```

That's it! This line associates the string `"sinh"` with a `FieldGenerator` . Even though `FieldFactory` doesn't know what type of `FieldGenerator` it is, it can make more copies by calling the `clone` member function. This is a useful technique for polymorphic objects in C++ called the "Virtual Constructor" idiom.

7.3 Parser internals

When a `FieldGenerator` is added using the `addGenerator` function, it is entered into a `std::map` which maps strings to `FieldGenerator` objects (**include/field_factory.hxx**):

```
223 map<string, FieldGenerator*> gen;
```

Parsing a string into a tree of `FieldGenerator` objects is done by first splitting the string up into separate tokens like operators like '*', brackets '(', names like 'sinh' and so on, then recognising patterns in the stream of tokens. Recognising tokens is done in **src/field/field_factory.cxx**:

```
259 char FieldFactory::nextToken() {
260  ...
```

This returns the next token, and setting the variable `char curtok` to the same value. This can be one of:

- -1 if the next token is a number. The variable `BoutReal curval` is set to the value of the token
- -2 for a string (e.g. "sinh", "x" or "pi"). This includes anything which starts with a letter, and contains only letters, numbers, and underscores. The string is stored in the variable `string curident` .
- 0 to mean end of input
- The character if none of the above. Since letters and numbers are taken care of (see above), this includes brackets and operators like '+' and '-'.

The parsing stage turns these tokens into a tree of `FieldGenerator` objects, starting with the `parse()` function

```
484 FieldGenerator* FieldFactory::parse(const string &input) {
485     ...
```

which puts the input string into a stream so that `nextToken()` can use it, then calls the `parseExpression()` function to do the actual parsing:

```
477 FieldGenerator* FieldFactory::parseExpression() {
478     ...
```

This breaks down expressions in stages, starting with writing every expression as

```
expression := primary [ op primary ]
```

i.e. a primary expression, and optionally an operator and another primary expression. Primary expressions are handled by the `parsePrimary()` function, so first `parsePrimary()` is called, and then `parseBinOpRHS` which checks if there is an operator, and if so calls `parsePrimary()` to parse it. This code also takes care of operator precedence by keeping track of the precedence of the current operator. Primary expressions are then further broken down and can consist of either a number, a name (identifier), a minus sign and a primary expression, or brackets around an expression:

```
primary := number
        := identifier
        := '-' primary
        := '(' expression ')'
        := '[' expression ']'
```

The minus sign case is needed to handle the unary minus e.g. `"-x"` . Identifiers are handled in `parseIdentifierExpr`() which handles either variable names, or functions

```
identifier := name
           := name '(' expression [ ',' expression [ ',' ... ] ] ')'
```

i.e. a name, optionally followed by brackets containing one or more expressions separated by commas. names without brackets are treated the same as those with empty brackets, so `"x"` is the same as `"x()"`. A list of inputs (`list<FieldGenerator*> args`;) is created, the `gen` map is searched to find the `FieldGenerator` object corresponding to the name, and the list of inputs is passed to the object's `clone` function.

8 Implementation

To control the behaviour of BOUT++ a set of options is used, with options organised into sections which can be nested. To represent this tree structure there is the `Options` class defined in **bout++/include/options.hxx**

```
class Options {
 public:
  // Setting options
  void set(const string &key,const int &val,const string &source="");
  ...
  // Testing if set
  bool isSet(const string &key);
  // Getting options
  void get(const string &key,int &val,const int &def,bool log=true);
  ...
  // Get a subsection. Creates if doesn't exist
  Options* getSection(const string &name);
};
```

To access the options, there is a static function (singleton)

```
  Options *options = Options::getRoot();
```

which gives the top-level (root) options class. Setting options is done using the `set()`↩ methods which are currently defined for `int`, `BoutReal`, `bool` and `string` . For example:

```
  options->set("nout", 10);       // Set an integer
  options->set("restart", true); // A bool
```

Often it's useful to see where an option setting has come from e.g. the name of the options file or "command line". To specify a source, pass it as a third argument:

```
options->set("nout", 10, "manual");
```

To create a section, just use `getSection` : if it doesn't exist it will be created.

```
Options *section = options->getSection("mysection");
section->set("myswitch", true);
```

To get options, use the `get`() method which take the name of the option, the variable to set, and the default value.

```
int nout;
options->get("nout", nout, 1);
```

Internally, `Options` converts all types to strings and does type conversion when needed, so the following code would work:

```
Options *options = Options::getRoot();
options->set("test", "123");
int val;
options->get("test", val, 1);
```

This is because often the type of the option is not known at the time when it's set, but only when it's requested.

By default, the `get` methods output a message to the log files giving the value used and the source of that value. To suppress this, set the `log` argument to `false` :

```
options->get("test", val, 1, false);
```

8.1 Reading options

To allow different input file formats, each file parser implements the `OptionParser` interface defined in **bout++/src/sys/options/optionparser.hxx**

```
class OptionParser {
 public:
  virtual void read(Options *options, const string &filename) = 0;
 private:
};
```

and so just needs to implement a single function which reads a given file name and inserts the options into the given `Options` object.

To use these parsers and read in a file, there is the `OptionsReader` class defined in **bout++/include/optionsreader.hxx**

```
class OptionsReader {
 public:
```

```
3   void read(Options *options, const char *file, ...);
4   void parseCommandLine(Options *options, int argc, char **argv);
5 };
```

This is a singleton object which is accessed using

```
1   OptionsReader *reader = OptionsReader::getInstance();
```

so to read a file **BOUT.inp** in a directory given in a variable `data_dir` the following code is used in **bout++.cxx**:

```
1   Options *options = Options::getRoot();
2   OptionsReader *reader = OptionsReader::getInstance();
3   reader->read(options, "%s/BOUT.inp", data_dir);
```

To parse command line arguments as options, the `OptionsReader` class has a method:

```
1   reader->parseCommandLine(options, argc, argv);
```

This is currently quite rudimentary and needs improving.

9 Time integration

9.1 Options

BOUT++ can be compiled with several different time-integration solvers , and at minimum should have Runge-Kutta (RK4) and PVODE (BDF/Adams) solvers available.

The solver library used is set using the `solver:type` option, so either in BOUT.inp:

```
[solver]
type = rk4  # Set the solver to use
```

or on the command line by adding `solver:type=pvode` for example:

```
mpirun -np 4 ./2fluid solver:type=rk4
```

NB: Make sure there are no spaces around the "=" sign: `solver:type =pvode` won't work (probably). Table 8 gives a list of time integration solvers, along with any compile-time options needed to make the solver available. Each solver can have its own settings which work in slightly different ways, but some common settings and which solvers they are used in are given in table 9. The most commonly changed options are the absolute and relative solver tolerances, `ATOL` and `RTOL` which should be varied to check convergence.

9.2 ODE integration

The Solver class can be used to solve systems of ODEs inside a physics model: Multiple Solver objects can exist besides the main one used for time integration. Example code is in

Table 8: Available time integration solvers

Name	Description	Compile options
euler	Euler explicit method	Always available
rk4	Runge-Kutta 4th-order explicit method	Always available
karniadakis	Karniadakis explicit method	Always available
pvode	1998 PVODE with BDF method	Always available
cvode	SUNDIALS CVODE. BDF and Adams methods	–with-cvode
ida	SUNDIALS IDA. DAE solver	–with-ida
petsc	PETSc TS methods	–with-petsc

Table 9: Time integration solver options

Option	Description	Solvers used
atol	Absolute tolerance	rk4, pvode, cvode, ida
rtol	Relative tolerance	rk4, pvode, cvode, ida
mxstep	Maximum internal steps per output step	rk4
max_timestep	Maximum timestep	rk4, cvode
timestep	Starting timestep	rk4, karniadakis, euler
adaptive	Adapt timestep? (Y/N)	rk4
use_precon	Use a preconditioner? (Y/N)	pvode, cvode, ida
mudq, mldq mukeep, mlkeep maxl	BBD preconditioner settings	pvode, cvode, ida
use_jacobian	Use user-supplied Jacobian? (Y/N)	cvode
adams_moulton	Use Adams-Moulton method rather than BDF	cvode
diagnose	Collect and print additional diagnostics	cvode

examples/test-integrate.

To use this feature, systems of ODEs must be represented by a class derived from `PhysicsModel` (see section 14).

```
1 class MyFunction : public PhysicsModel {
2  public:
3   int init(bool restarting) {
4     // Initialise ODE
5     // Add variables to solver as usual
6     solver->add(result, "result");
```

```
    ...
  }

  int rhs(BoutReal time) {
    // Specify derivatives of fields as usual
    ddt(result) = ...
  }
 private:
  Field3D result;
};
```

To solve this ODE, create a new Solver object:

```
Solver* ode = Solver::create(Options::getRoot()->getSection("ode"));
```

This will look in the section `[ode]` in the options file. **Important:** To prevent this solver overwriting the main restart files with its own restart files, either disable restart files:

```
[ode]
enablerestart = false
```

or specify a different directory to put the restart files:

```
[ode]
restartdir = ode  # Restart files ode/BOUT.restart.0.nc, ...
```

Create a model object, and pass it to the solver:

```
MyFunction* model = new MyFunction();
ode->setModel(model);
```

Finally tell the solver to perform the integration:

```
ode->solve(5, 0.1);
```

The first argument is the number of steps to take, and the second is the size of each step. These can also be specified in the options, so calling

```
ode->solve();
```

will cause ode to look in the input for `nout` and `timestep` options:

```
[ode]
nout = 5
timestep = 0.1
```

Finally, delete the model and solver when finished:

```
delete model;
delete solver;
```

Note: If an ODE needs to be solved multiple times, at the moment it is recommended to delete the solver, and create a new one each time.

9.3 Preconditioning

At every time step, an implicit scheme such as BDF has to solve a non-linear problem to find the next solution. This is usually done using Newton's method, each step of which involves solving a linear (matrix) problem. For N evolving variables is an $N \times N$ matrix and so can be very large. By default matrix-free methods are used, in which the Jacobian $\mathcal{J}$ is approximated by finite differences (see next subsection), and so this matrix never needs to be explicitly calculated. Finding a solution to this matrix can still be difficult, particularly as δt gets large compared with some time-scales in the system (i.e. a stiff problem).

A preconditioner is a function which quickly finds an approximate solution to this matrix, speeding up convergence to a solution. A preconditioner does not need to include all the terms in the problem being solved, as the preconditioner only affects the convergence rate and not the final solution. A good preconditioner can therefore concentrate on solving the parts of the problem with the fastest time-scales.

A simple example[5] is a coupled wave equation, solved in the `test-precon` example code:

$$\frac{\partial u}{\partial t} = \partial_{||} v \qquad \frac{\partial v}{\partial t} = \partial_{||} u \tag{7}$$

First, calculate the Jacobian of this set of equations by taking partial derivatives of the time-derivatives with respect to each of the evolving variables

$$\mathcal{J} = \begin{pmatrix} \frac{\partial}{\partial u}\frac{\partial u}{\partial t} & \frac{\partial}{\partial v}\frac{\partial u}{\partial t} \\ \frac{\partial}{\partial u}\frac{\partial v}{\partial t} & \frac{\partial}{\partial v}\frac{\partial v}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 & \partial_{||} \\ \partial_{||} & 0 \end{pmatrix} \tag{8}$$

In this case $\frac{\partial u}{\partial t}$ doesn't depend on u nor $\frac{\partial v}{\partial t}$ on v, so the diagonal is empty. Since the equations are linear, the Jacobian doesn't depend on u or v and so

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \mathcal{J}\begin{pmatrix} u \\ v \end{pmatrix} \tag{9}$$

In general for non-linear functions $\mathcal{J}$ gives the change in time-derivatives in response to changes in the state variables u and v.

In implicit time stepping, the preconditioner needs to solve an equation

$$\mathcal{I} - \gamma\mathcal{J} \tag{10}$$

[5]Taken from a talk by L.Chacon available here `https://bout.llnl.gov/pdf/workshops/2011/talks/Chacon_bout2011.pdf`

where $\mathcal{I}$ is the identity matrix, and γ depends on the time step and method (e.g. $\gamma = \delta t^2$ for backwards Euler method). For the simple wave equation problem, this is

$$\mathcal{I} - \gamma\mathcal{J} = \begin{pmatrix} 1 & -\gamma\partial_{||} \\ -\gamma\partial_{||} & 1 \end{pmatrix} \tag{11}$$

This matrix can be block inverted using Schur factorisation[6]

$$\begin{pmatrix} \mathbf{E} & \mathbf{U} \\ \mathbf{L} & \mathbf{D} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{I} & -\mathbf{E}^{-1}\mathbf{U} \\ 0 & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{E}^{-1} & 0 \\ 0 & \mathbf{P}_{Schur}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{I} & 0 \\ -\mathbf{L}\mathbf{E}^{-1} & \mathbf{I} \end{pmatrix} \tag{12}$$

where $\mathbf{P}_{Schur} = \mathbf{D} - \mathbf{L}\mathbf{E}^{-1}\mathbf{U}$ Using this, the wave problem becomes:

$$\begin{pmatrix} 1 & -\gamma\partial_{||} \\ -\gamma\partial_{||} & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & \gamma\partial_{||} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \left(1 - \gamma^2\partial_{||}^2\right)^{-1} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \gamma\partial_{||} & 1 \end{pmatrix} \tag{13}$$

The preconditioner is implemented by defining a function of the form

```
int precon(BoutReal t, BoutReal gamma, BoutReal delta) {
  ...
}
```

which takes as input the current time, the γ factor appearing above, and δ which is only important for constrained problems (not discussed here... yet). The current state of the system is stored in the state variables (here `u` and `v`), whilst the vector to be preconditioned is stored in the time derivatives (here `ddt(u)` and `ddt(v)`). At the end of the preconditioner the result should be in the time derivatives. A preconditioner which is just the identity matrix and so does nothing is therefore:

```
int precon(BoutReal t, BoutReal gamma, BoutReal delta) {
}
```

NOTE: This changed in github/bendudson on 15th Aug 2014. In older versions the result must be returned in the state variables

To implement the preconditioner in equation 13, first apply the rightmost matrix to the given vector:

$$\begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \gamma\partial_{||} & 1 \end{pmatrix} \begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} \tag{14}$$

[6] See paper `http://arxiv.org/abs/1209.2054` for an application to 2-fluid equations

```
int precon(BoutReal t, BoutReal gamma, BoutReal delta) {
  mesh->communicate(ddt(u));
  //ddt(u) = ddt(u);
  ddt(v) = gamma*Grad_par(ddt(u)) + ddt(v);
```

note that since the preconditioner is linear, it doesn't depend on u or v. As in the RHS function, since we are taking a differential of `ddt(u)`, it first needs to be communicated to exchange guard cell values.

The second matrix

$$\begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} \leftarrow \begin{pmatrix} 1 & 0 \\ 0 & \left(1 - \gamma^2 \partial_{||}^2\right)^{-1} \end{pmatrix} \begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} \tag{15}$$

doesn't alter u, but solves a parabolic equation in the parallel direction. There is a solver class to do this called `InvertPar` which solves the equation $\left(A + B\partial_{||}^2\right) x = b$ where A and B are `Field2D` or constants[7]. In `physics_init` we create one of these solvers:

```
InvertPar *inv; // Parallel inversion class
int physics_init(bool restarting) {
   ...
   inv = InvertPar::Create();
   inv->setCoefA(1.0);
   ...
}
```

In the preconditioner we then use this solver to update v:

```
  inv->setCoefB(-SQ(gamma));
  ddt(v) = inv->solve(ddt(v));
```

which solves $ddt(v) \leftarrow \left(1 - \gamma^2 \partial_{||}^2\right)^{-1} ddt(v)$. The final matrix just updates u using this new solution for v

$$\begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} \leftarrow \begin{pmatrix} 1 & \gamma\partial_{||} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \texttt{ddt(u)} \\ \texttt{ddt(v)} \end{pmatrix} \tag{16}$$

```
  mesh->communicate(ddt(v));
  ddt(u) = ddt(u) + gamma*Grad_par(ddt(v));
```

Finally, boundary conditions need to be imposed, which should be consistent with the conditions used in the RHS

[7] This `InvertPar` class can handle cases with closed field-lines and twist-shift boundary conditions for tokamak simulations

```
  ddt(u).applyBoundary("dirichlet");
  ddt(v).applyBoundary("dirichlet");
```

To use the preconditioner, pass the function to the solver in `physics_init`

```
1 int physics_init(bool restarting) {
2   solver->setPrecon(precon);
3   ...
4 }
```

then in the `BOUT.inp` settings file switch on the preconditioner

```
[solver]
type = cvode          # Need CVODE or PETSc
use_precon = true     # Use preconditioner
rightprec = false     # Use Right preconditioner (default left)
```

9.4 Jacobian function

9.5 DAE constraint equations

Using the IDA solver, BOUT++ can solve Differential Algebraic Equations (DAEs), in which algebraic constraints are used for some variables.

9.6 Monitoring the simulation output

Monitoring of the solution can be done at two levels: output monitoring, and timestep monitoring. Output monitoring occurs only when data is written to file, whereas timestep monitoring is every timestep and so (usually) much more frequent. Examples of both are in **examples/monitor** and **examples/monitor-newapi**.

Output monitoring: At every output timestep the solver calls a monitor function, which writes the output dump file, calculates and prints timing information and estimated time remaining. If you want to run additional code or write data to a different file, you can add monitor function(s).

You can call your output monitor function whatever you like, but it must have 4 inputs and return an int:

```
1 int my_output_monitor(Solver *solver, BoutReal simtime, int iter, int↩
    NOUT) {
2   ...
3 }
```

The first input is the solver object, the second is the current simulation time, the third is the output number, and the last is the total number of outputs requested. To get the solver to call this function every output time, put in your `physics_init` code:

```
  solver->addMonitor(my_output_monitor);
```

If you want to later remove a monitor, you can do so with

```
  solver->removeMonitor(my_output_monitor);
```

A simple example using this monitor is:

```
int my_output_monitor(Solver *solver, BoutReal simtime, int iter, int NOUT) {
  output.write("My monitor, time = %e, dt = %e\n",
      simtime, solver->getCurrentTimestep());
}

int physics_init(bool restarting) {
  solver->addMonitor(my_monitor);
}
```

See the monitor example (**examples/monitor**) for full code.

Timestep monitoring: This works in the same way as output monitoring. First define a monitor function:

```
int my_timestep_monitor(Solver *solver, BoutReal simtime, BoutReal lastdt) {
  ...
}
```

where `simtime` will again contain the current simulation time, and `lastdt` the last timestep taken. Add this function to the solver:

```
  solver->addTimestepMonitor(my_timestep_monitor);
```

Timestep monitoring is disabled by default, unlike output monitoring. To enable timestep monitoring, set in the options file (BOUT.inp):

```
[solver]
monitor_timestep = true
```

or put on the command line `solver:monitor_timestep=true` . When this is enabled, it will change how solvers like CVODE and PVODE (the default solvers) are used. Rather than being run in NORMAL mode, they will instead be run in SINGLE_STEP mode (see the SUNDIALS notes here:`http://computation.llnl.gov/casc/sundials/support/notes.html`). This may in some cases be less efficient.

10 Boundary conditions

NOTE: The boundary conditions are currently not set in the corner cells. Therefore: When using stecils which uses corner cells (like the Arakawa scheme) care must be taken, and the boundary conditions in the corner cells must be set manually.

Like the variable initialisation, boundary conditions can be set for each variable in individual sections, with default values in a section `[All]`. Boundary conditions are specified for each variable, being applied to variable itself during initialisation, and the time-derivatives at each timestep. They are a combination of a basic boundary condition, and optional modifiers.

When finding the boundary condition for a variable `var` on a boundary region, the options are checked in order from most to least specific:

- Section `var`, `bndry_` + region name. Depending on the mesh file, regions of the grid are given labels. Currently these are `core`, `sol`, `pf` and `target` which are intended for tokamak edge simulations. Hence the variables checked are `bndry_core`, `bndry_pf` etc.
- Section `var`, `bndry_` + boundary side. These names are `xin`, `xout`, `yup` and `ydown`.
- Section `var`, variable `bndry_all`
- The same settings again except in section `All`.

The default setting for everything is therefore `bndry_all` in the `All` section.

Boundary conditions are given names, with optional arguments in brackets. Currently implemented boundary conditions are:

- `dirichlet` - Set to zero
- `dirichlet(<number>)` - Set to some number e.g. `dirichlet(1)` sets the boundary to 1.0
- `neumann` - Zero gradient
- `robin` - A combination of zero-gradient and zero-value $af + b\frac{\partial f}{\partial x} = g$ where the syntax is `robin(a, b, g)`.
- `constgradient` - Constant gradient across boundary
- `zerolaplace` - Laplacian = 0, decaying solution (X boundaries only)

- `zerolaplace2` - Laplacian = 0, using coefficients from the Laplacian inversion and Delp2 operator.
- `constlaplace` - Laplacian = const, decaying solution (X boundaries only)

The zero- or constant-Laplacian boundary conditions works as follows:

$$\begin{aligned}\nabla_\perp^2 f =& 0 \\ \simeq & \quad g^{xx}\frac{\partial^2 f}{\partial x^2} + g^{zz}\frac{\partial^2 f}{\partial z^2}\end{aligned}$$

which when Fourier transformed in z becomes:

$$g^{xx}\frac{\partial^2 \hat{f}}{\partial x^2} - g^{zz}k_z^2\hat{f} = 0 \tag{17}$$

which has the solution

$$\hat{f} = Ae^{xk_z\sqrt{g^{zz}/g^{xx}}} + Be^{-xk_z\sqrt{g^{zz}/g^{xx}}} \tag{18}$$

Assuming that the solution should decay away from the domain, on the inner x boundary $B = 0$, and on the outer boundary $A = 0$. Boundary modifiers change the behaviour of boundary conditions, and more than one modifier can be used. Currently the following are available:

- `relax` - Relaxing boundaries. Evolve the variable towards the given boundary condition at a given rate
- `shifted` - Apply boundary conditions in orthogonal X-Z coordinates, rather than field-aligned
- `width` - Modifies the width of the region over which the boundary condition is applied

These are described in the following subsections.

10.1 Relaxing boundaries

All boundaries can be modified to be "relaxing" which are a combination of zero-gradient time-derivative, and whatever boundary condition they are applied to. The idea is that this prevents sharp discontinuities at boundaries during transients, whilst maintaining the desired boundary condition on longer time-scales. In some cases this can improve the numerical stability and timestep.

For example, `relax(dirichlet)` will make a field f at point i in the boundary follow a point $i-1$ in the domain:

$$\left.\frac{\partial f}{\partial t}\right|_i = \left.\frac{\partial f}{\partial t}\right|_{i-1} - f_i/\tau \tag{19}$$

where τ is a time-scale for the boundary (currently set to 0.1, but will be a global option). When the time-derivatives are slow close to the boundary, the boundary relaxes to the desired condition (Dirichlet in this case), but when the time-derivatives are large then the boundary approaches Neumann to reduce discontinuities.

By default, the relaxation rate is set to 10 (i.e. a time-scale of $\tau = 0.1$). To change this, give the rate as the second argument e.g. `relax(dirichlet, 2)` would relax to a Dirichlet boundary condition at a rate of 2.

10.2 Shifted boundaries

By default boundary conditions are applied in field-aligned coordinates, where y is along field-lines but x has a discontinuity at the twist-shift location. If radial derivatives are being done in shifted coordinates where x and z are orthogonal, then boundary conditions should also be applied in shifted coordinates. To do this, the `shifted` boundary modifier applies a z shift, applies the boundary condition, then shifts back. For example:

```
bndry_core = shifted( neumann )
```

would ensure that radial derivatives were zero in shifted coordinates on the core boundary.

10.3 Changing the width of boundaries

To change the width of a boundary region, the `width` modifier changes the width of a boundary region before applying the boundary condition, then changes the width back afterwards. To use, specify the boundary condition and the width, for example

```
bndry_core = width( neumann , 4 )
```

would apply a Neumann boundary condition on the innermost 4 cells in the core, rather than the usual 2. When combining with other boundary modifiers, this should be applied first e.g.

```
bndry_sol = width( relax( dirichlet ), 3)
```

would relax the last 3 cells towards zero, whereas

```
bndry_sol = relax( width( dirichlet, 3) )
```

would only apply to the usual 2, since relax didn't use the updated width.

Limitations:

1. Because it modifies then restores a globally-used BoundaryRegion, this code is not thread safe.
2. Boundary conditions can't be applied across processors, and no checks are done that the width asked for fits within a single processor.

10.4 Examples

This example is taken from the UEDGE benchmark test (in `examples/uedge-benchmark`):

```
[All]
bndry_all = neumann # Default for all variables, boundaries

[Ni]
bndry_target = neumann
bndry_core = relax(dirichlet(1.))   # 1e13 cm^-3 on core boundary
bndry_all  = relax(dirichlet(0.1))  # 1e12 cm^-3 on other boundaries

[Vi]
bndry_ydown = relax(dirichlet(-1.41648))   # -3.095e4/Vi_x
bndry_yup   = relax(dirichlet( 1.41648))
```

The variable `Ni` (density) is set to a Neumann boundary condition on the targets (yup and ydown), relaxes towards 1 on the core boundary, and relaxes to 0.1 on all other boundaries. Note that the `bndry_target = neumann` needs to be in the `Ni` section: If we just had

```
[All]
bndry_all = neumann # Default for all variables, boundaries

[Ni]
bndry_core = relax(dirichlet(1.))   # 1e13 cm^-3 on core boundary
bndry_all  = relax(dirichlet(0.1))  # 1e12 cm^-3 on other boundaries
```

then the "target" boundary condition for `Ni` would first search in the `[Ni]` section for `bndry_target`, then for `bndry_all` in the `[Ni]` section. This is set to `relax(dirichlet(0.1))`, not the Neumann condition desired.

10.5 Boundary regions

The boundary condition code (see section **??**) needs ways to loop over the boundary regions, without needing to know the details of the mesh.

At the moment two mechanisms are provided: A RangeIterator over upper and lower Y boundaries, and a vector of BoundaryRegion objects.

```
1 // Boundary region iteration
2 virtual const RangeIterator iterateBndryLowerY() const = 0;
3 virtual const RangeIterator iterateBndryUpperY() const = 0;
4
5 bool hasBndryLowerY();
6 bool hasBndryUpperY();
7
8 bool BoundaryOnCell; // NB: DOESN'T REALLY BELONG HERE
```

The `RangeIterator` class is an iterator which allows looping over a set of indices. Details are given in section **??**. For example, in **src/solver/solver.cxx** to loop over the upper Y boundary of a 2D variable `var`:

```
1 for(RangeIterator xi = mesh->iterateBndryUpperY(); !xi.isDone(); xi↩
     ++) {
2   ...
3 }
```

The `BoundaryRegion` class is defined in **include/boundary_region.hxx**

10.6 Boundary regions

Different regions of the boundary such as "core", "sol" etc. are labelled by the `Mesh` class (i.e. `BoutMesh`), which implements a member function defined in **mesh.hxx**:

```
150   // Boundary regions
151   virtual vector<BoundaryRegion*> getBoundaries() = 0;
```

This returns a vector of pointers to `BoundaryRegion` objects, each of which describes a boundary region with a label, a `BndryLoc` location (i.e. inner x, outer x, lower y, upper y or all), and iterator functions for looping over the points. This class is defined in **boundary_region.hxx**:

```
12 /// Describes a region of the boundary, and a means of iterating over↩
       it
13 class BoundaryRegion {
14   public:
15   BoundaryRegion();
16   BoundaryRegion(const string &name, int xd, int yd);
17   virtual ~BoundaryRegion();
18
```

```
19   string label; // Label for this boundary region
20
21   BndryLoc location; // Which side of the domain is it on?
22
23   int x,y; // Indices of the point in the boundary
24   int bx, by; // Direction of the boundary [x+dx][y+dy] is going ↩
        outwards
25
26   virtual void first() = 0;
27   virtual void next() = 0; // Loop over every element from inside out↩
         (in X or
28 Y first)
29   virtual void nextX() = 0; // Just loop over X
30   virtual void nextY() = 0; // Just loop over Y
31   virtual bool isDone() = 0; // Returns true if outside domain. Can ↩
        use this
32 with nested nextX, nextY
33 };
```

Example: To loop over all points in `BoundaryRegion *bndry` , use

```
for(bndry->first(); !bndry->isDone(); bndry->next()) {
  ...
}
```

Inside the loop, `bndry->x` and `bndry->y` are the indices of the point, whilst `bndry->bx` and `bndry->by` are unit vectors out of the domain. The loop is over all the points from the domain outwards i.e. the point `[bndry->x - bndry->bx][bndry->y - bndry->by]` will always be defined.

Sometimes it's useful to be able to loop over just one direction along the boundary. To do this, it is possible to use `nextX()` or `nextY()` rather than `next()`. It is also possible to loop over both dimensions using:

```
for(bndry->first(); !bndry->isDone(); bndry->nextX())
  for(; !bndry->isDone(); bndry->nextY()) {
    ...
  }
```

10.7 Boundary operations

On each boundary, conditions must be specified for each variable. The different conditions are imposed by `BoundaryOp` objects. These set the values in the boundary region such

that they obey e.g. Dirichlet or Neumann conditions. The `BoundaryOp` class is defined in **boundary_op.hxx**:

```
21 /// An operation on a boundary
22 class BoundaryOp {
23  public:
24   BoundaryOp() {bndry = NULL;}
25   BoundaryOp(BoundaryRegion *region)
26
27   // Note: All methods must implement clone, except for modifiers (↩
       see below)
28   virtual BoundaryOp* clone(BoundaryRegion *region, const list<string↩
       > &args);
29
30   /// Apply a boundary condition on field f
31   virtual void apply(Field2D &f) = 0;
32   virtual void apply(Field3D &f) = 0;
33
34   virtual void apply(Vector2D &f);
35
36   virtual void apply(Vector3D &f);
37
38   /// Apply a boundary condition on ddt(f)
39   virtual void apply_ddt(Field2D &f);
40   virtual void apply_ddt(Field3D &f);
41   virtual void apply_ddt(Vector2D &f);
42   virtual void apply_ddt(Vector3D &f);
43
44   BoundaryRegion *bndry;
45 };
```

(where the implementations have been removed for clarity). Which has a pointer to a `BoundaryRegion` object specifying which region this boundary is operating on.

Boundary conditions need to be imposed on the initial conditions (after `physics_init()`), and on the time-derivatives (after `physics_run()`). The `apply()` functions are therefore called during initialisation and given the evolving variables, whilst the `apply_ddt` functions are passed the time-derivatives.

To implement a boundary operation, as a minimum the `apply(Field2D)`, `apply(Field2D)` and `clone()` need to be implemented: By default the `apply(Vector)` will call the `apply(Field)` functions on each component individually, and the `apply_ddt()` functions just call the `apply()` functions.

Example: Neumann boundary conditions are defined in **boundary_standard.hxx**:

```
22 /// Neumann (zero-gradient) boundary condition
23 class BoundaryNeumann : public BoundaryOp {
24  public:
25   BoundaryNeumann() {}
26  BoundaryNeumann(BoundaryRegion *region):BoundaryOp(region) { }
27   BoundaryOp* clone(BoundaryRegion *region, const list<string> &args)↩
       ;
28   void apply(Field2D &f);
29   void apply(Field3D &f);
30 };
```

and implemented in **boundary_standard.cxx**

```
52 void BoundaryNeumann::apply(Field2D &f) {
53   // Loop over all elements and set equal to the next point in
54   for(bndry->first(); !bndry->isDone(); bndry->next())
55     f[bndry->x][bndry->y] = f[bndry->x - bndry->bx][bndry->y - bndry↩
         ->by];
56 }
57
58 void BoundaryNeumann::apply(Field3D &f) {
59   for(bndry->first(); !bndry->isDone(); bndry->next())
60     for(int z=0;z<mesh->ngz;z++)
61       f[bndry->x][bndry->y][z] = f[bndry->x - bndry->bx][bndry->y -
62 bndry->by][z];
63 }
```

This is all that's needed in this case since there's no difference between applying Neumann conditions to a variable and to its time-derivative, and Neumann conditions for vectors are just Neumann conditions on each vector component.

To create a boundary condition, we need to give it a boundary region to operate over:

```
BoundaryRegion *bndry = ...
BoundaryOp op = new BoundaryOp(bndry);
```

The `clone` function is used to create boundary operations given a single object as a template in `BoundaryFactory`. This can take additional arguments as a vector of strings - see explanation in section 10.9.

10.8 Boundary modifiers

To create more complicated boundary conditions from simple ones (such as Neumann conditions above), boundary operations can be modified by wrapping them up in a `BoundaryModifier` object, defined in **boundary_op.hxx**:

```
63 class BoundaryModifier : public BoundaryOp {
64  public:
65   virtual BoundaryOp* clone(BoundaryOp *op, const list<string> &args)↩
         = 0;
66  protected:
67   BoundaryOp *op;
68 };
```

Since `BoundaryModifier` inherits from `BoundaryOp`, modified boundary operations are just a different boundary operation and can be treated the same (Decorator pattern). Boundary modifiers could also be nested inside each other to create even more complicated boundary operations. Note that the `clone` function is different to the `BoundaryOp` one: instead of a `BoundaryRegion` to operate on, modifiers are passed a `BoundaryOp` to modify.

Currently the only modifier is `BoundaryRelax`, defined in **boundary_standard.hxx**:

```
64 /// Convert a boundary condition to a relaxing one
65 class BoundaryRelax : public BoundaryModifier {
66  public:
67   BoundaryRelax(BoutReal rate) {r = fabs(rate);}
68   BoundaryOp* clone(BoundaryOp *op, const list<string> &args);
69
70   void apply(Field2D &f);
71   void apply(Field3D &f);
72
73   void apply_ddt(Field2D &f);
74   void apply_ddt(Field3D &f);
75  private:
76   BoundaryRelax() {} // Must be initialised with a rate
77   BoutReal r;
78 };
```

10.9 Boundary factory

The boundary factory creates new boundary operations from input strings, for example turning "relax(dirichlet)" into a relaxing Dirichlet boundary operation on a given region. It is defined in **boundary_factory.hxx** as a Singleton, so to get a pointer to the boundary factory use

```
  BoundaryFactory *bfact = BoundaryFactory::getInstance();
```

and to delete this singleton, free memory and cleanup at the end use:

```
  BoundaryFactory::cleanup();
```

Because users should be able to add new boundary conditions during `physics_init()`, boundary conditions are not hard-wired into `BoundaryFactory`. Instead, boundary conditions must be registered with the factory, passing an instance which can later be cloned. This is done in **bout++.cxx** for the standard boundary conditions:

```
258  BoundaryFactory* bndry = BoundaryFactory::getInstance();
259  bndry->add(new BoundaryDirichlet(), "dirichlet");
260  ...
261  bndry->addMod(new BoundaryRelax(10.), "relax");
```

where the `add` function adds BoundaryOp objects, whereas `addMod` adds `BoundaryModifier` objects. **Note**: The objects passed to `BoundaryFactory` will be deleted when `cleanup()` is called.

When a boundary operation is added, it is given a name such as "dirichlet", and similarly for the modifiers ("relax" above). These labels and object pointers are stored internally in `BoundaryFactory` in maps defined in **boundary_factory.hxx**:

```
43  // Database of available boundary conditions and modifiers
44  map<string, BoundaryOp*> opmap;
45  map<string, BoundaryModifier*> modmap;
```

These are then used by `BoundaryFactory::create()`:

```
24  /// Create a boundary operation object
25  BoundaryOp* create(const string &name, BoundaryRegion *region);
26  BoundaryOp* create(const char* name, BoundaryRegion *region);
```

to turn a string such as "relax(dirichlet)" and a `BoundaryRegion` pointer into a `BoundaryOp` object. These functions are implemented in **boundary_factory.cxx**, starting around line 42. The parsing is done recursively by matching the input string to one of:

- `modifier(<expression>, arg1, ...)`
- `modifier(<expression>)`
- `operation(arg1, ...)`
- `operation`

the `<expression>` variable is then resolved into a BoundaryOp object by calling `create(<expression, region)`.

When an operator or modifier is found, it is created from the pointer stored in the `opmap` or `modmap` maps using the `clone` method, passing a `list<string>` reference containing any arguments. It's up to the operation implementation to ensure that the correct number of arguments are passed, and to parse them into floats or other types.

Example: The Dirichlet boundary condition can take an optional argument to change the value the boundary's set to. In **boundary_standard.cxx**:

```
13 BoutReal BoundaryDirichlet::clone(BoundaryRegion *region, const list<string>
14 &args) {
15   if(!args.empty()) {
16     // First argument should be a value
17     stringstream ss;
18     ss << args.front();
19
20     BoutReal val;
21     ss >> val;
22     return new BoundaryDirichlet(region, val);
23   }
24   return new BoundaryDirichlet(region);
25 }
```

If no arguments are passed i.e. the string was "dirichlet" or "dirichlet()" then the `args` list is empty, and the default value (0.0) is used. If one or more arguments is used then the first argument is parsed into a `BoutReal` type and used to create a new `BoundaryDirichlet` object. If more arguments are passed then these are just ignored; probably a warning should be printed.

To set boundary conditions on a field, `FieldData` methods are defined in **field_data.hxx**:

```
1 // Boundary conditions
2   void setBoundary(const string &name); ///< Set the boundary conditions
3   void setBoundary(const string &region, BoundaryOp *op); ///< Manually set
4   virtual void applyBoundary() {}
5   virtual void applyTDerivBoundary() {};
6  protected:
7   vector<BoundaryOp*> bndry_op; // Boundary conditions
```

The `setBoundary(const string &name)` method is implemented in **field_data.cxx**. It first gets a vector of pointers to `BoundaryRegions` from the mesh, then loops over these calling `BoundaryFactory::createFromOptions` for each one and adding the resulting boundary operator to the `bndry_op` vector.

11 Generating input grids

The simulation mesh describes the number and topology of grid points, the spacing between them, and the coordinate system. For many problems, a simple mesh can be created using options.

```
[mesh]
nx = 260  # X grid size
ny = 256  # Y grid size

dx = 0.1  # X mesh spacing
dy = 0.1  # Y mesh spacing
```

The above options will create a 260×256 mesh in X and Y (MZ option sets Z resolution), with mesh spacing of 0.1 in both directions. By default the coordinate system is Cartesian (metric tensor is the identity matrix), but this can be changed by specifying the metric tensor components.

Integer quantities such as `nx` must be numbers (like "260"), not expressions (like "256 + 2*MXG"). Real (floating-point) values can be expressions, allowing quite complicated analytic inputs. For example in the example `test-griddata`:

```
# Screw pinch

rwidth = 0.4

Rxy = 0.1 + rwidth*x  # Radius from axis      [m]
L   = 10              # Length of the device  [m]

dy = L/ny
hthe = 1.0

Zxy = L * y / (2*pi)

Bpxy = 1.0      # Axial field [T]
Btxy = 0.1*Rxy  # Azimuthal field [T]
Bxy = sqrt(Btxy^2 + Bpxy^2)

dr = rwidth / nx
dx = dr * Bpxy * Rxy
```

These expressions use the same mechanism as used for variable initialisation (section 7.0.2): `x` is a variable from 0 to 1 in the domain which is uniform in index space; `y` and `z` go from 0 to 2π. As with variable initialisation, common trigonometric and mathematical

functions can be used. In the above example, some variables depend on each other, for example `dy` depends on `L` and `ny`. The order in which these variables are defined doesn't matter, so `L` could be defined below `dy`, but circular dependencies are not allowed. If the variables are defined in the same section (as `dy` and `L`) then no section prefix is required. To refer to a variable in a different section, prefix the variable with the section name e.g. "`section:variable`".

More complex meshes can be created by supplying an input grid file to describe the grid points, geometry, and starting profiles. Currently BOUT++ supports either NetCDF, HDF5 or PDB format binary files. During startup, BOUT++ looks in the grid file for the following variables. If any are not found, a warning will be printed and the default values used.

- X and Y grid sizes (integers) `nx` and `ny` **REQUIRED**
- Differencing quantities in 2D arrays `dx[nx][ny]` and `dy[nx][ny]`. If these are not found they will be set to 1.
- Diagonal terms of the metric tensor g^{ij} `g11[nx][ny]`, `g22[nx][ny]`, and `g33[nx][ny]`. If not found, these will be set to 1.
- Off-diagonal metric tensor g^{ij} elements `g12[nx][ny]`, `g13[nx][ny]`, and `g23[nx][ny]`. If not found, these will be set to 0.
- Z shift for sheared grids `zshift[nx][ny]`. This is intended for dpsi derivatives in sheared coordinates. If not found, set to zero.

The remaining quantities determine the topology of the grid. These are based on tokamak single/double-null configurations, but can be adapted to many other situations.

- Separatrix locations `ixseps1`, and `ixseps2` If neither is given, both are set to nx (i.e. all points in closed "core" region). If only `ixseps1` is found, `ixseps2` is set to nx, and if only ixseps2 is found, ixseps1 is set to -1.
- Branch-cut locations `jyseps1_1`, `jyseps1_2`, `jyseps2_1`, and `jyseps2_2`
- Twist-shift matching condition `twistshift[nx]`. This is applied in the "core" region between indices `jyseps2_2`, and `jyseps1_1 + 1`, if enabled in the options file. If not given, this is set to zero.

NOTE: All input quantities should be normalised - no normalisation is performed by the BOUT++ code. Normalisation can be performed in the initialisation code, provided a call to `geometry()` is made after any changes to the metrics.
For users of BOUT, the radial derivative is `dx = dpsi / (bmag/1e4)`

The only quantities which are required are the sizes of the grid. If these are the only quantities specified, then the coordinates revert to Cartesian.

This section describes how to generate inputs for tokamak equilibria. If you're not interested in tokamaks then you can skip to the next section.

The directory `tokamak_grids` contains code to generate input grid files for tokamaks. These can be used by the `2fluid` and `highbeta_reduced` modules, and are (mostly) compatible with inputs to the BOUT-06 code.

Figure 2 shows the routines and file formats used in taking output from different codes and converting into input to BOUT++.

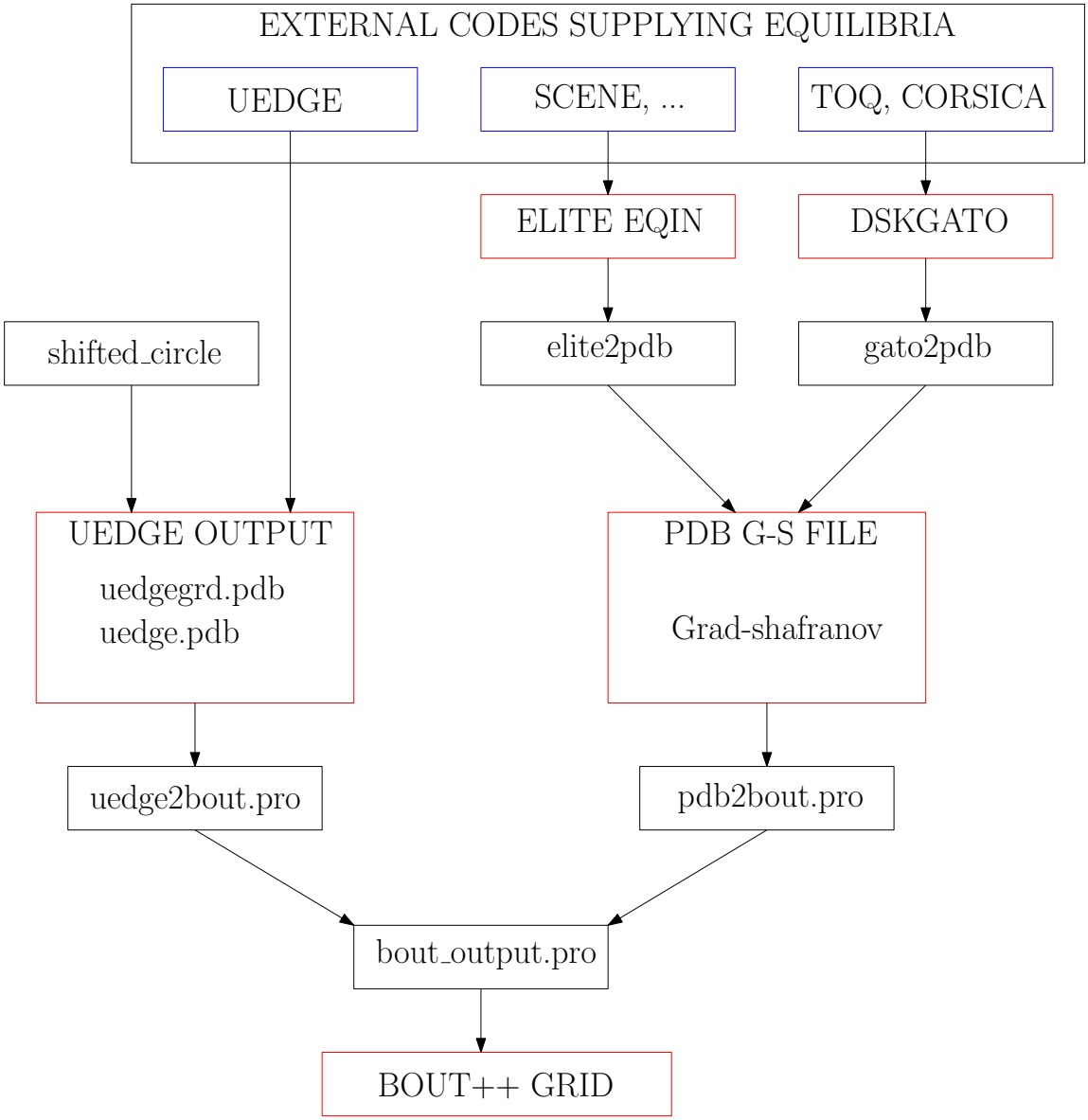


Figure 2: Generation of BOUT++ grid files. In red are the file formats, and in black the conversion routines. Blue are external codes.

11.1 BOUT++ Topology

11.1.1 Basic

In order to handle tokamak geometry BOUT++ contains an internal topology which is determined by the branch-cut locations (`jyseps1_1`, `jyseps1_2`, `jyseps2_1`, and `jyseps2_2`) and separatrix locations (`ixseps1` and `ixseps2`).

The separatrix locations, `ixseps1` and `ixseps2`, give the indices in the `x` domain where the first and second separatrices are located.

If `ixseps1 == ixseps2` then there is a single separatrix representing the boundary between the core region and the SOL region and the grid is a connected double null configuration. If `ixseps1 > ixseps2` then there are two separatrices and the inner separatrix is `ixseps2` so the tokamak is an upper double null. If `ixseps1 < ixseps2` then there are two separatrices and the inner separatrix is `ixseps1` so the tokamak is a lower double null.

In other words: Let us for illustrative purposes say that `ixseps1 > ixseps2` (see figure 3). Let us say that we have a field `f(x,y,z)` with a global `x`-index which includes ghost points. `f(x<=xseps1,y,z)`) will then be periodic in the `y`-direction, `f(xspes1<x<=xseps2,y,z)`) will have boundary condition in the `y`-direction set by the lowermost `ydown` and `yup`. If `f(xspes2<x,y,z)`) the boundary condition in the `y`-direction will be set by the uppermost `ydown` and `yup`. As for now, there is no difference between the two sets of upper and lower `ydown` and `yup` boundary conditions (unless manually specified, see section 12.5.1).

These values are set either in the grid file or in `BOUT.inp`. Figure 3 shows schematically how `ixseps` is used.

The branch cut locations, `jyseps1_1`, `jyseps1_2`, `jyseps2_1`, and `jyseps2_2`, split the `y` domain into logical regions defining the SOL, the PFR (private flux region) and the core of the tokamak. This is illustrated also in figure 3. If `jyseps1_2 == jyseps2_1` then the grid is a single null configuration, otherwise the grid is a double null configuration.

11.1.2 Advanced

The internal domain in BOUT++ is deconstructed into a series of logically rectangular subdomains with boundaries determined by the `ixseps` and `jyseps` parameters. The boundaries coinside with processor boundaries so the number of grid points within each subdomain must be an integer multiple of `ny/nypes` where `ny` is the number of grid points in `y` and `nypes` is the number of processors used to split the y domain. Processor communication across the domain boundaries is then handled internally. Figure 4 shows schematically how the different regions of a double null tokamak with `ixseps1 = ixseps2` are connected together via communications.

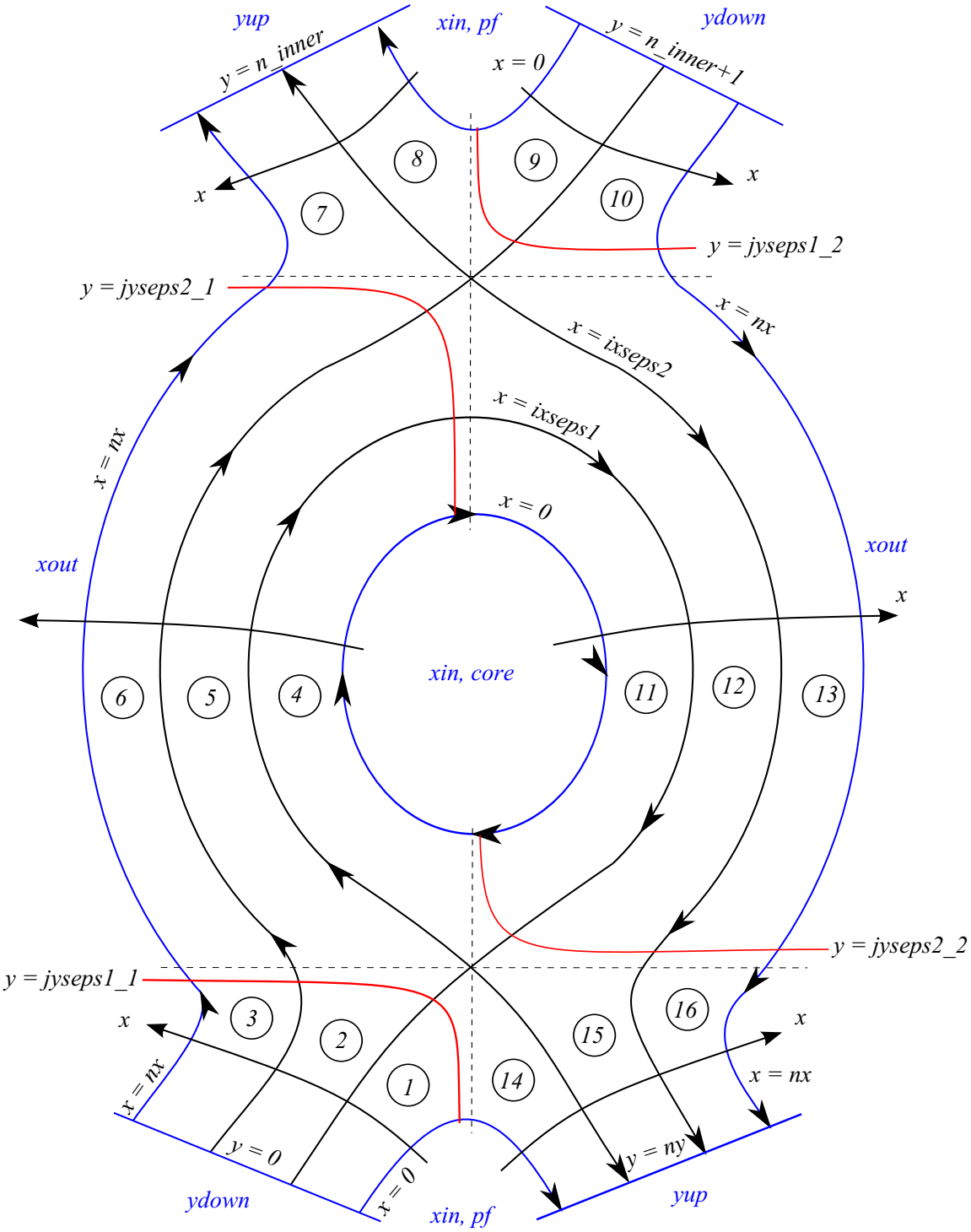


Figure 3: Deconstruction of a poloidal tokamak cross-section into logical domains using the parameters `ixseps1`, `ixseps2`, `jyseps1_1`, `jyseps1_2`, `jyseps2_1`, and `jyseps2_2`.

NOTE: To ensure that each subdomain follows logically, the `jyseps` indices must adhere to the following conditions:

- `jyseps1_1 > -1`
- `jyseps2_1` $\geq$ `jyseps1_1 + 1`
- `jyseps1_2` $\geq$ `jyseps2_1`
- `jyseps2_2` $\leq$ `ny -1`

To ensure that communications work branch cuts must align with processor boundaries.

11.1.3 Implementations

11.2 3D variables

BOUT++ was originally designed for tokamak simulations where the input equilibrium varies only in X-Y, and Z is used as the axisymmetric toroidal angle direction. In those cases, it is often convenient to have input grids which are only 2D, and allow the Z dimension to be specified independently, such as in the options file. The problem then is how to store 3D variables in the grid file?

Two representations are now supported for 3D variables:

1. A Fourier representation. If the size of the toroidal domain is not specified in the grid file (`nz` is not defined), then 3D fields are stored as Fourier components. In the Z dimension the coefficients must be stored as

$$[n = 0, n = 1(\text{real}), n = 1(\text{imag}), n = 2(\text{real}), n = 2(\text{imag}), \ldots] \tag{20}$$

   where n is the toroidal mode number. The size of the array must therefore be odd in the Z dimension, to contain a constant ($n = 0$) component followed by real/imaginary pairs for the non-axisymmetric components.

   If you are using IDL to create a grid file, there is a routine in `tools/idllib/bout3dvar.pro` for converting between BOUT++'s real and Fourier representation.

2. Real space, as values on grid points. If `nz` is set in the grid file, then 3D variables in the grid file must have size `nx`×`ny`×`nz`. These are then read in directly into `Field3D` variables as required.

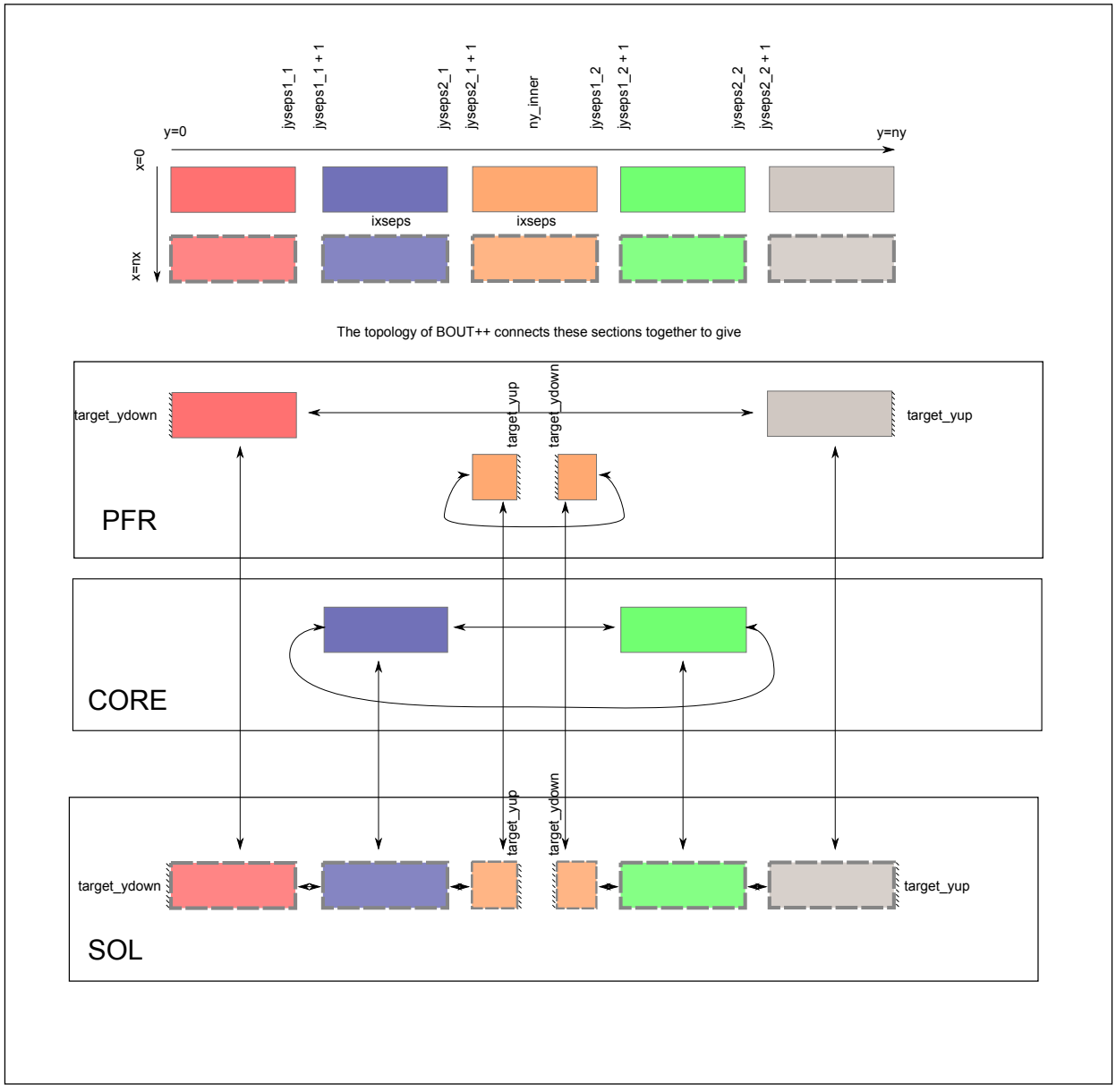


Figure 4: Schematic illustration of domain decomposition and communication in BOUT++ with `ixseps1 = ixseps2`.

11.3 From EFIT files

An IDL code called "Hypnotoad" has been developed to create BOUT++ input files from R-Z equilibria. This can read EFIT 'g' files, find flux surfaces, and calculate metric coefficients. The code is in **tools/tokamak_grids/gridgen**, and has its own manual under the **doc** subdirectory.

11.4 From ELITE and GATO files

Currently conversions exist for ELITE `.eqin` and GATO `dskgato` equilibrium files. Conversion of these into BOUT++ input grids is in two stages: In the first, both these input files are converted into a common NetCDF or PDB format which describes the Grad-Shafranov equilibrium. These intermediate files are then converted to BOUT++ grids using an interactive IDL script.

11.5 Generating equilibria

The directory `tokamak_grids/shifted_circle` contains IDL code to generate shifted circle (large aspect ratio) Grad-Shafranov equilibria.

11.6 Running pdb2bout

There are many options which are set interactively, so here's a run-through of the code (only showing most important outputs):

```
IDL> pdb2bout, "cbm18_dens6.dskgato.pdb", output="test.pdb"
***Maximum mu0p is       23071.7
Is this pressure (not mu0*pressure)?
```

This is needed because although many grid formats claim to store $\mu_0 P$, they actually store P. Since the given maximum value is very large, it must be in Pascals, so answer yes (y).

The grid will then be displayed along with the safety factor and pressure profiles against normalised ψ. In all three plots, a red line marks the location of the plasma edge. You must then choose the radial domain in normalised ψ:

```
Inner Psi boundary:0.6
Outer Psi boundary:1.2
Number of radial grid points:           69
Of which inside the plasma:           49
Is this range ok?
```

The plots will now also show two green lines for the inner and outer boundaries. Enter no (n) to specify a different range.

The code then checks to see if any plasma density of temperatures have been set in the input file:

```
====== SETTING PLASMA PROFILES =======
Some plasma parameters given in input file
Use given parameters?
```

Saying yes will just use the given values, but saying no will give you some more options:

```
Generating plasma profiles:
  1. Flat temperature profile
  2. Flat density profile
  3. Te proportional to density
Profile option:
```

The procedure is the same for each of these, so taking option 2 (flat density):

```
Setting flat density profile
Density [10^20 m^-3]:1.0
```

Anything can be entered here, depending on what you want to simulate. The code will ensure that whatever you enter, the equilibrium pressure is maintained. In this case the temperature is calculated from pressure and the specified density.

```
Maximum temperature (eV):      720.090
Is this ok?
```

NOTE: This is the maximum temperature anywhere on the input grid (i.e. in this case at $\psi = 0$), not just inside the chosen domain. Entering no will go back and you can specify a different density.

Earlier the radial resolution was printed, in this case 69 grid points. You can now change this if you need to:

```
Increase radial resolution?
```

Although it says increase, you can also decrease the resolution. Entering yes will allow you to enter a different number of radial grid points. It's recommended to use $2^n + 4$ grid points because this makes it easier to decompose the grid (4 cells for boundary, remainder equally divided between processors).

At this point, an orthogonal grid is generated:

```
======== GENERATING ORTHOGONAL COORDINATES FOR BOUT =========
Number of poloidal grid points: 64
Enter x index of equal hthe [0, 68] :35
```

Using 2^n points is highly recommended, but only because the points must be equally divided between processors. The x index of equal hthe shouldn't matter very much except for highly shaped plasmas. Recommend that you set it somewhere around the peak pressure gradient, or middle of the grid.

```
Interpolating Rxy
Interpolating Zxy
Is this ok?
```

Two plots are shown: On the left the original mesh, and on the right the new orthogonal mesh. If this doesn't look right you can enter 'no' and change the poloidal resolution and location of equal h_θ.

```
Add vacuum region?n
```

This is a little experimental, and extends the grid into vacuum. This is useful if the equilibrium supplied doesn't include a vacuum region. In this case we already have a vacuum region, so can answer no.

You're now presented with several options:

```
Equilibrium correction options:
  0  No correction
  1  RBt using force balance
  2  hthe and RBt using force balance and q (FAILS)
  3  hthe and RBt using force balance and jpar
Enter option:
```

Because the input Grad-Shafranov solution is probably not perfect to begin with, and has now been interpolated onto a new grid, the force balance in ballooning coordinates is not quite satisfied. These options attempt to correct the equilibrium slightly to ensure force balance, the given q profile, and the given $j_{||}$ profile. Option 1 can sometimes work well, other times it can fail to converge (as in this case). It's safe to just use option 0.

```
Calculating poloidal arc length dthe
Maximum difference in hthe:       0.23551123
Maximum percentage difference:        16.745859
Use new hthe?
```

A key metric in the BOUT/BOUT++ coordinates is the poloidal arc length h_θ. A plot will shot this quantity calculated geometrically (solid line), and calculated by enforcing force balance (red symbols) at the outboard midplane. The difference between these two methods is an indication of the quality of the Grad-Shafranov solution. Entering 'y' will use the "new" h_θ calculated from force balance, whilst 'n' will use the h_θ calculated geometrically. Personally. i prefer to make sure force balance is satisfied so enter 'y'.

```
Checking parallel current
****Equilibrium has -ve toroidal field
```

Because of the varied and confusing ways different codes define the poloidal and toroidal directions, this code currently just sets Bp and Bt positive, and then uses the expression for Jpar to work out what sign Bt should have. This is fine if you just want an equilibrium, but for detailed comparison to experiment where the sign of Bt may/will make a difference this needs to be changed.

Jpar calculated from quantities such as Bp, Bt and hthe is now shown as red symbols, with the jpar from the original Grad-Shafranov solution as a black line. Like the hthe display, this is a good consistency check.

```
Use new Jpar?
```

Entering 'y' will use the calculated jpar i.e. consistent with the other grid quantities, but probably more noisy and slightly different to the original. Entering 'n' will use the original jpar profiles.

```
q is negative. Reversing values from equilibrium
```

This can be printed because the q profile given in the grid file is almost always positive, whereas qsafe calculated by integrating the pitch angle can be positive or negative. In this case the toroidal field has been set negative (see above), and so qinty is negative too.

```
Use new qsafe?
```

As with hthe and jpar, the qsafe specified in the original grid file is plotted as a black line, and the value calculated by integrating quantities on the new mesh is shown as red symbols. Entering 'y' uses the values consistent on the new grid, whilst 'n' uses the original safety factor profile. In most cases i'd prefer the grid to be consistent, rather than being identical to the input, so answer 'y'. You may have to do some experimentation though.

```
****Minimum pressure is very small:       0.0000000
****Setting minimum pressure to 1% of maximum
```

This is because having negative pressures is very bad for BOUT/BOUT++ runs, and can easily be caused by overshoots or even rounding error when the pressure is too low. Because the equilibrium doesn't depend on absolute pressure, this just adds a constant pressure across the entire profile.

Finally, the grid file is written to PDB format

```
Cannot write 2 dimensional double dx. Writing as float
.
.
.
```

These warnings are because the PDB2IDL library currently doesn't have any functions for writing doubles, and pdb2bout does calculations in double precision. The output is therefore converted to single-precision floats.

12 Fluid equations

Once you have tried some example codes, and generally got the hang of running BOUT++ and analysing the results, there will probably come a time when you want to change the equations being solved. This section uses the ideal MHD equations as an example, demonstrating how a BOUT++ physics module is put together. It assumes you have a working knowledge of C or C++, but you don't need to be an expert - most of the messy code is hidden away from the physics module. There are several good books on C and C++, but I'd recommend online tutorials over books because there are a lot more of them, they're quicker to scan through, and they're cheaper.

When going through this section, it may help to refer to the finished code, which is given in the file `mhd.cxx` in the BOUT++ examples directory. The equations to be solved are:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\mathbf{v}\cdot\nabla\rho - \rho\nabla\cdot\mathbf{v} \\
\frac{\partial p}{\partial t} &= -\mathbf{v}\cdot\nabla p - \gamma p\nabla\cdot\mathbf{v} \\
\frac{\partial \mathbf{v}}{\partial t} &= -\mathbf{v}\cdot\nabla\mathbf{v} + \frac{1}{\rho}\left(-\nabla p + (\nabla\times\mathbf{B})\times\mathbf{B}\right) \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla\times(\mathbf{v}\times\mathbf{B})
\end{aligned}$$

There are two ways to specify a set of equations to solve in BOUT++. For advanced users, an object-oriented interface is available and described in section 14. The simplest way to start is to use a C-like interface and define two functions:

```
int physics_init(bool restarting) {
  return 0;
}

int physics_run(BoutReal t) {
  return 0;
}
```

The first of these is called once at the start of the simulation, and should set up the problem, specifying which variables are to be evolved. The argument `restarting` is false the first time a problem is run, and true if loading the state from a restart file.

The second function `physics_run` is called every time-step, and should calculate the time-derivatives for a given state. In both cases returning non-zero tells BOUT++ that an error occurred.

12.1 Variables

We need to define the variables to evolve as global variables (so they can be used in `physics_init` and `physics_run`.

> **NOTE**: Version 0.85 and earlier needed two variables to be defined, so if you're upgrading then you can remove the time-derivative variables

For ideal MHD, we need two 3D scalar fields density ρ and pressure p, and two 3D vector fields velocity v, and magnetic field B:

```
Field3D rho, p; // 3D scalar fields
Vector3D v, B;  // 3D vector fields

int physics_init(bool restarting) {
}
```

Scalar and vector fields behave much as you would expect: `Field3D` objects can be added, subtracted, multiplied, divided and exponentiated, so the following examples are all valid operations:

```
Field3D a, b, c;
BoutReal r;

a = b + c; a = b - c;
a = b * c; a = r * b;
a = b / c; a = b / r; a = r / b;
a = b ^ c; a = b ^ r; a = r ^ b;
```

Similarly, vector objects can be added/subtracted from each other, multiplied/divided by scalar fields and real numbers, for example:

```
Vector3D a, b, c;
Field3D f;
BoutReal r;

a = b + c; a = b - c;
a = b * f; a = b * r;
a = b / f; a = b / r;
```

In addition the dot and cross products are represented by `*` and $\wedge$ symbols:

```
Vector3D a, b, c;
Field3D f;

f = a * b // Dot-product
a = b ^ c // Cross-product
```

For both scalar and vector field operations, so long as the result of an operation is of the correct type, the usual C/C++ shorthand notation can be used:

```
Field3D a, b;
Vector3D v, w;

a += b; v *= a; v -= w; v ^= w; // valid
v *= w; // NOT valid: result of dot-product is a scalar
```

NOTE: In C++ the $\wedge$ operator has lower precedence than the `*` or `+` operators. To be safe, always put exponentiation and cross-product operations in brackets

12.2 Evolution equations

At this point we can tell BOUT++ which variables to evolve, and where the state and time-derivatives will be stored. This is done using the `bout_solve(variable, name)` function in `physics_init`:

```
int physics_init(bool restarting) {
  bout_solve(rho, "density");
  bout_solve(p,   "pressure");
  bout_solve(v,   "v");
  bout_solve(B,   "B");

  return 0;
}
```

The name given to this function will be used in the output and restart data files. These will be automatically read and written depending on input options (see section 6). Input

options based on these names are also used to initialise the variables.

If the name of the variable in the output file is the same as the variable name, you can use a shorthand macro. In this case, we could use this shorthand for `v` and `B`:

```
SOLVE_FOR(v);
SOLVE_FOR(B);
```

To make this even shorter, we can use macros `SOLVE_FOR2`, `SOLVE_FOR3`, ..., `SOLVE_FOR6` to shorten our initialisation code to

```
int physics_init(bool restarting) {
  bout_solve(rho, "density");
  bout_solve(p,   "pressure");
  SOLVE_FOR2(v, B);

  return 0;
}
```

The equations to be solved can now be written in the `physics_run` function. The value passed to the function (`BoutReal t`) is the simulation time - only needed if your equations contain time-dependent sources or similar terms. To refer to the time-derivative of a variable `var`, use `ddt(var)`. The ideal MHD equations can be written as:

```
int physics_run(BoutReal t) {
  ddt(rho) = -V_dot_Grad(v, rho) - rho*Div(v);
  ddt(p) = -V_dot_Grad(v, p) - gamma*p*Div(v);
  ddt(v) = -V_dot_Grad(v, v) + ( (Curl(B)^B) - Grad(p) ) / rho;
  ddt(B) = Curl(v^B);
}
```

Where the differential operators `vector = Grad(scalar)`, `scalar = Div(vector)`, and `vector = Curl(vector)` are used. For the density and pressure equations, the $\mathbf{v} \cdot \nabla \rho$ term could be written as `v*Grad(rho)`, but this would then use central differencing in the Grad operator. Instead, the function `V_dot_Grad` uses upwinding methods for these advection terms. In addition, the `Grad` function will not operate on vector objects (since result is neither scalar nor vector), so the $\mathbf{v} \cdot \nabla \mathbf{v}$ term CANNOT be written as `v*Grad(v)`.

12.3 Input options

Note that in the above equations the extra parameter `gamma` has been used. To enable this to be set in the input options file (see section 6), we use the `options` object in the initialisation function:

```
BoutReal gamma;
```

```
2
3  int physics_init(bool restarting) {
4    Options *globalOptions = Options::getRoot();
5    Options *options = globalOptions->getSection("mhd");
6
7    options->get("gamma", gamma, 5.0/3.0);
```

This specifies that an option called "gamma" in a section called "mhd" should be put into the variable `gamma`. If the option could not be found, or was of the wrong type, the variable should be set to a default value of 5/3. The value used will be printed to the output file, so if gamma is not set in the input file the following line will appear:

```
Option mhd / gamma = 1.66667 (default)
```

This function can be used to get integers and booleans. To get strings, there is the function (`char* options.getString(section, name)`. To separate options specific to the physics model, these options should be put in a separate section, for example here the "mhd" section has been specified. To save having to write the section name for every option, there is the `setSection` function:

```
1  BoutReal gamma;
2  int someint;
3
4  int physics_init(bool restarting) {
5    Options *globalOptions = Options::getRoot();
6    Options *options = globalOptions->getSection("mhd");
7
8    options->get("gamma", gamma, 5.0/3.0);
9    options->get("someint", someint, 0);
```

Most of the time, the name of the variable (e.g. `gamma`) will be the same as the identifier in the options file ("gamma"). In this case, there is the macro

```
OPTION(options, gamma, 5.0/3.0);
```

which is equivalent to

```
options->get("gamma", gamma, 5.0/3.0);
```

See section 6 for more details of how to use the input options.

12.4 Communication

If you plan to run BOUT++ on more than one processor, any operations involving y derivatives will require knowledge of data stored on other processors. To handle the necessary

parallel communication, there is the `mesh->communicate` function. This takes care of where the data needs to go to/from, and only needs to be told which variables to transfer.

If you only need to communicate a small number (up to 5 currently) of variables then just call the `mesh->communicate` function directly. For the MHD code, we need to communicate the variables `rho,p,v,B` at the beginning of the `physics_run` function before any derivatives are calculated:

```
1 int physics_run(BoutReal t) {
2   mesh->communicate(rho, p, v, B);
```

If you need to communicate lots of variables, or want to change at run-time which variables are evolved (e.g. depending on input options), then you can create a group of variables and communicate them later. To do this, first create a `FieldGroup` object , in this case called `comms` , then use the add method. This method does no communication, but records which variables to transfer when the communication is done later.

```
1  FieldGroup comms;
2
3  int physics_init() {
4    .
5    .
6    .
7    comms.add(rho);
8    comms.add(p);
9    comms.add(v);
10   comms.add(B);
11
12   return 0;
13 }
```

The `comms.add()` routine can be given up to 6 variables at once (there's no practical limit on the total number of variables which are added to a `FieldGroup`), so this can be shortened to

```
1  FieldGroup comms;
2
3  int physics_init() {
4    .
5    .
6    .
7    comms.add(rho, p, v, B);
8
9    return 0;
10 }
```

To perform the actual communication, call the `mesh->communicate` function with the group. In this case we need to communicate all these variables before performing any calculations, so call this function at the start of the `physics_run` routine:

```
int physics_run(BoutReal t) {
  mesh->communicate(comms);
  .
  .
  .
```

In many situations there may be several groups of variables which can be communicated at different times. The function `mesh->communicate` consists of a call to `mesh->send` followed by `mesh->wait` which can be done separately to interleave calculations and communications. This will speed up the code if parallel communication bandwidth is a problem for your simulation.

In our MHD example, the calculation of `ddt(rho)` and `ddt(p)` does not require `B`, so we could first communicate `rho`, `p`, and `v`, send `B` and do some calculations whilst communications are performed:

```
int physics_run(BoutReal t) {
  mesh->communicate(rho, p, v); // sends and receives rho, p and v
  comm_handle ch = mesh->send(B);// only send B

  ddt(rho) = ...
  ddt(p) = ...

  mesh->wait(ch); // now wait for B to arrive

  ddt(v) = ...
  ddt(B) = ...

  return 0;
}
```

This scheme is not used in `mhd.cxx`, partly for clarity, and partly because currently communications are not a significant bottleneck (too much inefficiency elsewhere!).

> **NOTE**: Before using the result of a differential operator as input to another differential operator, communications must be performed for the intermediate result

When a differential is calculated, points on neighbouring cells are assumed to be in the guard cells. There is no way to calculate the result of the differential in the guard cells, and so after every differential operator the values in the guard cells are invalid. Therefore, if you take the output of one differential operator and use it as input to another differen-

tial operator, you must perform communications (and set boundary conditions) first. See section 15.

12.5 Boundary conditions

All evolving variables have boundary conditions applied automatically after the `physics_run` has finished. Which condition is applied depends on the options file settings (see section 10). If you want to disable this and apply your own boundary conditions then set boundary condition to `none` in the `BOUT.inp` options file.

In addition to evolving variables, it's sometimes necessary to impose boundary conditions on other quantities which are not explicitly evolved.

The simplest way to set a boundary condition is to specify it as text, so to apply a Dirichlet boundary condition:

```
1   Field3D var;
2   ...
3   var.applyBoundary("dirichlet");
```

The format is exactly the same as in the options file. Each time this is called it must parse the text, create and destroy boundary objects. To avoid this overhead and have different boundary conditions for each region, it's better to set the boundary conditions you want to use first in `physics_init`, then just apply them every time:

```
1  Field3D var;
2
3  int physics_init() {
4    ...
5    var.setBoundary("myVar");
6    ...
7  }
8
9  int physics_run(BoutReal t) {
10   ...
11   var.applyBoundary();
12   ...
13 }
```

This will look in the options file for a section called `"[myvar]"` (upper or lower case doesn't matter) in the same way that evolving variables are handled. In fact this is precisely what is done: inside `bout_solve` (or `SOLVE_FOR`) the `setBoundary` method is called, and then after `physics_run` the applyBoundary() method is called on each evolving variable. This method also gives you the flexibility to apply different boundary conditions on different boundary

regions (e.g. radial boundaries and target plates); the first method just applies the same boundary condition to all boundaries.

Another way to set the boundaries is to copy them from another variable:

```
Field3D a, b;
  ...
  a.setBoundaryTo(b); // Copy b's boundaries into a
  ...
```

12.5.1 Custom boundary conditions

The boundary conditions supplied with the BOUT++ library cover the most common situations, but cannot cover all of them. If the boundary condition you need isn't available, then it's quite straightforward to write your own. First you need to make sure that your boundary condition isn't going to be overwritten. To do this, set the boundary condition to "none" in the BOUT.inp options file, and BOUT++ will leave that boundary alone. For example:

```
[P]
bndry_all = dirichlet
bndry_xin = none
bndry_xout = none
```

would set all boundaries for the variable "P" to zero value, except for the X inner and outer boundaries which will be left alone for you to modify.

To set an X boundary condition, it's necessary to test if the processor is at the left boundary (first in X), or right boundary (last in X). Note that it might be both if `NXPE = 1`, or neither if `NXPE > 2`.

```
  Field3D f;
  ...
  if(mesh->firstX()) {
    // At the left of the X domain
    // set f[0:1][*][*] i.e. first two points in X, all Y and all Z
    for(int x=0; x < 2; x++)
      for(int y=0; y < mesh->ngy; y++)
        for(int z=0; z < mesh->ngz; z++) {
          f[x][y][z] = ...
        }
  }
  if(mesh->lastX()) {
    // At the right of the X domain
    // Set last two points in X
```

```
  for(int x=mesh->ngx-2; x < mesh->ngx; x++)
    for(int y=0; y < mesh->ngy; y++)
      for(int z=0; z < mesh->ngz; z++) {
        f[x][y][z] = ...
      }
}
```

note the size of the local mesh including guard cells is given by `mesh->ngx`, `mesh->ngy`, and `mesh->ngz`. The functions `mesh->firstX()` and `mesh->lastX()` return true only if the current processor is on the left or right of the X domain respectively.

Setting custom Y boundaries is slightly more complicated than X boundaries, because target or limiter plates could cover only part of the domain. Rather than use a `for` loop to iterate over the points in the boundary, we need to use a more general iterator:

```
Field3D f;
...
RangeIterator it = mesh->iterateBndryLowerY();
for(it.first(); !it.isDone(); it++) {
  // it.ind contains the x index
  for(int y=2;y>=0;y--)  // Boundary width 3 points
    for(int z=0;z<mesh->ngz;z++) {
      ddt(f)[it.ind][y][z] = 0.;  // Set time-derivative to zero in↩
          boundary
    }
}
```

This would set the time-derivative of f to zero in a boundary of width 3 in Y (from 0 to 2 inclusive). In the same way `mesh->iterateBndryUpperY()` can be used to iterate over the upper boundary:

```
RangeIterator it = mesh->iterateBndryUpperY();
for(it.first(); !it.isDone(); it++) {
  // it.ind contains the x index
  for(int y=mesh->ngy-3;y<mesh->ngy;y--)  // Boundary width 3 ↩
     points
    for(int z=0;z<mesh->ngz;z++) {
      ddt(f)[it.ind][y][z] = 0.;  // Set time-derivative to zero in↩
          boundary
    }
}
```

12.6 Initial profiles

Up to this point the code is evolving total density, pressure etc. This has advantages for clarity, but has problems numerically: For small perturbations, rounding error and tolerances in the time-integration mean that linear dispersion relations are not calculated correctly. The solution to this is to write all equations in terms of an initial "background" quantity and a time-evolving perturbation, for example $\rho(t) \to \rho_0 + \tilde{\rho}(t)$. For this reason, **the initialisation of all variables passed to the `bout_solve` function is a combination of small-amplitude gaussians and waves; the user is expected to have performed this separation into background and perturbed quantities.**

To read in a quantity from a grid file, there is the `grid.get` function:

```
1 Field2D Ni0; // Background density
2
3 int physics_init(bool restarting) {
4   ...
5   mesh->get(Ni0, "Ni0");
6   ...
7 }
```

As with the input options, most of the time the name of the variable in the physics code will be the same as the name in the grid file to avoid confusion. In this case, you can just use

```
1 GRID_LOAD(Ni0);
```

which is equivalent to

```
1 mesh->get(Ni0, "Ni0");
```

12.7 Output variables

BOUT++ always writes the evolving variables to file, but often it's useful to add other variables to the output. For convenience you might want to write the normalised starting profiles or other non-evolving values to file. For example:

```
1   Field2D Ni0;
2   ...
3   GRID_LOAD(Ni0);
4   dump.add(Ni0, "Ni0", 0);
```

where the '0' at the end means the variable should only be written to file once at the start of the simulation. For convenience there are some macros e.g.

```
SAVE_ONCE(Ni0);
```

is equivalent to

```
dump.add(Ni0, "Ni0", 0);
```

In some situations you might also want to write some data to a different file. To do this, create a Datafile object:

```
Datafile mydata;
```

in physics_init, you then:

1. (optional) Initialise the file, passing it the options to use. If you skip this step, default (sane) options will be used. This just allows you to enable/disable, use parallel I/O, set whether files are opened and closed every time etc.

   ```
   mydata = Datafile(Options::getRoot()->getSection("mydata"));
   ```

   which would use options in a section [mydata] in BOUT.inp

2. Open the file for writing

   ```
   mydata.openw("mydata.nc")
   ```

   By default this only specifies the file name; actual opening of the file happens later when the data is written. If you are not using parallel I/O, the processor number is also inserted into the file name before the last ".", so mydata.nc" becomes "mydata.0.nc", "mydata.1.nc" etc. The file format used depends on the extension, so ".nc" will open NetCDF, ".hdf5" an HDF5 file, ".pdb" a PDB file etc.

   (see e.g. src/fileio/datafile.cxx line 139, which calls src/fileio/dataformat.cxx line 23, which then calls the file format interface e.g. src/fileio/impls/netcdf/nc_format.cxx line 172).

3. Add variables to the file

   ```
   mydata.add(variable, "name") ;  // Not evolving. Every time the ↩
      file is
   written, this will be overwritten
   mydata.add(variable2, "name2", 1); // Evolving. Will output a ↩
      sequence of values
   ```

Whenever you want to write values to the file, for example in physics_run or a monitor, just call

```
mydata.write();
```

To collect the data afterwards, you can specify the prefix to collect. In Python:

```
>>> var = collect("name", prefix="mydata")
```

or in IDL:

```
IDL> var = collect(var="name", prefix="mydata")
```

By default the prefix is "BOUT.dmp".

13 Fluid equations 2: reduced MHD

The MHD example presented previously covered some of the functions available in BOUT++, which can be used for a wide variety of models. There are however several other significant functions and classes which are commonly used, which will be illustrated using the `reconnect-2field` example. This is solving equations for $A_{||}$ and vorticity U

$$\begin{aligned}\frac{\partial U}{\partial t} &= -\frac{1}{B}\mathbf{b}_0 \times \nabla\phi \cdot \nabla U + B^2\nabla_{||}\left(j_{||}/B\right)\\ \frac{\partial A_{||}}{\partial t} &= -\frac{1}{\hat{\beta}}\nabla_{||}\phi - \eta\frac{1}{\hat{\beta}}j_{||}\end{aligned}$$

with ϕ and $j_{||}$ given by

$$\begin{aligned}U &= \frac{1}{B}\nabla_\perp^2\phi\\ j_{||} &= -\nabla_\perp^2 A_{||}\end{aligned}$$

First create the variables which are going to be evolved, ensure they're communicated

```
Field3D U, Apar; // Evolving variables

int physics_init(bool restarting) {

  SOLVE_FOR2(U, Apar);
}

int physics_run(BoutReal t) {
  mesh->communicate(U, Apar);

}
```

In order to calculate the time derivatives, we need the auxiliary variables ϕ and $j_{||}$. Calculating $j_{||}$ from $A_{||}$ is a straightforward differential operation, but getting ϕ from U means inverting a Laplacian.

```
1  Field3D U, Apar;
2  Field3D phi, jpar; // Auxilliary variables
3
4  int physics_init(bool restarting) {
5    SOLVE_FOR2(U, Apar);
6    SAVE_REPEAT2(phi, jpar); // Save variables in output file
7    return 0;
8  }
9
10 int physics_run(BoutReal t) {
11   phi = invert_laplace(mesh->Bxy*U, phi_flags); // Solve for phi
12   mesh->communicate(U, Apar, phi);  // Communicate phi
13   jpar = -Delp2(Apar);      // Calculate jpar
14   mesh->communicate(jpar); // Communicate jpar
15   return 0;
16 }
```

Note that the Laplacian inversion code takes care of boundary regions, so `U` doesn't need to be communicated first. The differential operator `Delp2` , like all differential operators, needs the values in the guard cells and so `Apar` needs to be communicated before calculating `jpar` . Since we will need to take derivatives of `jpar` later, this needs to be communicated as well.

```
1  int physics_run(BoutReal t) {
2    ...
3    mesh->communicate(jpar);
4
5    ddt(U) = -b0xGrad_dot_Grad(phi, U) + SQ(mesh->Bxy)*Grad_par(Jpar / ↩
       mesh->Bxy)
6    ddt(Apar) = -Grad_par(phi) / beta_hat - eta*jpar / beta_hat; }
```

13.1 Printing messages/warnings

In order to print to screen and/or a log file, the object `output` is provided. This provides two different ways to write output: the C (`printf`) way, and the C++ stream way. This is because each method can be clearer in different circumstances, and people have different tastes in these matters.

The C-like way (which is the dominant way in BOUT++) is to use the `write` function,

which works just like `printf`, and takes all the same codes (it uses `sprintf` internally).

```
output.write(const char *format, ...)
```

For example:

```
output.write("This is an integer: %d, and this a real: %e\n", 5, 2.0)
```

For those who prefer the C++ way of doing things, a completely equivalent way is to treat `output` as you would `cout`:

```
output << "This is an integer: " << 5 << ", and this a real: " << 2.0
    << endl;
```

which will produce exactly the same result as the `output.write` call above.

On all processors, anything sent to `output` will be written to a log file called `BOUT.log.#` with # replaced by the processor number. On processor 0, anything written to the output will be written to screen (stdout), in addition to the log file. Unless there is a really good reason not to, please use this `output` object when writing text output.

13.2 Error handling

Finding where bugs have occurred in a (fairly large) parallel code is a difficult problem. This is more of a concern for developers of BOUT++ (see the developers manual), but it is still useful for the user to be able to hunt down bug in their own code, or help narrow down where a bug could be occurring.

If you have a bug which is easily reproduceable i.e. it occurs almost immediately every time you run the code, then the easiest way to hunt down the bug is to insert lots of `output.write` statements (see section 13.1). Things get harder when a bug only occurs after a long time of running, and/or only occasionally. For this type of problem, a useful tool can be the message stack. At the start of a section of code, put a message onto the stack:

```
   msg_stack.push("Some message here");
```

which can also take arguments in `printf` format, as with `output.write`. At the end of the section of code, take the message off the stack again:

```
   msg_stack.pop();
```

If an error occurs, the message stack is printed out, and this can then help track down where the error originated.

14 Object-orientated interface

If you prefer to create classes rather than global variables and C functions for your physics model, this can be done using a (somewhat experimental) interface. To see the difference, compare **examples/advect1d/gas_compress.cxx** with **examples/advect1d-newapi/gas_compress.cxx**. The disadvantage of this interface is that it's marginally more complicated to set up, but it has several advantages: It makes splitting the model into multiple files easier (sharing global variables is a pain), models can be combined together to enable coupling of models, and BOUT++ can be more easily used alongside other libraries. For large models, it's recommended to use this method. Converting C-style interface to a class is also quite straightforward, and discussed below.

In a header file (e.g. **examples/advect1d-newapi/gas_compress.hxx**), first put

```
#include <bout/physicsmodel.hxx>
```

(do NOT include **boutmain.hxx**, as that defines the C-like interface and a `main()` function).

Next define a class which inherits from `PhysicsModel`

```
class GasCompress : public PhysicsModel {
protected:
  int init(bool restarting);
  int rhs(BoutReal t);
private:
  // Evolving variables, parameters etc. here
};
```

As a minimum, you need to define the initialisation function `init` (it's a pure virtual member of PhysicsModel, so if you don't you'll get a compile-time error). Any variables being evolved should now be members of this class. If you are converting a C-style model, just move all the global variables into the `private` section.

Next create a source file (e.g. **examples/advect1d-newapi/gas_compress.cxx**, which includes your header file

```
#include "gas_compress.hxx"
```

Then implement the init and rhs functions:

```
int GasCompress::init(bool restarting) {
  ...
}

int GasCompress::rhs(BoutReal t) {
  ...
}
```

To convert simple physics models, just rename `physics_init` to `YourModel::init` , and `physics_run` to `YourModel::run` .

Finally, you need to create a `main()` function for your code. The easiest way to do this is to use the macro `BOUTMAIN` :

```
BOUTMAIN(GasCompress);
```

This is defined in **include/bout/physicsmodel.hxx**, and expands to

```
int main(int argc, char **argv) {
  BoutInitialise(argc, argv); // Initialise BOUT++

  GasCompress *model = new GasCompress(); // Create a model

  Solver *solver = Solver::create(); // Create a solver
  solver->setModel(model); // Specify the model to solve
  solver->addMonitor(bout_monitor); // Monitor the solver

  solver->solve(); // Run the solver

  delete model;
  delete solver;
  BoutFinalise(); // Finished with BOUT++
  return 0;
}
```

If you like, you can define your own `main()` function, making it easier to combine BOUT++ with other libraries.

15 Differential operators

There are a huge number of possible ways to perform differencing in computational fluid dynamics, and BOUT++ is intended to be able to implement a large number of them. This means that the way differentials are handled internally is quite involved; see the developer's manual for full gory details. Much of the time this detail is not all that important, and certainly not while learning to use BOUT++. Default options are therefore set which work most of the time, so you can start using the code without getting bogged down in these details.

In order to handle many different differencing methods and operations, many layers are used, each of which handles just part of the problem. The main division is between differencing methods (such as 4th-order central differencing), and differential operators (such as $\nabla_{||}$).

15.1 Differencing methods

Methods are implemented on 5-point stencils, and are divided into three categories:

- Central-differencing methods, for diffusion operators $\frac{df}{dx}$, $\frac{d^2f}{dx^2}$. Each method has a short code, and currently include
  - `C2`: 2^{nd} order $f_{-1} - 2f_0 + f_1$
  - `C4`: 4^{th} order $\left(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2\right)/12$
  - `W2`: 2^{nd} order CWENO
  - `W3`: 3^{rd} order CWENO
  - `FFT`: Fourier Transform method in Z (axisymmetric) direction only
- Upwinding methods for advection operators $v_x \frac{df}{dx}$
  - `U1`: 1^{st} order upwinding
  - `U4`: 4^{th} order upwinding
  - `W3`: 3^{rd} order Weighted Essentially Non-Oscillatory (WENO)[7]
- Flux conserving and limiting methods for terms of the form $\frac{d}{dx}\left(v_x f\right)$
  - `SPLIT`: split into upwind and central terms $\frac{d}{dx}\left(v_x f\right) = v_x \frac{df}{dx} + f\frac{dv_x}{dx}$
  - `NND`: Non-oscillatory, containing No free parameters and Dissipative (NND) scheme[8]

Both of these methods avoid overshoots (Gibbs phenomena) at sharp gradients such as shocks, but the simple 1st-order method has very large artificial diffusion. WENO schemes are a development of the ENO reconstruction schemes which combine good handling of sharp-gradient regions with high accuracy in smooth regions.

To use these differencing operators directly, add the following to the top of your physics module

```
1 #include <derivs.hxx>
```

By default the method used will be the one specified in the options input file (see section 6.6), but most of these methods can take an optional `DIFF\_METHOD` argument, specifying exactly which method to use.

Table 10: Coordinate derivatives

Function	Formula
DDX(f)	$\partial f/\partial x$
DDY(f)	$\partial f/\partial y$
DDZ(f)	$\partial f/\partial z$
D2DX2(f)	$\partial^2 f/\partial x^2$
D2DY2(f)	$\partial^2 f/\partial y^2$
D2DZ2(f)	$\partial^2 f/\partial z^2$
D2DX4(f)	$\partial^4 f/\partial x^4$
D2DY4(f)	$\partial^4 f/\partial y^4$
D2DZ4(f)	$\partial^4 f/\partial z^4$
D2DXDZ(f)	$\partial^2 f/\partial x\partial z$
D2DYDZ(f)	$\partial^2 f/\partial y\partial z$
VDDX(f, g)	$f\partial g/\partial x$
VDDY(f, g)	$f\partial g/\partial y$
VDDZ(f, g)	$f\partial g/\partial z$
FDDX(f, g)	$\partial/\partial x\,(f*g)$
FDDY(f, g)	$\partial/\partial x\,(f*g)$
FDDZ(f, g)	$\partial/\partial x\,(f*g)$

15.2 Non-uniform meshes

examples/test-nonuniform seems to not work? Setting `non_uniform = true` in the BOUT.inp options file enables corrections to second derivatives in X and Y. This correction is given by writing derivatives as:

$$\frac{\partial f}{\partial x} \simeq \frac{1}{\Delta x}\frac{\partial f}{\partial i} \tag{21}$$

where i is the cell index number. The second derivative is therefore given by

$$\frac{\partial^2 f}{\partial x^2} \simeq \frac{1}{\Delta x^2}\frac{\partial^2 f}{\partial i^2} + \frac{1}{\Delta x}\frac{\partial f}{\partial x}\cdot\frac{\partial}{\partial i}\left(\frac{1}{\Delta x}\right) \tag{22}$$

The correction factor $\partial/\partial i\,(1/\Delta x)$ can be calculated automatically, but you can also specify `d2x` in the grid file which is

$$\texttt{d2x} = \frac{\partial \Delta x}{\partial i} = \frac{\partial^2 x}{\partial i^2} \tag{23}$$

The correction factor is then calculated from `d2x` using

$$\frac{\partial}{\partial i}\left(\frac{1}{\Delta x}\right) = -\frac{1}{\Delta x^2}\frac{\partial \Delta x}{\partial i} \tag{24}$$

15.3 General operators

These are differential operators which are for a general coordinate system.

$$\begin{array}{rcll} \mathbf{v} = & \nabla f & \texttt{Vector} = & \texttt{Grad(Field)} \\ f = & \nabla \cdot \mathbf{a} & \texttt{Field} = & \texttt{Div(Vector)} \\ \mathbf{v} = & \nabla \times \mathbf{a} & \texttt{Vector} = & \texttt{Curl(Vector)} \\ f = & \mathbf{v} \cdot \nabla g & \texttt{Field} = & \texttt{V\_dot\_Grad(Vector, Field)} \\ \mathbf{v} = & \mathbf{a} \cdot \nabla \mathbf{c} & \texttt{Vector} = & \texttt{V\_dot\_Grad(Vector, Vector)} \\ f = & \nabla^2 f & \texttt{Field} = & \texttt{Laplace(Field)} \end{array} \tag{25}$$

$$\begin{aligned} \nabla\phi =& \frac{\partial\phi}{\partial u^i}\nabla u^i \rightarrow (\nabla\phi)_i = \frac{\partial\phi}{\partial u^i} \\ \nabla \cdot A =& = \frac{1}{J}\frac{\partial}{\partial u^i}\left(Jg^{ij}A_j\right) \\ \nabla^2\phi =& G^j\frac{\partial\phi}{\partial u^i} + g^{ij}\frac{\partial^2\phi}{\partial u^i \partial u^j} \end{aligned}$$

where we have defined

$$G^j = \frac{1}{J}\frac{\partial}{\partial u^i}\left(Jg^{ij}\right)$$

not to be confused with the Cristoffel symbol of the second kind (see the coordinates manual for more details).

15.4 Clebsch operators

Another set of operators assume that the equilibrium magnetic field is written in Clebsch form as

$$\mathbf{B}_0 = \nabla z \times \nabla x \qquad B_0 = \frac{\sqrt{g_{yy}}}{J} \tag{26}$$

where

$$\mathbf{B}_0 = |\mathbf{B}_0|\,\mathbf{b}_0 = B_0\mathbf{b}_0 \tag{27}$$

is the background *equilibrium* magnetic field.

Table 11: Clebsch operators

Function	Formula
`Grad_par`	$\partial_{\|\|}^0 = \mathbf{b}_0 \cdot \nabla = \frac{1}{\sqrt{g_{yy}}}\frac{\partial}{\partial y}$
`Div_par`	$\nabla_{\|\|}^0 f = B_0 \partial_{\|\|}^0 \left(\frac{f}{B_0}\right)$
`Grad2_par2`	$\partial_{\|\|}^2 \phi = \partial_{\|\|}^0 \left(\partial_{\|\|}^0 \phi\right) = \frac{1}{\sqrt{g_{yy}}}\frac{\partial}{\partial y}\left(\frac{1}{\sqrt{g_{yy}}}\right)\frac{\partial \phi}{\partial y} + \frac{1}{g_{yy}}\frac{\partial^2 \phi}{\partial y^2}$
`Laplace_par`	$\nabla_{\|\|}^2 \phi = \nabla \cdot \mathbf{b}_0 \mathbf{b}_0 \cdot \nabla \phi = \frac{1}{J}\frac{\partial}{\partial y}\left(\frac{J}{g_{yy}}\frac{\partial \phi}{\partial y}\right)$
`Laplace_perp`	$\nabla_\perp^2 = \nabla^2 - \nabla_{\|\|}^2$
`Delp2`	Perpendicular Laplacian, neglecting all y derivatives The `Laplacian` solver performs the inverse operation
`brackets`	Poisson brackets The Arakawa option, neglects the parallel y derivatives

We have that

$$\mathbf{b}_0 \cdot \nabla\phi \times \nabla A = \frac{1}{J\sqrt{g_{yy}}}\left[\left(g_{yy}\frac{\partial \phi}{\partial z} - g_{yz}\frac{\partial \phi}{\partial y}\right)\frac{\partial A}{\partial x} + \left(g_{yz}\frac{\partial \phi}{\partial x} - g_{xy}\frac{\partial \phi}{\partial z}\right)\frac{\partial A}{\partial y} + \left(g_{xy}\frac{\partial \phi}{\partial y} - g_{yy}\frac{\partial \phi}{\partial x}\right)\frac{\partial A}{\partial z}\right]$$

$$\nabla_\perp \equiv \nabla - \boldsymbol{b}\left(\boldsymbol{b} \cdot \nabla\right) \qquad \boldsymbol{b} \cdot \nabla = \frac{1}{JB}\frac{\partial}{\partial y} \tag{28}$$

$$\boldsymbol{b} = \frac{1}{JB}\boldsymbol{e}_y = \frac{1}{JB}\left[g_{xy}\nabla x + g_{yy}\nabla y + g_{yz}\nabla z\right] \tag{29}$$

In a Clebsch coordinate system $\boldsymbol{B} = \nabla z \times \nabla x = \frac{1}{J}\boldsymbol{e}_y$, $g_{yy} = \boldsymbol{e}_y \cdot \boldsymbol{e}_y = J^2 B^2$, and so the ∇y term cancels out:

$$\nabla_\perp = \nabla x\left(\frac{\partial}{\partial x} - \frac{g_{xy}}{(JB)^2}\frac{\partial}{\partial y}\right) + \nabla z\left(\frac{\partial}{\partial z} - \frac{g_{yz}}{(JB)^2}\frac{\partial}{\partial y}\right)$$

15.5 The bracket operators

The bracket operator `brackets(phi, f, method)` aims to differentiate equations on the form

$$-\frac{\nabla\phi \times \boldsymbol{b}}{B} \cdot \nabla f$$

NOTE: The bracket operators in BOUT++ are using Clebsch coordinates, and returns $-\frac{\nabla\phi\times\boldsymbol{b}}{B}\cdot\nabla f$ rather than $-\nabla\phi\times\boldsymbol{b}\cdot\nabla f$.

Notice that when we use the Arakawa scheme, y-derivatives are neglected. An example of usage of the brackets can be found in for example **examples/MMS/advection** or **examples/blob2d**.

15.6 Setting differencing method

16 Staggered grids

Until now all quantities have been cell-centred i.e. both velocities and conserved quantities were defined at the same locations. This is because these methods are simple and this was the scheme used in the original BOUT. This class of methods can however be susceptible to grid-grid oscillations, and so most shock-capturing schemes involve densities and velocities (for example) which are not defined at the same location: their grids are staggered.

By default BOUT++ runs with all quantities at cell centre. To enable staggered grids, set

```
StaggerGrids = true
```

in the top section of the `BOUT.inp` file. The **test-staggered** example illustrates how to use staggered grids in BOUT++.

There are four possible locations in a grid cell where a quantity can be defined in BOUT++: centre, lower X, lower Y, and lower Z. These are illustrated in figure 5. To

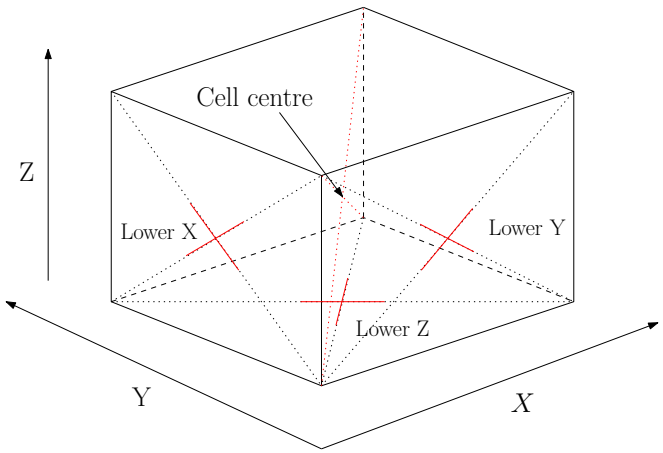


Figure 5: Locations in a grid cell where quantities may be defined.

specify the location of a variable, use the method `setLocation()` with one of the locations `CELL\_CENTRE`, `CELL\_XLOW`, `CELL\_YLOW`, or `CELL\_ZLOW` .

> **NOTE**: If setting the location of an evolving variable, this should be done **before** the call to `bout_solve` or `SOLVE_FOR`

The key lines in the **test-staggered** example which specify the locations of the evolving variables are

```
Field3D n, v;

int physics_init(bool restart) {
  v.setLocation(CELL_YLOW); // Staggered relative to n
  SOLVE_FOR2(n, v);
  ...
```

which makes the velocity `v` staggered to the lower side of the cell in Y, whilst the density n remains cell centred.

Arithmetic operations between staggered quantities are handled by interpolating them to the same location according to the algorithm in figure 6. If performing an operation

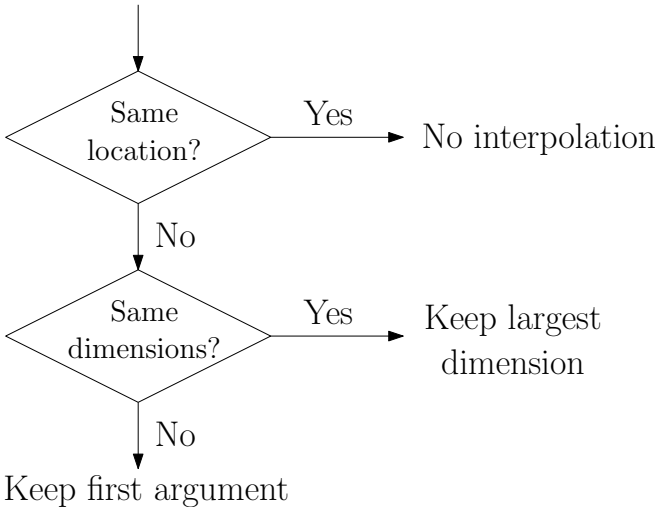


Figure 6: How the cell location of an arithmetic operation (`+,-,*,/,`$\wedge$) is decided

between variables defined at two different locations, the order of the variables matter: the result will be defined at the locations of the **left** variable. For example, `n*v` would be `CELL_CENTRE` because this is the location of `n` , whilst `v*n` would be `CELL_YLOW` . Relying on this behaviour could lead to trouble, to make your code clearer it's probably best to use the interpolation routines. Include the header file

```
#include <interpolation.hxx>
```

then use the `interp_to(field, location)` function. Using this, `interp_to(n, CELL_YLOW)*v` would be `CELL_YLOW` as `n` would be interpolated.

Differential operators by default return fields which are defined at the same location as their inputs, so here `Grad_par(v)` would be `CELL_YLOW` . If this is not what is wanted, give the location of the result as an additional argument: `Grad_par(v, CELL_CENTRE)` uses staggered differencing to produce a result which is defined at the cell centres. As with the arithmetic operators, if you ask for the result to be staggered in a different direction from the input then the differencing will be to cell centre and then be interpolated. For example `Grad_par(v, CELL_XLOW)` would first perform staggered differencing from `CELL_YLOW` to get a result at `CELL_CENTRE`, and then interpolate the result to `CELL_XLOW` .

Advection operators which take two arguments return a result which is defined at the location of the field being advected. For example `Vpar_Grad_par(v, f)` calculates $v\nabla_{||}f$ and returns a result at the same location as `f`. If `v` and `f` are defined at the same locations then centred differencing is used, if one is centred and the other staggered then staggered differencing is used, and if both are staggered to different locations then the behaviour is less well defined (don't do it). As with other differential operators, the required location of the result can be given as an optional argument.

> **NOTE**: There are subtleties with boundary conditions when staggering variables. The test-staggered example manually applies a boundary condition to make the width of the boundary wider

17 Advanced methods

This section describes the more advanced methods which can be used to speed up simulations using implicit time stepping schemes. At the time of writing (Dec '12), they can be used with either the SUNDIALS CVODE or PETSc solvers.

17.1 Global field gather / scatter

In BOUT++ each processor performs calculations on a sub-set of the mesh, and communicates with other processors primarily through exchange of guard cells (the `mesh->communicate` function). If you need to gather data from the entire mesh onto a single processor, then this can be done using either 2D or 3D `GlobalFields` .

First include the header file

```
1 #include <bout/globalfield.hxx>
```

which defines both `GlobalField2D` and `GlobalField3D` . To create a 3D global field, pass it the mesh pointer:

```
1   GlobalField3D g3d(mesh);
```

By default all data will be gathered onto processor 0. To change this, specify which processor the data should go to as the second input

```
GlobalField3D g3d(mesh, processor);
```

Gather and scatter methods are defined:

```
Field3D localData;
// Set local data to some value

g3d.gather(localData);  // Gathers all data onto one processor

localData = g3d.scatter(); // Scatter data back
```

Note: Boundary guard cells are **not** handled by the scatter step, as this would mean handling branch-cuts etc. To obtain valid data in the guard and Y boundary cells, you will need to communicate and set Y boundaries.

Note: Gather and Scatter are global operations, so all processors must call these functions.

Once data has been gathered, it can be used on one processor. To check if the data is available, call the method `dataIsLocal()`, which will return `true` only on one processor

```
if(g3d.dataIsLocal()) {
  // Data is available on this processor

}
```

The sizes of the global array are available through `xSize()`, `ySize()` and `zSize()` methods. The data itself can be accessed indirectly using `(x,y,z)` operators:

```
for(int x=0; x<g3d.xSize(); x++)
  for(int y=0; y<g3d.ySize(); y++)
    for(int z=0; z<g3d.zSize(); z++)
      output.write("Value at (%d,%d,%d) is %e\n",
      x,y,z,
      g3d(x,y,z) );
```

or by getting a pointer to the underlying data, which is stored as a 1D array:

```
BoutReal *data = g3d.getData();
nx = g3d.xSize();
ny = g3d.ySize();
nz = g3d.zSize();

data[x*ny*nz + y*nz + z]; // Value at g3d(x,y,z)
```

See the example **examples/test-globalfield** for more examples.

17.2 LaplaceXY

Perpendicular Laplacian solver in X-Y.

$$\begin{aligned}\nabla_\perp f &= \nabla f - \mathbf{b}\left(\mathbf{b}\cdot\nabla\right) \\ &= \left(\frac{\partial f}{\partial x} - \frac{g_{xy}}{g_{yy}}\frac{\partial f}{\partial y}\right)\nabla x + \left(\frac{\partial f}{\partial z} - \frac{g_{yz}}{g_{yy}}\frac{\partial f}{\partial y}\right)\nabla z\end{aligned}$$

In 2D (X-Y), the g_{xy} component can be dropped since this depends on integrated shear I which will cancel with the g_{xz} component. The z derivative is zero and so this simplifies to

$$\nabla_\perp f = \frac{\partial f}{\partial x}\nabla x - \frac{g_{yz}}{g_{yy}}\frac{\partial f}{\partial y}\nabla z$$

The divergence operator in conservative form is

$$\nabla\cdot\mathbf{A} = \frac{1}{J}\frac{\partial}{\partial u^i}\left(Jg^{ij}A_j\right)$$

and so the perpendicular Laplacian in X-Y is

$$\nabla_\perp^2 = \frac{1}{J}\frac{\partial}{\partial x}\left(Jg^{xx}\frac{\partial f}{\partial x}\right) - \frac{1}{J}\frac{\partial}{\partial y}\left(Jg^{yz}\frac{g_{yz}}{g_{yy}}\frac{\partial f}{\partial y}\right)$$

In field-aligned coordinates, the metrics in the y derivative term become:

$$g^{yz}\frac{g_{yz}}{g_{yy}} = \frac{B_{tor}}{B^2}\frac{1}{h_\theta^2}$$

In the LaplaceXY operator this is implemented in terms of fluxes at cell faces.

$$\frac{1}{J}\frac{\partial}{\partial x}\left(Jg^{xx}\frac{\partial f}{\partial x}\right) \quad\rightarrow\quad \frac{1}{J_i\mathrm{dx_i}}\left[J_{i+1/2}g^{xx}_{i+1/2}\left(\frac{f_{i+1}-f_i}{\mathrm{dx}_{i+1/2}}\right) - J_{i-1/2}g^{xx}_{i-1/2}\left(\frac{f_i-f_{i-1}}{\mathrm{dx}_{i-1/2}}\right)\right]$$

Notes:

- The ShiftXderivs option must be true for this to work, since it assumes that $g^{xz} = 0$

17.3 LaplaceXZ

This is a Laplacian inversion code in X-Z, similar to the `Laplacian` solver described in section 6.4. The difference is in the form of the Laplacian equation solved, and the approach used to derive the finite difference formulae. The equation solved is:

$$\nabla\cdot\left(A\nabla_\perp f\right) + Bf = b \tag{30}$$

where A and B are coefficients, b is the known RHS vector (e.g. vorticity), and f is the unknown quantity to be calculated (e.g. potential). The Laplacian is written in conservative form like the `LaplaceXY` solver, and discretised in terms of fluxes through cell faces.

$$\frac{1}{J}\left(JAg^{xx}\frac{\partial f}{\partial x}\right) + \frac{1}{J}\left(JAg^{zz}\frac{\partial f}{\partial z}\right) + Bf = b \tag{31}$$

The header file is `include/bout/invert/laplacexz.hxx`. The solver is constructed by using the `LaplaceXZ::create` function:

```
LaplaceXZ *lap = LaplaceXZ::create(mesh);
```

Note that a pointer to a `Mesh` object must be given, which for now is the global variable `mesh`. By default the options section `laplacexz` is used, so to set the type of solver created, set in the options

```
[laplacexz]
type = petsc  # Set LaplaceXZ type
```

or on the command-line `laplacexz:type=petsc`.

The coefficients must be set using `setCoefs`. All coefficients must be set at the same time:

```
lap->setCoefs(1.0, 0.0);
```

Constants, `Field2D` or `Field3D` values can be passed. If the implementation doesn't support `Field3D` values then the average over z will be used as a `Field2D` value.

To perform the inversion, call the `solve` function:

```
Field3D vort = ...;

Field3D phi = lap->solve(vort, 0.0);
```

The second input to `solve` is an initial guess for the solution, which can be used by iterative schemes e.g. using PETSc.

17.3.1 Implementations

The currently available implementations are:

- `cyclic`: This implementation assumes coefficients are constant in Z, and uses FFTs in z and a complex tridiagonal solver in x for each z mode (the `CyclicReduction` solver). Code in `src/invert/laplacexz/impls/cyclic/`.

- `petsc`: This uses the PETSc KSP interface to solve a matrix with coefficients varying in both x and z. To improve efficiency of direct solves, a different matrix is used

for preconditioning. When the coefficients are updated the preconditioner matrix is not usually updated. This means that LU factorisations of the preconditioner can be re-used. Since this factorisation is a large part of the cost of direct solves, this should greatly reduce the run-time.

17.3.2 Test case

The code in `examples/test-laplacexz` is a simple test case for `LaplaceXZ`. First it creates a `LaplaceXZ` object:

```
LaplaceXZ *inv = LaplaceXZ::create(mesh);
```

For this test the `petsc` implementation is the default:

```
[laplacexz]
type = petsc
ksptype = gmres # Iterative method
pctype  = lu  # Preconditioner
```

By default the LU preconditioner is used. PETSc's built-in factorisation only works in serial, so for parallel solves a different package is needed. This is set using:

```
factor_package = superlu_dist
```

This setting can be "petsc" for the built-in (serial) code, or one of "superlu", "superlu_dist", "mumps", or "cusparse".

Then we set the coefficients:

```
inv->setCoefs(Field3D(1.0),Field3D(0.0));
```

Note that the scalars need to be cast to fields (Field2D or Field3D) otherwise the call is ambiguous. Using the PETSc command-line flag `-mat_view ::ascii_info` information on the assembled matrix is printed:

```
$ mpirun -np 2 ./test-laplacexz -mat_view ::ascii_info
...
Matrix Object: 2 MPI processes
type: mpiaij
rows=1088, cols=1088
total: nonzeros=5248, allocated nonzeros=5248
total number of mallocs used during MatSetValues calls =0
  not using I-node (on process 0) routines
...
```

which confirms that the matrix element pre-allocation is setting the correct number of non-zero elements, since no additional memory allocation was needed.

A field to invert is created using FieldFactory:

```
Field3D rhs = FieldFactory::get()->create3D("rhs",
                                            Options::getRoot(),
                                            mesh);
```

which is currently set to a simple function in the options:

```
rhs = sin(x - z)
```

and then the system is solved:

```
Field3D x = inv->solve(rhs, 0.0);
```

Using the PETSc command-line flags `-ksp_monitor` to monitor the iterative solve, and `-mat_superlu_dist_statprint` to monitor SuperLU_dist we get:

```
      Nonzeros in L       19984
       Nonzeros in U       19984
       nonzeros in L+U     38880
       nonzeros in LSUB    11900
       NUMfact space (MB) sum(procs):  L\U     0.45    all     0.61
       Total highmark (MB):  All       0.62    Avg     0.31    Max     0.36
       Mat conversion(PETSc->SuperLU_DIST) time (max/min/avg):
                            4.69685e-05 / 4.69685e-05 / 4.69685e-05
       EQUIL time             0.00
       ROWPERM time           0.00
       COLPERM time           0.00
       SYMBFACT time          0.00
       DISTRIBUTE time        0.00
       FACTOR time            0.00
       Factor flops    1.073774e+06    Mflops    222.08
       SOLVE time             0.00
       SOLVE time             0.00
       Solve flops     8.245800e+04    Mflops     28.67
  0 KSP Residual norm 5.169560044060e+02
       SOLVE time             0.00
       Solve flops     8.245800e+04    Mflops     60.50
       SOLVE time             0.00
       Solve flops     8.245800e+04    Mflops     49.86
  1 KSP Residual norm 1.359142853145e-12
```

So after the initial setup and factorisation, the system is solved in one iteration using the LU direct solve.

As a test of re-using the preconditoner, the coefficients are then modified:

```
inv->setCoefs(Field3D(2.0),Field3D(0.1));
```

and solved again:

```
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     84.15
  0 KSP Residual norm 5.169560044060e+02
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     90.42
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     98.51
  1 KSP Residual norm 2.813291076609e+02
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     94.88
  2 KSP Residual norm 1.688683980433e+02
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     87.27
  3 KSP Residual norm 7.436784980024e+01
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     88.77
  4 KSP Residual norm 1.835640800835e+01
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     89.55
  5 KSP Residual norm 2.431147365563e+00
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     88.00
  6 KSP Residual norm 5.386963293959e-01
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     93.50
  7 KSP Residual norm 2.093714782067e-01
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     91.91
  8 KSP Residual norm 1.306701698197e-02
        SOLVE time             0.00
        Solve flops     8.245800e+04    Mflops     89.44
  9 KSP Residual norm 5.838501185134e-04
        SOLVE time             0.00
```

```
        Solve flops     8.245800e+04    Mflops     81.47
```

Note that this time there is no factorisation step, but the direct solve is still very effective.

17.3.3 Blob2d comparison

The example `examples/blob2d-laplacexz` is the same as `examples/blob2d` but with `LaplaceXZ` rather than `Laplacian`.

Tests on one processor: Using Boussinesq approximation, so that the matrix elements are not changed, the cyclic solver produces output

```
1.000e+02        125       8.28e-01    71.8    8.2    0.4    0.6   18.9
2.000e+02         44       3.00e-01    69.4    8.1    0.4    2.1   20.0
```

whilst the PETSc solver with LU preconditioner outputs

```
1.000e+02        146       1.15e+00    61.9   20.5    0.5    0.9   16.2
2.000e+02         42       3.30e-01    58.2   20.2    0.4    3.7   17.5
```

so the PETSc direct solver seems to take only slightly longer than the cyclic solver. For comparison, GMRES with Jacobi preconditioning gives:

```
1.000e+02        130       2.66e+00    24.1   68.3    0.2    0.8    6.6
2.000e+02         78       1.16e+00    33.8   54.9    0.3    1.1    9.9
```

and with SOR preconditioner

```
1.000e+02        124       1.54e+00    38.6   50.2    0.3    0.4   10.5
2.000e+02         45       4.51e-01    46.8   37.8    0.3    1.7   13.4
```

When the Boussinesq approximation is not used, the PETSc solver with LU preconditioning, re-setting the preconditioner every 100 solves gives:

```
1.000e+02        142       3.06e+00    23.0   70.7    0.2    0.2    6.0
2.000e+02         41       9.47e-01    21.0   72.1    0.3    0.6    6.1
```

i.e. around three times slower than the Boussinesq case. When using jacobi preconditioner:

```
1.000e+02        128       2.59e+00    22.9   70.8    0.2    0.2    5.9
2.000e+02         68       1.18e+00    26.5   64.6    0.2    0.6    8.1
```

For comparison, the `Laplacian` solver using the tridiagonal solver as preconditioner gives:

```
1.000e+02        222       5.70e+00    17.4   77.9    0.1    0.1    4.5
2.000e+02        172       3.84e+00    20.2   74.2    0.2    0.2    5.2
```

or with Jacobi preconditioner:

```
1.000e+02        107       3.13e+00    15.8   79.5    0.1    0.2    4.3
2.000e+02        110       2.14e+00    23.5   69.2    0.2    0.3    6.7
```

The `LaplaceXZ` solver does not appear to be dramatically faster **in serial** than the `Laplacian` solver when the matrix coefficients are modified every solve. When matrix elements are not modified then the solve time is competitive with the tridiagonal solver.

As a test, timing only the `setCoefs` call for the non-Boussinesq case gives

```
1.000e+02        142       1.86e+00    83.3    9.5    0.2    0.3    6.7
2.000e+02         41       5.04e-01    83.1    8.0    0.3    1.2    7.3
```

so around 9% of the run-time is in setting the coefficients, and the remaining $\sim 60\%$ in the solve itself.

18 Eigenvalue solver

By using the SLEPc library, BOUT++ can be used as an eigenvalue solver to find the eigenvectors and eigenvalues of sets of equations.

18.1 Configuring with SLEPc

The BOUT++ interface has been tested with SLEPc version 3.4.3, itself compiled with PETSc 3.4.2. SLEPc version 3.4 should work, but other versions will not yet.

18.2 SLEPc options

Time derivatives can be taken directly from the RHS function, or by advancing the simulation in time by a relatively large increment. This second method acts to damp high frequency components

18.3 Examples

18.3.1 Wave in a box

`examples/eigen-box`

19 Testing

Two types of tests are currently used in BOUT++ to catch bugs as early as possible: Unit tests, which check a small piece of the code separately, and a test suite which runs the entire code on a short problem. Unit tests can be run using the **src/unit_tests** Python script. This searches through the directories looking for an executable script called **unit_test**, runs them, and collates the results. Not many tests are currently available as much of the code is too tightly coupled. If done correctly, the unit tests should describe and check the behavior of each part of the code, and hopefully the number of these will increase over time. The test suite is in the **examples** directory, and is run using the **test_suite** python script. At the top of this file is a list of the subdirectories to run (e.g. **test-io**, **test-laplace**, and **interchange-instability**). In each of those subdirectories the script **runtest** is executed, and the return value used to determine if the test passed or failed.

All tests should be short, otherwise it discourages people from running the tests before committing changes. A few minutes or less on a typical desktop, and ideally only a few seconds. If you have a large simulation which you want to stop anyone breaking, find starting parameters which are as sensitive as possible so that the simulation can be run quickly.

19.1 Method of Manufactured Solutions

The Method of Manufactured solutions (MMS) is a rigorous way to check that a numerical algorithm is implemented correctly. A known solution is specified (manufactured), and it is possible to check that the code output converges to this solution at the expected rate.

To enable testing by MMS, switch an input option "mms" to true:

```
1 [solver]
2 mms = true
```

This will have the following effect:

1. For each evolving variable, the solution will be used to initialise and to calculate the error

19.2 Choosing manufactured solutions

Manufactured solutions must be continuous and have continuous derivatives. Common mistakes:

- Don't use terms multiplying coordinates together e.g. `x * z` or `y * z`. These are not periodic in y and/or z, so will give strange answers and usually no convergence. Instead use `x * sin(z)` or similar, which are periodic.

19.3 Timing

To time parts of the code, and calculate the percentage of time spent in communications, file I/O, etc. there is the `Timer` class defined in **include/bout/sys/timer.hxx**. To use it, just create a `Timer` object at the beginning of the function you want to time:

```
#include <bout/sys/timer.hxx>

void someFunction() {
  Timer timer("test")
  ...
}
```

Creating the object starts the timer, and since the object is destroyed when the function returns (since it goes out of scope) the destructor stops the timer.

```
class Timer {
public:
  Timer();
  Timer(const std::string &label);
  ~Timer();

  double getTime();
  double resetTime();
};
```

The empty constructor is equivalent to setting `label = ""` . Constructors call a private function `getInfo()` , which looks up the `timer_info` structure corresponding to the label in a `map<string, timer_info*>` . If no such structure exists, then one is created. This structure is defined as:

```
struct timer_info {
  double time;    ///< Total time
  bool running;   ///< Is the timer currently running?
  double started; ///< Start time
};
```

Since each timer can only have one entry in the map, creating two timers with the same label at the same time will lead to trouble. Hence this code is **not** thread-safe.

The member functions `getTime()` and `resetTime()` both return the current time. Whereas `getTime()` only returns the time without modifying the timer, `resetTime()` also resets the timer to zero.

If you don't have the object, you can still get and reset the time using static methods:

```
double Timer::getTime(const std::string &label);
```

```
2 double Timer::resetTime(const std::string &label);
```

These look up the `timer_info` structure, and perform the same task as their non-static namesakes. These functions are used by the monitor function in **bout++.cxx** to print the percentage timing information.

20 Examples

The code and input files in the `examples/` subdirectory are for research, demonstrating BOUT++, and to check for broken functionality. Some proper unit tests have been implemented, but this is something which needs improving. The examples which were published in [1, 2] were `drift-instability`, `interchange-instability` and `orszag-tang`.

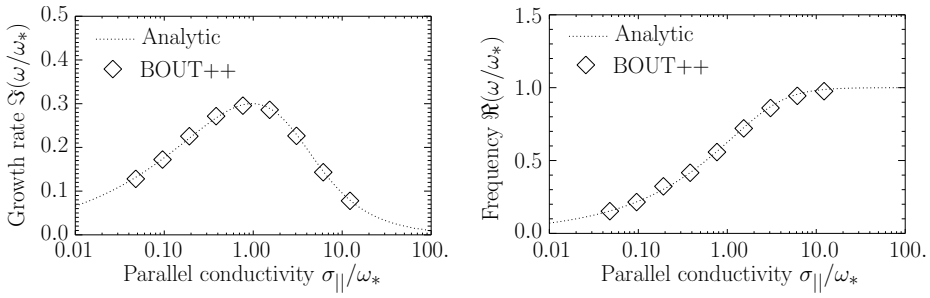
20.1 advect1d

The model in `gas_compress.cxx` solves the compressible gas dynamics equations for the density n, velocity $\mathbf{V}$, and pressure P:

20.2 drift-instability

The physics code `2fluid.cxx` implements a set of reduced Braginskii 2-fluid equations, similar to those solved by the original BOUT code. This evolves 6 variables: Density, electron and ion temperatures, parallel ion velocity, parallel current density and vorticity.

Input grid files are the same as the original BOUT code, but the output format is different.



(a) Growth rate (b) Real Frequency

Figure 7: Resistive Drift wave instability test. Dashed lines are analytic results, diamonds from BOUT++ simulations

20.3 em-drift

20.4 gyro-gem

20.5 interchange-instability

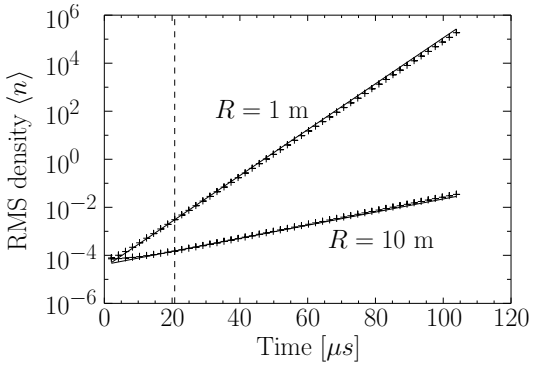


Figure 8: Interchange instability test. Solid lines are from analytic theory, symbols from BOUT++ simulations, and the RMS density is averaged over z. Vertical dashed line marks the reference point, where analytic and simulation results are set equal

20.6 jorek-compare

20.7 lapd-drift

20.8 orszag-tang

The file `mhd.cxx` solves the full MHD equations for the full values (perturbation + initial), whilst the file `mhd_perturb.cxx` solves for a perturbation about the equilibrium.

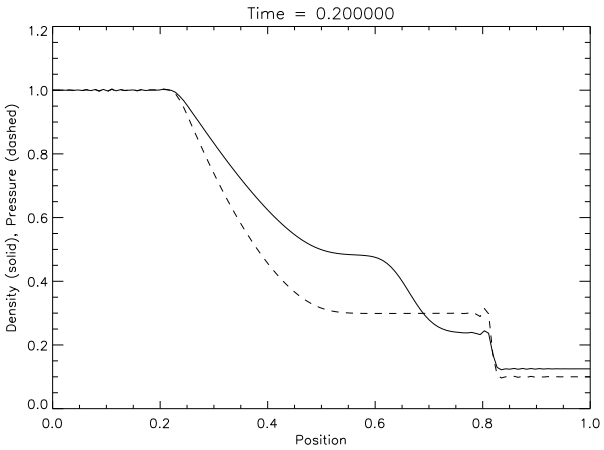


Figure 9: Sod shock-tube problem for testing shock-handling methods

20.9 shear-alfven-wave

20.10 sod-shock

20.11 uedge-benchmark

21 Notes

21.1 Compile options

Compiling with `-DCHECK` enables a lot of checks of operations performed by the field objects. This is very useful for debugging a code, and can be omitted once bugs have been removed.

For (sometimes) more useful error messages, there is the `-DTRACK` option. This keeps track of the names of variables and includes these in error messages.

21.2 Adaptive grids

Two types of adaptive grids can be used in BOUT++: Moving meshes, and changing resolution.

21.2.1 Moving meshes

During either the initialisation, or the simulation itself, the metric tensors can be modified. This could be used to make the coordinate system time-dependent. Since currently the metric tensors are 2D fields, this would only allow axisymmetric motion. Changing the tensors to be 3D objects is however possible with fairly small modification to the code.

Whenever one of the metrics g^{ij} are changed, a call to `geometry()` must be made.

21.2.2 Changing resolution

NOTE: Not implemented yet - this just for discussion

Since all 2D and 3D fields/vectors are located internally in global lists, the resolution of the grid can be changed when required by interpolation. **This requires a new, more efficient implementation of the Fields classes**.

References

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[2] B D Dudson, M V Umansky, X Q Xu, P B Snyder, and H R Wilson. BOUT++: a framework for parallel plasma fluid simulations. *arXiv*, physics.plasm-ph:0810.5757, Nov 2008.

[3] M V Umansky, X Q Xu, B Dudson, and L L LoDestro. *BOUT Code Manual*. LLNL, June 2006. Available from www.mfescience.org/bout/.

[4] M V Umansky, X Q Xu, B Dudson, L L LoDestro, and J R Myra. Status and verification of edge plasma turbulence code bout. *Comp. Phys. Comm.*, page doi:10.1016/j.cpc.2008.12.012, 2008.

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A Machine-specific installation

A.1 Archer

As of 30th April 2014, the following configuration should work

```
> module swap PrgEnv-cray PrgEnv-gnu/5.1.29
> module load fftw
> module load netcdf/4.1.3
```

B Installing PACT

There are two ways to install PACT, and usually one of them will work on a given system.

B.1 Self-extracting package

This is probably the easiest method (when it works). Download one of the "Executable UNIX distribution files" from the PACT website and run:

```
./pact07_07_18-src -sl -i $HOME/local/
```

The "-sl" flag tells it to generate shared libraries. If you don't plan on using IDL to read/write PDB files, then you can omit this. The "-i $HOME/local/" tells PACT to install in your home directory/local.

If this script fails, you will usually have to resort to either trying to understand DSYS, or going with the second method below.

B.2 PACT source distribution

The second method is to use a .tar.gz PACT source file. Here the version used is `pact-2.1.0.tar.gz`.

```
~/ $ cd install
~/install/ $ tar -xzvf pact-2.1.0.tar.gz
~/install/ $ cd pact-2.1.0/
~/install/pact-2.1.0/ $ ./configure --prefix=$HOME/local --enable-shared
```

NOTE: On Franklin, PACT will compile without the –enable-shared option, but not with it. This is OK if you just want to run BOUT++, but the shared libraries are needed for reading the results into IDL (the PDB2IDL library)

At this point, the installation may fail with the following error:

```
configure: WARNING: yacc is a symbolic link to bison
configure: WARNING: bison is not a supported type of yacc
configure: error: No working yacc found
```

If this happens, you need to first install Berkeley Yacc into your home directory

```
 ~/install/ $ ls
byacc.tar.gz       netcdf-tar -xzvf byacc.tar.gz4.0.1.tar.gz  pact-2.1.0.tar.gz
fftw-3.2.1.tar.gz  pact-2.1.0           sundials-2.4.0.tar.gz

 ~/install/ $ tar -xzvf byacc.tar.gz
 ~/install/ $ cd byacc-20080826/
 ~/install/byacc-20080826/ $ ./configure --prefix=$HOME/local
 ~/install/byacc-20080826/ $ gmake
 ~/install/byacc-20080826/ $ mkdir ~/local/bin
 ~/install/byacc-20080826/ $ cp yacc ~/local/bin/
```

NB: We're copying the yacc executable manually because "gmake install" doesn't seem to work, and the fix which works for PACT (see later) doesn't work here.

Add this directory to your path:

```
 ~/install/byacc-20080826/ $ setenv PATH $HOME/local/bin:$PATH
```

You can check that this has worked by running "which yacc", which should then print your home directory /local/bin/yacc. You could also add this to your .profile startup scripts. Now go back to PACT:

```
 ~/install/byacc-20080826/ $ cd ../pact-2.1.0
 ~/install/pact-2.1.0/ $ ./configure --prefix=$HOME/local --enable-shared
 ~/install/pact-2.1.0/ $ gmake
 ~/install/pact-2.1.0/ $ gmake install
```

The last step may fail with a strange error message like:

```
The current directory must be set to the ITT directory.
Change the default to the ITT directory and re-run
this script.
```

This happens when the wrong "install" is being used. Check by running:

```
 ~/install/byacc-20080826/ $ which install
```

This should print "/usr/bin/install", but if not then run

```
~/install/byacc-20080826/ $ ln -s /usr/bin/install ~/local/bin/
~/install/pact-2.1.0/ $ ./configure --prefix=$HOME/local
~/install/pact-2.1.0/ $ gmake
~/install/pact-2.1.0/ $ gmake install
```

NOTE: configure needs to be run again after messing with install.
This should now install PACT into your local directory.

C Compiling and running under AIX

Most development and running of BOUT++ is done under Linux, with the occasional FreeBSD and OSX. The configuration scripts are therefore heavily tested on these architectures. IBM's POWER architecture however runs AIX, which has some crucial differences which make compiling a pain.

- Under Linux/BSD, it's usual for a Fortran routine `foo` to appear under C as `foo_`, whilst under AIX the name is unchanged
- MPI compiler scripts are usually given the names `mpicc` and either `mpiCC` or `mpicxx`. AIX uses `mpcc` and `mpCC`.
- Like BSD, the `make` command isn't compatible with GNU make, so you have to run `gmake` to compile everything.
- The POWER architecture is big-endian, different to the little endian Intel and AMD chips. This can cause problems with binary file formats.

C.1 SUNDIALS

To compile SUNDIALS, use

```
$ export CC=cc
$ export CXX=xlC
$ export F77=xlf
$ export OBJECT_MODE=64
$ ./configure --prefix=$HOME/local/ --with-mpicc=mpcc --with-mpif77=mpxlf CFLAGS=-maix64
```

You may get an error message like:

```
make: Not a recognized flag: w
```

This is because the AIX `make` is being used, rather than `gmake`. The easiest way to fix this is to make a link to `gmake` in your local bin directory:

```
$ ln -s /usr/bin/gmake $HOME/local/bin/make
```

Running `which make` should now point to this `local/bin/make`, and if not then you need to make sure that your bin directory appears first in the `PATH`:

```
export PATH=$HOME/local/bin:$PATH
```

If you see an error like this:

```
ar: 0707-126 ../../src/sundials/sundials_math.o is not valid with the current object fil
        Use the -X option to specify the desired object mode.
```

then you need to set the environment variable `OBJECT_MODE`

```
export OBJECT_MODE=64
```

Configuring BOUT++, you may get the error:

```
configure: error: C compiler cannot create executables
```

In that case, you can try using:

```
./configure CFLAGS="-maix64"
```

When compiling, you may see warnings

```
xlC_r: 1501-216 (W) command option -64 is not recognized - passed to ld
```

At this point, the main BOUT++ library should compile, and you can try compiling one of the examples.

```
ld: 0711-317 ERROR: Undefined symbol: .NcError::NcError(NcError::Behavior)
ld: 0711-317 ERROR: Undefined symbol: .NcFile::is_valid() const
ld: 0711-317 ERROR: Undefined symbol: .NcError::~NcError()
ld: 0711-317 ERROR: Undefined symbol: .NcFile::get_dim(const char*) const
```

This is probably because the NetCDF libraries are 32-bit, whilst BOUT++ has been compiled as 64-bit. You can try compiling BOUT++ as 32-bit:

```
$ export OBJECT_MODE=32
$ ./configure CFLAGS="-maix32"
$ gmake
```

If you still get undefined symbols, then go back to 64-bit, and edit make.config, replacing `-lnetcdf_c++` with -lnetcdf64_c++, and `-lnetcdf` with -lnetcdf64. This can be done by running:

```
$ sed 's/netcdf/netcdf64/g' make.config > make.config.new
$ mv make.config.new make.config
```

D BOUT++ functions (alphabetical)

This is a list of functions which can be called by users writing a physics module. For a full list of functions, see the Reference manual, DOxygen documentation, and source code.

- `Field = ` **abs**`(Field | Vector)`
- `(Communicator).` **add**`(Field | Vector)`
  Add a variable to a communicator object.
- **apply_boundary**`(Field. ‘‘name’’)`
- `Field = ` **b0xGrad_dot_Grad**`(Field, Field, CELL_LOC)`
- **bout_solve**`(Field, Field, ‘‘name’’)`
- **bout_solve**`(Vector, Vector, ‘‘name’’)`
- `(Communicator).` **clear**`()`
  Remove all variables from a Communicator object
- `Field = ` **cos**`(Field)`
- `Field = ` **cosh**`(Field)`
- `Vector = ` **Curl**`(Vector)`
- `Field = ` **Delp2**`(Field)`
  $\nabla_\perp^2$ operator
- `Field = ` **Div**`(Vector)`
  Divergence of a vector
- `Field = ` **Div_par**`(Field f)`
  Parallel divergence $B_0\mathbf{b}\cdot\nabla\left(f/B_0\right)$
- **dump.add**`(Field, ‘‘name’’, 1/0)`
- `Field = ` **filter**`(Field, modenr)`
- **geometry_derivs**`()`
  Calculates useful quantities from the metric tensor. Call this every time the metric tensor is changed.
- `Vector = ` **Grad**`(Field)`

- `Field =` **Grad_par**`(Field)`
- `Field =` **Grad2_par2**`(Field)`
- **grid_load**`(BoutReal, ‘‘name’’)`
  Load a scalar real from the grid file
- **grid_load2d**`(Field2D, ‘‘name’’)`
  Load a 2D scalar field from the grid file
- **grid_load3d**`(Field3D, ‘‘name’’)`
  Load a 3D scalar field from the grid file
- **invert_laplace**`(Field input, Field output, flags, Field2D *A)`
- `Field =` **invert_parderiv**`(Field2D|BoutReal A, Field2D|BoutReal B, Field3D r)`
  Inverts an equation `A*x + B*Grad2_par2(x) = r`
- `Field =` **Laplacian**`(Field)`
- `Field3D =` **low_pass**`(Field3D, max_modenr)`
- `BoutReal =` **max**`(Field)`
- `BoutReal =` **min**`(Field)`
- **msg_stack.pop**`( |int)`
  Remove a message from the top of the stack. If a message ID is passed, removes all messages back to that point.
- `int =` **msg_stack.push**`(‘‘format’’, ...)`
  Put a message onto the stack. Works like `printf` (and `output.write`).
- **options.get**`(‘‘name’’, variable, default)`
  Get an integer, real or boolean value from the options file. If not in the file, the default value is used. The value used is printed to log file.
- **options.setSection**`(‘‘name’’)` Set the section name in the input file
- **output** $<<$ `values`
  Behaves like cout for stream output
- **output.write**`(‘‘format’’, ...)`
  Behaves like printf for formatted output

- `(Communicator).`**receive**`()`
  Receive data from other processors. Must be preceded by a `send` call.
- `(Communicator).`**run**`()`
  Sends and receives data.
- `(Communicator).`**send**`()`
  Sends data to other processors (and posts receives). This must be followed by a call to `receive()` before calling send again, or adding new variables.
- `(Field3D).`**setLocation(CELL_LOC)**
- `(Field3D).`**ShiftZ(bool)**
- `Field = `**sin**`(Field)`
- `Field = `**sinh**`(Field)`
- **solver.setPrecon**`(PhysicsPrecon)`
  Set a preconditioner function
- `Field = `**sqrt(Field)**
- `Field = `**tan**`(Field)`
- `Field = `**tanh**`(Field)`
- `Field = `**V_dot_Grad**`(Vector v, Field f)`
  Calculates an advection term $\mathbf{v} \cdot \nabla f$
- `Vector = `**V_dot_Grad**`(Vector v, Vector u)`
  Advection term $\mathbf{v} \cdot \nabla \mathbf{u}$
- `Field = `**Vpar_Grad_par**`(Field v, Field f)`
- `Field3D = `**where**`(Field2D test, Field|BoutReal gt0, Field|BoutReal lt0)`
  Chooses between two values, depending on sign of `test`.

E IDL routines

List of IDL routines available in idllib. There are broadly three categories of routine:

- Completely general routines which could be useful outside BOUT++ work

  - Data plotting and animation: **contour2** and **showdata**
  - File reading and writing: **file_open**, **file_read** etc.
  - User input and output: **get_float**, **get_integer**, **get_yesno** and **str**
  - FFT routines for integrating, differentiating and filtering: **fft_integrate**, **fft_deriv**, **fft_filter**

- Routines for BOUT++, but not specific to any application
  - Modifying restart files: **expand_restarts**, **scale_restarts** and **split_restarts**
  - Processing 3D variables for input grid: **bout3dvar**

- Routines specifically for tokamak simulations
  - Reading A- and G-EQDSK format files into IDL: **read_aeqdsk** and **read_neqdsk**
  - Plotting results: **polslice**, **plotpolslice**

Here the format is
name, arguments, [optional arguments]

- var = **bout3dvar** (var)
  Converts 3D variables to and from BOUT++'s Fourier representation which is used for input grids. By default converts from [x,y,z] to [x,y,f]
  - **/reverse** Convert from [x,y,f] to [x,y,z]
  - **nf**=nf Set number of frequencies in the result
  - **nz**=nz When using /reverse, set number of Z points in the result

- var = **collect**()
  Read in data from a set of BOUT++ dump files
  - **var** = "name of variable"
  - **path** = "path/to/variable/"
  - **xind**, **yind**, **zind**, **tind** = [min, max] index pairs
  - **t_array** = Output 1D array of times

- **contour2**, data [, x, y]
  This is a replacement for the IDL contour which includes a scale color bar.
  - **data** can be either 2D (x,y) or 3D (x,y,t). If data is 3D then the color is scaled to the entire range.

  - **x** is an optional 2D (x,y) array of X coordinates
  - **y** is an optional 2D (x,y) array of Y coordinates
  - **t**=t is a time index for 3D data
  - **nlev**=nlev
  - **centre**=centre Make zero the middle of the color range (white if redblue)
  - **redblue**=redblue Use a blue-white-red color scheme
  - **revcolor**=revcolor Reverse color scheme

- **expand_restarts**, newz
  Increases the number of Z points in restart files. Together with scale_restarts and split_restarts, this makes it easier to modify a linear simulation as a start for non-linear runs.

  - **newz** is the new value of NZ
  - **path**=path Input path
  - **output**=output Output path
  - **format**=format File extension of output

- result = **fft_deriv** (var1d)
  Calculates the derivative of a variable on a periodic domain.

- result = **fft_filter** (var, nf) Fourier filter a variable on a periodic domain. Arguments are a 1D variable and the number of Fourier components to keep

- result = **fft_integrate** (var1d) Integrates a variable on a periodic domain.

  - **loop**=loop The loop integral is returned in this variable

- **file_close**, handle
  Close a file opened using file_open()

- list = **file_list** (handle)
  Return a list of variable names in the file

- integer = **file_ndims** (handle , “variable”)
  Get the number of dimensions of a variable

- handle = **file_open** (“file”)
  Open a PDB or NetCDF file. File type is inferred from file name

  - **/write** Open file for writing (default is read only)
  - **/create** Create a new file, over-writing if already exists

- var = **file_read** (handle, "variable")
  - **inds** = [xmin, xmax, ymin, ymax, ...]

- float = **get_float** ("prompt")
  Ask the user for a float, using the given prompt

- integer = **get_integer** ("prompt")
  Ask the user for an integer

- integer = **get_yesno** ("prompt")
  Ask for a yes (1) or no (0) answer

- result = **gmres** (x0, operator, b)
  General Minimal Residual (GMRES)
  - **x0** is the starting guess at the solution
  - **operator**
  - **b**

  Optional arguments
  - **restart**=restart
  - **max_iter**=max_iter
  - **tol**=tol
  - **stats**=stats
  - **show**=show
  - **output**=output

- result = **int_func** ([x,] f)
  Integrate a function, always using the maximum number of grid-points possible for highest accuracy

- bool = **is_pow2** (value)
  Returns 1 (true) if the given number is a power of 2, 0 (false) otherwise

- **plotpolslice**, var3d, grid
  Takes a slice through a field-aligned tokamak domain, showing a poloidal cross-section.

  - **var3d** is a 3D (x,y,z) variable to plot. Needs all of the points to work properly.
  - **grid** is a structure from importing a grid file

  Optional arguments:

  - **period**=period
  - **zangle**=zangle
  - **nlev**=nlev
  - **yr**=yr
  - **profile**=profile
  - **output**=output
  - **lines**=lines
  - **linecol**=linecol
  - **filter**=filter

- **polslice**, data, gridfile
  Plots a 2D poloidal contour for single or double-null configurations, including color bar.

  - **xstart**=xstart X index where the data begins. Useful if only part of the domain has been collected
  - **ystart**=ystart Y index where data begins

- struct = **read_aeqdsk** ("filename")
  Reads an A-EQDSK file. Format is specified here: `https://fusion.gat.com/THEORY/efit/a_eqdsk.html`

- struct = **read_neqdsk** ("filename")
  Reads in an 'neqdsk' or G-EQDSK formatted tokamak equilibrium file. Format of G-EQDSK file is specified here: `https://fusion.gat.com/THEORY/efit/g_eqdsk.html`

- stringarray = **regex_extract** (line, pattern)
  Extract all matches to Regular Expression pattern contained in line. Useful for extracting numbers from FORTRAN-formatted text files.

  - **line** Input string
  - **pattern** Regular expression pattern to match

  - **nmatch**=nmatch

- var = **reverse_inds** (var)
  Reverse array indices e.g. `arr[t,z,y,x] -> arr[x,y,z,t]`. Works on up to 5 dimensional variables

- **safe_colors**
  Sets the color table to useful values for plotting.

  - **/first** Sets the first 10 colors to specific values, otherwise sets last 7

- **scale_restarts**, factor

  - **path**=path Path to the restart files (default is current directory '.')
  - **format**=format Specify what the file format is, otherwise goes on the file name

- **showdata**, data
  Display animations of 1D,2D and 3D data. Defaults:

  - 2D data Animate a line plot
  - 3D data Animate a surface plot
  - 4D data Animate a poloidal cross-section (tokamaks only)

  Optional arguments:

  - **/addsym** For 2D data (1D plots), add symbols to mark data points
  - **az**=angle Rotate surface plots
  - **/bw** Make contour plots grey scale
  - **chars**=size character size
  - **/contour** For 3D input, show color contour plot
  - **delay**=time Time delay between plots (default 0.2 seconds)
  - **/noscale** By default, all plots are on the same scale. This changes the scale for each plot's range
  - **profile**=array Background profile. Data is 3D: profile is 1D (X). Data is 4D -¿ profile is 2D (X,Y)
  - **yr**=[min,max] Y range

- result = **sign** (var)
  This returns +1 if the variable is > 0, -1 otherwise

- **spectrum**
- **split_restarts**, [nxpe], nype
  split restart files between a different number of processors
  - **nxpe** is an optional argument giving the number of processors in the X direction
  - **nype** is the number of processors in the Y direction
  - **path**=path Input path
  - **output**=output Output path
  - **format**=format File extension of output
- string = **str** (value)
  Convert a value to a string with whitespace trimmed. Arrays are converted to a comma-separated list in brackets.
- result = **zfamp** (var4d)
  Given a 4D variable [x,y,z,t], returns the Fourier amplitudes in [x,y,f,t]
- var = **zshift** (var, shift)
  Shifts a variable in the Z direction, useful for mapping between field-aligned and orthogonal coordinates.
  - **period**=period How many domains fit in 2π. Default is 1 (full torus)

F Python routines (alphabetical)

F.1 boututils

- `class Datafile` provides a convenient way to read and write NetCDF or HDF5 files. There are many different NetCDF libraries available for Python, so this class tries to provide a consistent interface to many of them, as well as to h5py.
- `deriv`()
- `determineNumberOfCPUs`()
- `file_import`() reads the contents of a NetCDF file into a dictionary
- `integrate`()
- `launch`()
- `linear_regression`()

F.2 boutdata

- `collect`() provides an interface to read BOUT++ data outputs, returning NumPy arrays of data. It deals with the processor layout, working out which file contains each part of the domain.

```
1    from boutdata.collect import collect
2
3    t = collect("t_array")  # Collect the time values
```

- `pol_slice`() takes a 3 or 4-D data set for a toroidal equilibrium, and calculates a slice through it at fixed toroidal angle.

- `gen_surface`() is a generator for iterating over flux surfaces

F.3 bout_runners

`bout_runners` contains classes which gives an alternative way of running BOUT++ simulations either normally using the class `basic_runner` , or on a cluster through a generated Portable Batch System (PBS) script using the child class `PBS_runner` . Examples can be found in **examples/bout_runners_example/**.

NOTE: `bout_runners` is currently only tested on clusters using `TORQUE`

`bout_runners` is especially useful if one needs to make several runs with only small changes in the options (which is normally written in **BOUT.inp** or in the command-line), as is the case when performing a parameter scan, or when performing a MMS test.

Instead of making several runs with several different input files with only small changes in the option, one can with `bout_runners` specify the changes as member data of an instance of the appropriate `bout_runners` class. One way to do this is to write a *driver* in the same directory as the executable. The *driver* is just a python script which imports `bout_runners` , creates an instance, specifies the running option as member data of that instance and finally calls the member function `self.execute_runs`() .

In addition, the `bout_runners` provides a way to run any python post-processing script after finished simulations (as long as it accept at least one parameter containing the folder name(s) of the run(s)). If the simulations have been performed using the `PBS_runner` , the post-processing function will be submitted to the cluster (although it is possible to submit it to a different queue, using a different amount of nodes etc.).

When the function `self.execute_runs`() is executed, a folder structure like the one presented in figure 10 is created. **BOUT.inp** is copied to the folder of execution, where the **BOUT.*.dmp** files are stored. Secondly a list of combination of the options specified in the driver is made. Eventually unset options are obtained from **BOUT.inp** or given a default value if the option is nowhere to be found.

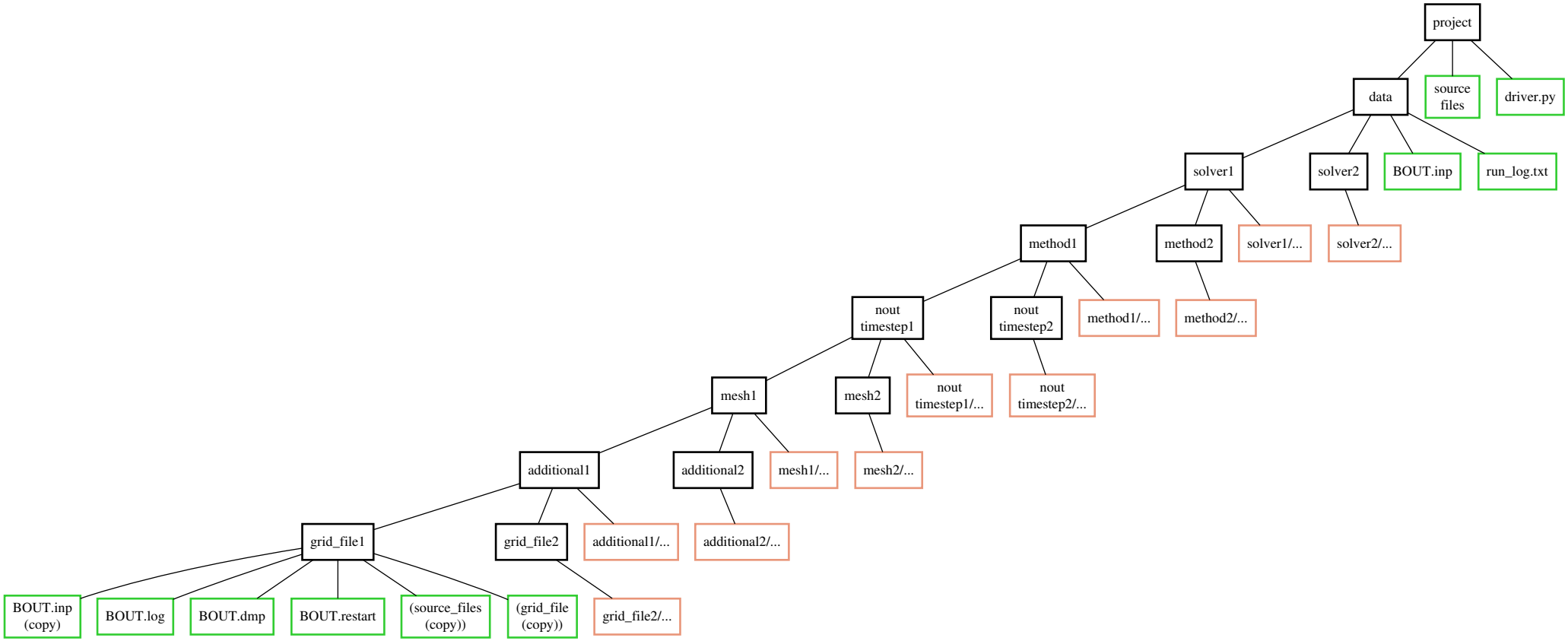

Figure 10: Longest possible folder tree made by the `self.execute_runs()` function.