Dedalus Project Documentation

Dedalus Collaboration

Oct 16, 2018

Contents

CHAPTER 1

About Dedalus

Dedalus is a flexible framework for solving partial differential equations using spectral methods. The code is open-source and developed by a team of researchers working on problems in astrophysical and geophysical fluid dynamics.

The code is written primarily in Python and features an easy-to-use interface, including text-based equation entry. Our numerical algorithm produces highly sparse systems for a wide variety of equations on spectrally-discretized domains. These systems are efficiently solved using compiled libraries and multidimensional parallelization though MPI.

CHAPTER 2

Doc Contents

2.1 Installing Dedalus

2.1.1 Installing the Dedalus Package

Dedalus is a Python 3 package that includes custom C-extensions (compiled with Cython) and that relies on MPI, FFTW (linked to MPI), HDF5, and a basic scientific-Python stack: numpy, scipy, mpi4py (linked to the same MPI), and h5py.

If you have the necessary C dependencies (MPI, FFTW+MPI, and HDF5), as well as Python 3, you should be able to install Dedalus from PyPI or build it from source. Otherwise, see one of the alternate sections below for instructions for building the dependency stack.

Installing from PyPI

We currently only provide Dedalus on PyPI as a source distribution so that the Cython extensions are properly linked to your FFTW library at build-time. To install Dedalus from PyPI, first set the `FFTW_PATH` environment variable to the prefix paths for FFTW and then install using pip:

```
export FFTW_PATH=/path/to/your/fftw_prefix
pip3 install dedalus
```

Building from source

Alternately, to build the lastest version of Dedalus from source: clone the repository, set the `FFTW_PATH` variable, install the build requirements, and install using pip:

```
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
export FFTW_PATH=/path/to/your/fftw_prefix
```

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```
pip3 install -r requirements.txt
pip3 install .
```

Updating Dedalus

If Dedalus was installed from PyPI, it can be updated using:

```
export FFTW_PATH=/path/to/your/fftw_prefix
pip3 install --upgrade Dedalus
```

If Dedalus was built from source, it can be updated by first pulling new changes from the source repository, and then reinstalling with pip:

```
cd /path/to/dedalus/repo
hg pull
hg update
export FFTW_PATH=/path/to/your/fftw_prefix
pip3 install -r requirements.txt
pip3 install --upgrade --force-reinstall .
```

Uninstalling Dedalus

If Dedalus was installed using pip, it can be uninstalled using:

```
pip3 uninstall dedalus
```

2.1.2 Conda Installation

We preliminarily support installation through conda via a custom script that allows you to link against custom MPI/FFTW/HDF5 libraries, or opt for the builds of those packages that are available through conda.

First, install conda/miniconda for your system if you don't already have it, following the instructions from conda. Then download the Dedalus conda installation script from this link or using:

```
wget https://raw.githubusercontent.com/DedalusProject/conda_dedalus/master/install_
↪conda.sh
```

Modify the options at the top of the script to link against custom MPI/FFTW/HDF5 libraries, choose between OpenBLAS and MKL-based numpy and scipy, and set the name of the resulting conda environment. Then activate the base conda environment and run the script to build a new conda environment with Dedalus and its dependencies, as requested:

```
conda activate base
bash install_conda.sh
```

2.1.3 Installation Script

Dedalus provides an all-in-one installation script that will build an isolated stack containing a Python installation and the other dependencies needed to run Dedalus. In most cases, the script can be modified to link with system installations of FFTW, MPI, and linear algebra libraries.

You can get the installation script from this link, or download it using:

```
wget https://bitbucket.org/dedalus-project/dedalus/raw/tip/docs/install.sh
```

and execute it using:

```
bash install.sh
```

The installation script has been tested on a number of Linux distributions and OS X. If you run into trouble using the script, please get in touch on the user list.

2.1.4 Manual Installation

Below are instructions for building the dependency stack on a variety of machines and operating systems:

Install notes for Mac OS X (10.9)

These instructions assume you're starting with a clean Mac OS X system, which will need `python3` and all scientific packages installed.

Mac OS X cookbook

```
#!bash

# Homebrew
ruby -e "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/
↪install)"
brew update
brew doctor
# ** Fix any errors raised by brew doctor before proceeding **

# Prep system
brew install gcc
brew install swig

# Python 3
brew install python3

# Scientific packages for Python 3
brew tap homebrew/science
brew install suite-sparse
pip3 install nose
pip3 install numpy
pip3 install scipy
brew install libpng
brew install freetype
pip3 install matplotlib

# MPI
brew install openmpi
pip3 install mpi4py

# FFTW
```

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```
brew install fftw --with-mpi

# HDF5
brew install hdf5
pip3 install h5py

# Dedalus
# ** Change to the directory where you want to keep the Dedalus repository **
brew install hg
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
pip3 install -r requirements.txt
python3 setup.py build_ext --inplace
```

Detailed install notes for Mac OS X (10.9)

Preparing a Mac system

First, install Xcode from the App Store and seperately install the Xcode Command Line Tools. To install the command line tools, open Xcode, go to `Preferences`, select the `Downloads` tab and `Components`. These command line tools install `make` and other requisite tools that are no longer automatically included in Mac OS X (as of 10.8).

Next, you should install the Homebrew package manager for OS X. Run the following from the Terminal:

```
#!bash
ruby -e "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/
↪install)"
brew update
brew doctor
```

Cleanup any problems identified by `brew doctor` before proceeding.

To complete the `scipy` install process, we'll need `gfortran` from `gcc` and `swig`, which you can install from Homebrew:

```
#!bash
brew install gcc
brew install swig
```

Install Python 3

Now, install python3 from Homebrew:

```
#!bash
brew install python3
```

Scientific packages for Python3

Next install the numpy and scipy scientific packages. To adequately warn you before proceeding, properly installing numpy and scipy on a Mac can be a frustrating experience.

Start by proactively installing UMFPACK from suite-sparse, located in homebrew-science on https://github.com/Homebrew/homebrew-science. Failing to do this may lead to a series of perplexing UMFPACK errors during the scipy install.

```
#!bash
brew tap homebrew/science
brew install suite-sparse
```

Now use pip, the (the standard Python package management system, installed with Python via Homebrew) to install `nose`, `numpy`, and `scipy` in order:

```
#!bash
pip3 install nose
pip3 install numpy
pip3 install scipy
```

The `scipy` install can fail in a number of surprising ways. Be especially wary of custom settings to `LDFLAGS`, `CPPFLAGS`, etc. within your shell; these may cause the `gfortran` compile step to fail spectacularly.

Also install `matplotlib`, the main Python plotting library, along with its dependencies, using Homebrew and pip:

```
#!bash
brew install libpng
brew install freetype
pip3 install matplotlib
```

Other libraries

Dedalus is parallelized using MPI, and we recommend using the Open MPI library on OS X. The Open MPI library and Python wrappers can be installed using Homebrew and pip:

```
#!bash
brew install openmpi
pip3 install mpi4py
```

Dedalus uses the FFTW library for transforms and parallelized transposes, and can be installed using Homebrew:

```
#!bash
brew install fftw --with-mpi
```

Dedalus uses HDF5 for data storage. The HDF5 library and Python wrappers can be installed using Homebrew and pip:

```
#!bash
brew install hdf5
pip3 install h5py
```

Installing the Dedalus package

Dedalus is managed using the Mercurial distributed version control system, and hosted online though Bitbucket. Mercurial (referred to as `hg`) can be installed using homebrew, and can then be used to download the latest copy of Dedalus (note: you should change to the directory where you want the put the Dedalus repository):

```
#!bash
brew install hg
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
```

A few other Python packages needed by Dedalus are listed in the `requirements.txt` file in the Dedalus repository, and can be installed using pip:

```
#!bash
pip3 install -r requirements.txt
```

You then need to build Dedalus's Cython extensions from within the repository using the `setup.py` script. This step should be perfomed whenever updates are pulled from the main repository (but it is only strictly necessary when the Cython extensions are modified).

```
#!bash
python3 setup.py build_ext --inplace
```

Finally, you need to add the Dedalus repository to the Python search path so that the `dedalus` package can be imported. To do this, add the following to your `~/.bash_profile`, substituting in the path to the Dedalus repository you cloned using Mercurial:

```
# Add Dedalus repository to Python search path
export PYTHONPATH=<PATH/TO/DEDALUS/REPOSITORY>:$PYTHONPATH
```

Other resources

http://www.lowindata.com/2013/installing-scientific-python-on-mac-os-x/

http://stackoverflow.com/questions/12574604/scipy-install-on-mountain-lion-failing

https://github.com/jonathansick/dotfiles/wiki/Notes-for-Mac-OS-X

Install notes for TACC/Stampede

Install notes for building our python3 stack on TACC/Stampede, using the intel compiler suite. Many thanks to Yaakoub El Khamra at TACC for help in sorting out the python3 build and numpy linking against a fast MKL BLAS.

On Stampede, we can in principle either install with a `gcc/mpvapich2/fftw3` stack with `OpenBLAS`, or with an `intel/mvapich2/fftw3 stack` with `MKL`. Mpvaich2 is causing problems for us, and this appears to be a known issue with `mvapich2/1.9`, so for now we must use the `intel/mvapich2/fftw3` stack, which has `mvapich2/2.0b`. The intel stack should also, in principle, allow us to explore auto-offloading with the Xenon MIC hardware accelerators. Current `gcc` instructions can be found under NASA Pleiades.

Modules

Here is my current build environment (from running `module list`)

1. TACC-paths
2. Linux
3. cluster-paths
4. TACC

5. cluster
6. intel/14.0.1.106
7. mvapich2/2.0b

Note: To get here from a gcc default do the following:

module unload mkl module swap gcc intel/14.0.1.106

In the `intel` compiler stack, we need to use `mvapich2/2.0b`, which then implies `intel/14.0.1.106`. Right now, TACC has not built `fftw3` for this stack, so we'll be doing our own FFTW build.

See the Stampede user guide for more details. If you would like to always auto-load the same modules at startup, build your desired module configuration and then run:

```
module save
```

For ease in structuring the build, for now we'll define:

```
export BUILD_HOME=$HOME/build_intel
```

Python stack

Building Python3

Create ~\build_intel and then proceed with downloading and installing Python-3.3:

```
cd ~/build_intel
wget http://www.python.org/ftp/python/3.3.3/Python-3.3.3.tgz
tar -xzf Python-3.3.3.tgz
cd Python-3.3.3

# make sure you have the python patch, put it in Python-3.3.3
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/python_intel_patch.
↪tar
tar xvf python_intel_patch.tar

./configure --prefix=$BUILD_HOME \
                     CC=icc CFLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                     CXX=icpc CPPFLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                     F90=ifort F90FLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                     --enable-shared LDFLAGS="-lpthread" \
                     --with-cxx-main=icpc --with-system-ffi

make
make install
```

To successfully build `python3`, the key is replacing the file `ffi64.c`, which is done automatically by downloading and unpacking this crude patch `python_intel_patch.tar` in your `Python-3.3.3` directory. Unpack it in `Python-3.3.3` (`tar xvf python_intel_patch.tar` line above) and it will overwrite `ffi64.c`. If you forget to do this, you'll see a warning/error that `_ctypes` couldn't be built. This is important.

Here we are building everything in `~/build_intel`; you can do it whereever, but adjust things appropriately in the above instructions. The build proceeeds quickly (few minutes).

Installing FFTW3

We need to build our own FFTW3, under intel 14 and mvapich2/2.0b:

```
wget http://www.fftw.org/fftw-3.3.3.tar.gz
tar -xzf fftw-3.3.3.tar.gz
cd fftw-3.3.3

./configure --prefix=$BUILD_HOME \
                      CC=mpicc \
                      CXX=mpicxx \
                      F77=mpif90 \
                      MPICC=mpicc MPICXX=mpicxx \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads
make
make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Updating shell settings

At this point, `python3` is installed in `~/build_intel/bin/`. Add this to your path and confirm (currently there is no `python3` in the default path, so doing a `which python3` will fail if you haven't added `~/build_intel/bin`).

On Stampede, login shells (interactive connections via ssh) source only `~/.bash_profile`, `~/.bash_login` or `~/.profile`, in that order, and do not source `~/.bashrc`. Meanwhile non-login shells only launch `~/.bashrc` (see Stampede user guide).

In the bash shell, add the following to `.bashrc`:

```
export PATH=~/build_intel/bin:$PATH
export LD_LIBRARY_PATH=~/build_intel/lib:$LD_LIBRARY_PATH
```

and the following to `.profile`:

```
if [ -f ~/.bashrc ]; then . ~/.bashrc; fi
```

(from bash reference manual) to obtain the same behaviour in both shell types.

Installing pip

We'll use `pip` to install our python library depdencies. Instructions on doing this are available here and summarized below. First download and install setup tools:

```
cd ~/build
wget https://bitbucket.org/pypa/setuptools/raw/bootstrap/ez_setup.py
python3 ez_setup.py
```

Then install `pip`:

```
wget --no-check-certificate https://raw.github.com/pypa/pip/master/contrib/get-pip.py
python3 get-pip.py --cert /etc/ssl/certs/ca-bundle.crt
```

Now edit `~/.pip/pip.conf`:

```
[global]
cert = /etc/ssl/certs/ca-bundle.crt
```

You will now have `pip3` and `pip` installed in `~/build/bin`. You might try doing `pip -V` to confirm that `pip` is built against python 3.3. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Numpy and BLAS libraries

Building numpy against MKL

Now, acquire `numpy` (1.8.0):

```
cd ~/build_intel
wget http://sourceforge.net/projects/numpy/files/NumPy/1.8.0/numpy-1.8.0.tar.gz
tar -xvf numpy-1.8.0.tar.gz
cd numpy-1.8.0
wget http://lcd-www.colorado.edu/bpbrown/dedalus_documentation/_downloads/numpy_intel_
↪patch.tar
tar xvf numpy_inte_patch.tar
```

This last step saves you from needing to hand edit two files in `numpy/distutils`; these are `intelccompiler.py` and `fcompiler/intel.py`. I've built a crude patch, `numpy_intel_patch.tar` which can be auto-deployed by within the `numpy-1.8.0` directory by the instructions above. This will unpack and overwrite:

```
numpy/distutils/intelccompiler.py
numpy/distutils/fcompiler/intel.py
```

We'll now need to make sure that `numpy` is building against the MKL libraries. Start by making a `site.cfg` file:

```
cp site.cfg.example site.cfg
emacs -nw site.cfg
```

Edit `site.cfg` in the `[mkl]` section; modify the library directory so that it correctly point to TACC's `$MKLROOT/lib/intel64/`. With the modules loaded above, this looks like:

```
[mkl]
library_dirs = /opt/apps/intel/13/composer_xe_2013_sp1.1.106/mkl/lib/intel64
include_dirs = /opt/apps/intel/13/composer_xe_2013_sp1.1.106/mkl/include
mkl_libs = mkl_rt
lapack_libs =
```

These are based on intels instructions for compiling numpy with ifort and they seem to work so far.

Then proceed with:

```
python3 setup.py config --compiler=intelem build_clib --compiler=intelem build_ext --
↪compiler=intelem install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://lcd-www.colorado.edu/bpbrown/dedalus_documentation/_downloads/numpy_test_
↪full
chmod +x numpy_test_full
./numpy_test_full
```

or do so manually by launching `python3` and then doing:

```
import numpy as np
np.__config__.show()
```

If you've installed `nose` (with `pip3 install nose`), we can further test our numpy build with:

```
np.test()
np.test('full')
```

We fail `np.test()` with two failures, while `np.test('full')` has 3 failures and 19 errors. But we do successfully link against the fast BLAS libraries (look for `FAST BLAS` output, and fast dot product time).

Note: We should check what impact these failed tests have on our results.

Python library stack

After `numpy` has been built (see links above) we will proceed with the rest of our python stack. Right now, all of these need to be installed in each existing virtualenv instance (e.g., `openblas`, `mkl`, etc.).

For now, skip the venv process.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Download an install in your appropriate `~/venv/INSTANCE` directory:

```
wget http://sourceforge.net/projects/scipy/files/scipy/0.13.2/scipy-0.13.2.tar.gz
tar -xvf scipy-0.13.2.tar.gz
cd scipy-0.13.2
```

Then run

```
python3 setup.py config --compiler=intelem --fcompiler=intelem build_clib \
                                        --compiler=intelem --fcompiler=intelem build_
↪ext \
                                        --compiler=intelem --fcompiler=intelem install
```

Installing mpi4py

This should just be pip installed:

```
pip3 install mpi4py==2.0.0
```

Note: If we use use

```
pip3 install mpi4py
```

then stampede tries to pull version 0.6.0 of mpi4py. Hence the explicit version pull above.

Installing cython

This should just be pip installed:

```
pip3 install -v https://pypi.python.org/packages/source/C/Cython/Cython-0.20.tar.gz
```

The Feb 11, 2014 update to cython (0.20.1) seems to have broken (at least with intel compilers).:

```
pip3 install cython
```

Installing matplotlib

This should just be pip installed:

```
pip3 install -v https://downloads.sourceforge.net/project/matplotlib/matplotlib/
↪matplotlib-1.3.1/matplotlib-1.3.1.tar.gz
```

Note: If we use use

```
pip3 install matplotlib
```

then stampede tries to pull version 1.1.1 of matplotlib. Hence the explicit version pull above.

Installing sympy

Do this with a regular pip install:

```
pip3 install sympy
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O:

```
wget http://www.hdfgroup.org/ftp/HDF5/current/src/hdf5-1.8.12.tar
tar xvf hdf5-1.8.12.tar
cd hdf5-1.8.12
./configure --prefix=$BUILD_HOME \
                    CC=mpicc \
                    CXX=mpicxx \
                    F77=mpif90 \
                    MPICC=mpicc MPICXX=mpicxx \
                    --enable-shared --enable-parallel
make
make install
```

Installing h5py

Next, install h5py. We wish for full HDF5 parallel goodness, so we can do parallel file access during both simulations and post analysis as well. This will require building directly from source (see Parallel HDF5 in h5py for further details). Here we go:

```
git clone https://github.com/h5py/h5py.git
cd h5py
export CC=mpicc
export HDF5_DIR=$BUILD_HOME
python3 setup.py configure --mpi
python3 setup.py build
python3 setup.py install
```

After this install, `h5py` shows up as an `.egg` in `site-packages`, but it looks like we pass the `suggested demo2.py` test from Parallel HDF5 in h5py.

Installing h5py with collectives

We've been exploring the use of collectives for faster parallel file writing. To build that version of the h5py library:

```
git clone https://github.com/andrewcollette/h5py.git
cd h5py
git checkout mpi_collective
export CC=mpicc
export HDF5_DIR=$BUILD_HOME
python3 setup.py configure --mpi
python3 setup.py build
python3 setup.py install
```

To enable collective outputs within dedalus, edit `dedalus2/data/evaluator.py` and replace:

```
# Assemble nonconstant subspace
subshape, subslices, subdata = self.get_subspace(out)
dset = task_group.create_dataset(name=name, shape=subshape, dtype=dtype)
dset[subslices] = subdata
```

with

```
# Assemble nonconstant subspace
subshape, subslices, subdata = self.get_subspace(out)
dset = task_group.create_dataset(name=name, shape=subshape, dtype=dtype)
```

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```
with dset.collective:
    dset[subslices] = subdata
```

Alternatively, you can see this same edit in some of the forks (Lecoanet, Brown).

Note: There are some serious problems with this right now; in particular, there seems to be an issue with empty arrays causing h5py to hang. Troubleshooting is ongoing.

Dedalus2

With the modules set as above, set:

```
export BUILD_HOME=$HOME/build_intel
export FFTW_PATH=$BUILD_HOME
export MPI_PATH=$MPICH_HOME
export HDF5_DIR=$BUILD_HOME
export CC=mpicc
```

Then change into your root dedalus directory and run:

```
python setup.py build_ext --inplace
```

Our new stack (`intel/14`, `mvapich2/2.0b`) builds to completion and runs test problems successfully. We have good scaling in limited early tests.

Running Dedalus on Stampede

Source the appropriate virtualenv:

```
source ~/venv/openblas/bin/activate
```

or:

```
source ~/venv/mkl/bin/activate
```

grab an interactive dev node with `idev`. Play.

Skipped libraries

Installing freetype2

Freetype is necessary for matplotlib

```
cd ~/build
wget http://sourceforge.net/projects/freetype/files/freetype2/2.5.2/freetype-2.5.2.
↪tar.gz
tar -xvf freetype-2.5.2.tar.gz
cd freetype-2.5.2
./configure --prefix=$HOME/build
```

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```
make
make install
```

Note: Skipping for now

Installing libpng

May need this for matplotlib?:

```
cd ~/build
wget http://prdownloads.sourceforge.net/libpng/libpng-1.6.8.tar.gz
./configure --prefix=$HOME/build
make
make install
```

Note: Skipping for now

UMFPACK

We may wish to deploy UMFPACK for sparse matrix solves. Keaton is starting to look at this now. If we do, both numpy and scipy will require UMFPACK, so we should build it before proceeding with those builds.

UMFPACK requires AMD (another package by the same group, not processor) and SuiteSparse_config, too.

If we need UMFPACK, we can try installing it from `suite-sparse` as in the Mac install. Here are links to UMFPACK docs and Suite-sparse

Note: We'll check and update this later. (1/9/14)

All I want for christmas is suitesparse

Well, maybe :) Let's give it a try, and lets grab the whole library:

```
wget http://www.cise.ufl.edu/research/sparse/SuiteSparse/current/SuiteSparse.tar.gz
tar xvf SuiteSparse.tar.gz

<edit SuiteSparse_config/SuiteSparse_config.mk>
```

Note: Notes from the original successful build process:

Just got a direct call from Yaakoub. Very, very helpful. Here's the quick rundown.

He got _ctypes to work by editing the following file:

> vim /work/00364/tg456434/yye00/src/Python-3.3.3/Modules/_ctypes/libffi/src/x86/ffi64.c

Do build with intel 14 use mvapich2/2.0b Will need to do our own build of fftw3

set mpicc as c compiler rather than icc, same for CXX, FC and others, when configuring python. should help with mpi4py.

in mpi4py, can edit mpi.cfg (non-pip install).

Keep Yaakoub updated with direct e-mail on progress.

Also, Yaakoub is spear-heading TACCs efforts in doing auto-offload to Xenon Phi.

Beware of disk quotas if you're trying many builds; I hit 5GB pretty fast and blew my matplotlib install due to quota limits :)

Installing virtualenv (skipped)

In order to test multiple numpys and scipys (and really, their underlying BLAS libraries), we will use `virtualenv`:

```
pip3 install virtualenv
```

Next, construct a virtualenv to hold all of your python modules. We suggest doing this in your home directory:

```
mkdir ~/venv
```

Python3

Note: With help from Yaakoub, we now build `_ctypes` successfully.

Also, the mpicc build is much, much slower than icc. Interesting. And we crashed out. Here's what we tried with mpicc:

```
./configure --prefix=$BUILD_HOME \
                CC=mpicc CFLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                CXX=mpicxx CPPFLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                F90=mpif90 F90FLAGS="-mkl -O3 -xHost -fPIC -ipo" \
                --enable-shared LDFLAGS="-lpthread" \
                --with-cxx-main=mpicxx --with-system-ffi
```

Install notes for NASA/Pleiades

Best performance is coming from our newly developed Pleaides/Intel/MKL stack; we've retained our gcc/openblas build for future use.

Install notes for NASA/Pleiades: Intel stack

An initial Pleiades environment is pretty bare-bones. There are no modules, and your shell is likely a csh varient. To switch shells, send an e-mail to support@nas.nasa.gov; I'll be using `bash`.

Then add the following to your `.profile`:

```
# Add your commands here to extend your PATH, etc.

module load comp-intel
module load git
module load openssl
module load emacs

export BUILD_HOME=$HOME/build

export PATH=$BUILD_HOME/bin:$BUILD_HOME:/$PATH  # Add private commands to PATH

export LD_LIBRARY_PATH=$BUILD_HOME/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=/nasa/openssl/1.0.1h/lib/:$LD_LIBRARY_PATH

export CC=mpicc

#pathing for Dedalus
export LOCAL_MPI_VERSION=openmpi-1.10.1
export LOCAL_MPI_SHORT=v1.10

# falling back to 1.8 until we resolve tcp wireup errors
# (probably at runtime with MCA parameters)
export LOCAL_MPI_VERSION=openmpi-1.8.6
export LOCAL_MPI_SHORT=v1.8

export LOCAL_PYTHON_VERSION=3.5.0
export LOCAL_NUMPY_VERSION=1.10.1
export LOCAL_SCIPY_VERSION=0.16.1
export LOCAL_HDF5_VERSION=1.8.15-patch1
export LOCAL_MERCURIAL_VERSION=3.6

export MPI_ROOT=$BUILD_HOME/$LOCAL_MPI_VERSION
export PYTHONPATH=$BUILD_HOME/dedalus:$PYTHONPATH
export MPI_PATH=$MPI_ROOT
export FFTW_PATH=$BUILD_HOME
export HDF5_DIR=$BUILD_HOME

# Openmpi forks:
export OMPI_MCA_mpi_warn_on_fork=0

# don't mess up Pleiades for everyone else
export OMPI_MCA_btl_openib_if_include=mlx4_0:1
```

Doing the entire build took about 2 hours. This was with several (4) open ssh connections to Pleaides to do poor-mans-parallel building (of python, hdf5, fftw, etc.), and one was on a dev node for the openmpi compile. The openmpi compile is time intensive and mus be done first. The fftw and hdf5 libraries take a while to build. Building scipy remains the most significant time cost.

Python stack

Interesting update. Pleiades now appears to have a python3 module. Fascinating. It comes with matplotlib (1.3.1), scipy (0.12), numpy (1.8.0) and cython (0.20.1) and a few others. Very interesting. For now we'll proceed with our usual build-it-from-scratch approach, but this should be kept in mind for the future. No clear mpi4py, and the `mpi4py` install was a hangup below for some time.

Building Openmpi

The suggested `mpi-sgi/mpt` MPI stack breaks with mpi4py; existing versions of openmpi on Pleiades are outdated and suffer from a previously identified bug (v1.6.5), so we'll roll our own. This needs to be built on a compute node so that the right memory space is identified.:

```
# do this on a main node (where you can access the outside internet):
cd $BUILD_HOME
wget http://www.open-mpi.org/software/ompi/$LOCAL_MPI_SHORT/downloads/$LOCAL_MPI_
↪VERSION.tar.gz
tar xvf $LOCAL_MPI_VERSION.tar.gz

# get ivy-bridge compute node
qsub -I -q devel -l select=1:ncpus=24:mpiprocs=24:model=has -l walltime=02:00:00

# once node exists
cd $BUILD_HOME
cd $LOCAL_MPI_VERSION
./configure \
    --prefix=$BUILD_HOME \
    --enable-mpi-interface-warning \
    --without-slurm \
    --with-tm=/PBS \
    --without-loadleveler \
    --without-portals \
    --enable-mpirun-prefix-by-default \
    CC=icc CXX=icc FC=ifort

make -j
make install
```

These compilation options are based on `/nasa/openmpi/1.6.5/NAS_config.sh`, and are thanks to advice from Daniel Kokron at NAS. Compiling takes about 10-15 minutes with make -j.

Building Python3

Create `$BUILD_HOME` and then proceed with downloading and installing Python-3.4:

```
cd $BUILD_HOME
wget https://www.python.org/ftp/python/$LOCAL_PYTHON_VERSION/Python-$LOCAL_PYTHON_
↪VERSION.tgz --no-check-certificate
tar xzf Python-$LOCAL_PYTHON_VERSION.tgz
cd Python-$LOCAL_PYTHON_VERSION

./configure --prefix=$BUILD_HOME \
                    OPT="-mkl -O3 -axCORE-AVX2 -xSSE4.2 -fPIC -ipo -w -vec-report0 -
↪opt-report0" \
                    FOPT="-mkl -O3 -axCORE-AVX2 -xSSE4.2 -fPIC -ipo -w -vec-report0 -
↪opt-report0" \
                    CC=mpicc CXX=mpicxx F90=mpif90 \
                    LDFLAGS="-lpthread" \
                    --enable-shared --with-system-ffi \
                    --with-cxx-main=mpicxx --with-gcc=mpicc

make
make install
```

The previous intel patch is no longer required.

Installing pip

Python 3.4 now automatically includes pip. We suggest you do the following immediately to suppress version warning messages:

```
pip3 install --upgrade pip
```

On Pleiades, you'll need to edit `.pip/pip.conf`:

```
[global]
cert = /etc/ssl/certs/ca-bundle.trust.crt
```

You will now have `pip3` installed in `$BUILD_HOME/bin`. You might try doing `pip3 -V` to confirm that `pip3` is built against python 3.4. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

Installing mpi4py

This should be pip installed:

```
pip3 install mpi4py
```

Installing FFTW3

We need to build our own FFTW3, under intel 14 and mvapich2/2.0b, or under openmpi:

```
 wget http://www.fftw.org/fftw-3.3.4.tar.gz
 tar -xzf fftw-3.3.4.tar.gz
 cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=mpicc        CFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      CXX=mpicxx CPPFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      F77=mpif90  F90FLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      MPICC=mpicc MPICXX=mpicxx \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads
 make
 make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Installing cython

This should just be pip installed:

```
pip3 install cython
```

Numpy and BLAS libraries

Numpy will be built against a specific BLAS library. On Pleiades we will build against the Intel MKL BLAS.

Building numpy against MKL

Now, acquire `numpy` (1.9.2):

```
cd $BUILD_HOME
wget http://sourceforge.net/projects/numpy/files/NumPy/$LOCAL_NUMPY_VERSION/numpy-
↪$LOCAL_NUMPY_VERSION.tar.gz
tar -xvf numpy-$LOCAL_NUMPY_VERSION.tar.gz
cd numpy-$LOCAL_NUMPY_VERSION
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_pleiades_intel_
↪patch.tar
tar xvf numpy_pleiades_intel_patch.tar
```

This last step saves you from needing to hand edit two files in `numpy/distutils`; these are `intelccompiler.py` and `fcompiler/intel.py`. I've built a crude patch, `numpy_pleiades_intel_patch.tar` which is auto-deployed within the `numpy-$LOCAL_NUMPY_VERSION` directory by the instructions above. This will unpack and overwrite:

```
numpy/distutils/intelccompiler.py
numpy/distutils/fcompiler/intel.py
```

This differs from prior versions in that "-xhost" is replaced with "-axCORE-AVX2 -xSSE4.2". NOTE: this is now updated for Haswell.

We'll now need to make sure that `numpy` is building against the MKL libraries. Start by making a `site.cfg` file:

```
cp site.cfg.example site.cfg
emacs -nw site.cfg
```

Note: If you're doing many different builds, it may be helpful to have the numpy site.cfg shared between builds. If so, you can edit ~/.numpy-site.cfg instead of site.cfg. This is per site.cfg.example.

Edit `site.cfg` in the `[mkl]` section; modify the library directory so that it correctly point to TACC's `$MKLROOT/lib/intel64/`. With the modules loaded above, this looks like:

```
[mkl]
library_dirs = /nasa/intel/Compiler/2015.3.187/composer_xe_2015.3.187/mkl/lib/intel64/
include_dirs = /nasa/intel/Compiler/2015.3.187/composer_xe_2015.3.187/mkl/include
mkl_libs = mkl_rt
lapack_libs =
```

These are based on intels instructions for compiling numpy with ifort and they seem to work so far.

Then proceed with:

```
python3 setup.py config --compiler=intelem build_clib --compiler=intelem build_ext --
↪compiler=intelem install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_test_full
chmod +x numpy_test_full
./numpy_test_full
```

We succesfully link against fast BLAS and the test results look normal.

Python library stack

After `numpy` has been built we will proceed with the rest of our python stack.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Dong a pip install fails, so we'll keep doing it the old fashioned way:

```
wget http://sourceforge.net/projects/scipy/files/scipy/$LOCAL_SCIPY_VERSION/scipy-
↪$LOCAL_SCIPY_VERSION.tar.gz
tar -xvf scipy-$LOCAL_SCIPY_VERSION.tar.gz
cd scipy-$LOCAL_SCIPY_VERSION
python3 setup.py config --compiler=intelem --fcompiler=intelem build_clib \
                                        --compiler=intelem --fcompiler=intelem build_
↪ext \
                                        --compiler=intelem --fcompiler=intelem install
```

Note: We do not have umfpack; we should address this moving forward, but for now I will defer that to a later day.

Installing matplotlib

This should just be pip installed. However, we're hitting errors with qhull compilation in every part of the 1.4.x branch, so we fall back to 1.3.1:

```
pip3 install matplotlib==1.3.1
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O:

```
wget http://www.hdfgroup.org/ftp/HDF5/releases/hdf5-$LOCAL_HDF5_VERSION/src/hdf5-
↪$LOCAL_HDF5_VERSION.tar.gz
tar xzvf hdf5-$LOCAL_HDF5_VERSION.tar.gz
cd hdf5-$LOCAL_HDF5_VERSION
./configure --prefix=$BUILD_HOME \
                    CC=mpicc         CFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                    CXX=mpicxx CPPFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                    F77=mpif90  F90FLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                    MPICC=mpicc MPICXX=mpicxx \
                    --enable-shared --enable-parallel
make
make install
```

H5PY via pip

This can now just be pip installed (>=2.6.0):

```
pip3 install h5py
```

For now we drop our former instructions on attempting to install parallel h5py with collectives. See the repo history for those notes.

Installing Mercurial

On NASA Pleiades, we need to install mercurial itself. I can't get mercurial to build properly on intel compilers, so for now use gcc:

```
cd $BUILD_HOME
wget http://mercurial.selenic.com/release/mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
tar xvf mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
cd mercurial-$LOCAL_MERCURIAL_VERSION
module load gcc
export CC=gcc
make install PREFIX=$BUILD_HOME
```

I suggest you add the following to your `~/.hgrc`:

```
[ui]
username = <your bitbucket username/e-mail address here>
editor = emacs

[web]
cacerts = /etc/ssl/certs/ca-bundle.crt

[extensions]
graphlog =
color =
convert =
mq =
```

Dedalus

Preliminaries

Then do the following:

```
cd $BUILD_HOME
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
pip3 install -r requirements.txt
python3 setup.py build_ext --inplace
```

Running Dedalus on Pleiades

Our scratch disk system on Pleiades is `/nobackup/user-name`. On this and other systems, I suggest soft-linking your scratch directory to a local working directory in home; I uniformly call mine `workdir`:

```
ln -s /nobackup/bpbrown workdir
```

Long-term mass storage is on LOU.

Install notes for NASA/Pleiades: Intel stack with MPI-SGI

Here we build using the recommended MPI-SGI environment, with Intel compilers. An initial Pleiades environment is pretty bare-bones. There are no modules, and your shell is likely a csh varient. To switch shells, send an e-mail to support@nas.nasa.gov; I'll be using `bash`.

Then add the following to your `.profile`:

```
# Add your commands here to extend your PATH, etc.

module load mpi-sgi/mpt
module load comp-intel
module load git
module load openssl
module load emacs

export BUILD_HOME=$HOME/build

export PATH=$BUILD_HOME/bin:$BUILD_HOME:/$PATH  # Add private commands to PATH

export LD_LIBRARY_PATH=$BUILD_HOME/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=/nasa/openssl/1.0.1h/lib/:$LD_LIBRARY_PATH

# proper wrappers for using Intel rather than GNU compilers,
# Thanks to Daniel Kokron at NASA.
export MPICC_CC=icc
export MPICXX_CXX=icpc

export CC=mpicc

#pathing for Dedalus
export LOCAL_PYTHON_VERSION=3.5.0
export LOCAL_NUMPY_VERSION=1.10.1
```

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```
export LOCAL_SCIPY_VERSION=0.16.1
export LOCAL_HDF5_VERSION=1.8.15-patch1
export LOCAL_MERCURIAL_VERSION=3.6

export PYTHONPATH=$BUILD_HOME/dedalus:$PYTHONPATH
export MPI_PATH=$MPI_ROOT
export FFTW_PATH=$BUILD_HOME
export HDF5_DIR=$BUILD_HOME

# Pleaides workaround for QP errors 8/25/14 from NAS (only for MPI-SGI)
export MPI_USE_UD=true
```

Python stack

Here we use the recommended MPI-SGI compilers, rather than our own openmpi.

Building Python3

Create `$BUILD_HOME` and then proceed with downloading and installing Python-3.4:

```
cd $BUILD_HOME
wget https://www.python.org/ftp/python/$LOCAL_PYTHON_VERSION/Python-$LOCAL_PYTHON_
↪VERSION.tgz --no-check-certificate
tar xzf Python-$LOCAL_PYTHON_VERSION.tgz
cd Python-$LOCAL_PYTHON_VERSION
./configure --prefix=$BUILD_HOME \
                     OPT="-w -vec-report0 -opt-report0" \
                     FOPT="-w -vec-report0 -opt-report0" \
                     CFLAGS="-mkl -O3 -ipo -axCORE-AVX2 -xSSE4.2 -fPIC" \
                     CPPFLAGS="-mkl -O3 -ipo -axCORE-AVX2 -xSSE4.2 -fPIC" \
                     F90FLAGS="-mkl -O3 -ipo -axCORE-AVX2 -xSSE4.2 -fPIC" \
                     CC=mpicc  CXX=mpicxx F90=mpif90  \
                     --with-cxx-main=mpicxx --with-gcc=mpicc \
                     LDFLAGS="-lpthread" \
                    --enable-shared --with-system-ffi

make
make install
```

The previous intel patch is no longer required.

Installing pip

Python 3.4 now automatically includes pip.

On Pleiades, you'll need to edit `.pip/pip.conf`:

```
[global]
cert = /etc/ssl/certs/ca-bundle.trust.crt
```

You will now have `pip3` installed in `$BUILD_HOME/bin`. You might try doing `pip3 -V` to confirm that `pip3` is built against python 3.4. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

We suggest doing the following immediately to suppress version warning messages:

```
pip3 install --upgrade pip
```

Installing mpi4py

This should be pip installed:

```
pip3 install mpi4py
```

version >=2.0.0 seem to play well with mpi-sgi.

Installing FFTW3

We build our own FFTW3:

```
 wget http://www.fftw.org/fftw-3.3.4.tar.gz
 tar -xzf fftw-3.3.4.tar.gz
 cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=icc        CFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      CXX=icpc CPPFLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      F77=ifort  F90FLAGS="-O3 -axCORE-AVX2 -xSSE4.2" \
                      MPICC=icc MPICXX=icpc \
                      LDFLAGS="-lmpi" \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads
 make -j
 make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Installing cython

This should just be pip installed:

```
pip3 install cython
```

Numpy and BLAS libraries

Numpy will be built against a specific BLAS library. On Pleiades we will build against the OpenBLAS libraries.

All of the intel patches, etc. are unnecessary in the gcc stack.

Building numpy against MKL

Now, acquire `numpy` (1.10.1):

```
cd $BUILD_HOME
wget http://sourceforge.net/projects/numpy/files/NumPy/$LOCAL_NUMPY_VERSION/numpy-
↪$LOCAL_NUMPY_VERSION.tar.gz
tar -xvf numpy-$LOCAL_NUMPY_VERSION.tar.gz
cd numpy-$LOCAL_NUMPY_VERSION
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_pleiades_intel_
↪patch.tar
tar xvf numpy_pleiades_intel_patch.tar
```

This last step saves you from needing to hand edit two files in `numpy/distutils`; these are `intelccompiler.py` and `fcompiler/intel.py`. I've built a crude patch, `numpy_pleiades_intel_patch.tar` which is auto-deployed within the `numpy-$LOCAL_NUMPY_VERSION` directory by the instructions above. This will unpack and overwrite:

```
numpy/distutils/intelccompiler.py
numpy/distutils/fcompiler/intel.py
```

This differs from prior versions in that "-xhost" is replaced with "-axCORE-AVX2 -xSSE4.2". I think this could be handled more gracefully using a extra_compile_flag option in the site.cfg.

We'll now need to make sure that `numpy` is building against the MKL libraries. Start by making a `site.cfg` file:

```
cp site.cfg.example site.cfg
emacs -nw site.cfg
```

Edit `site.cfg` in the `[mkl]` section; modify the library directory so that it correctly point to TACC's `$MKLROOT/lib/intel64/`. With the modules loaded above, this looks like:

```
[mkl]
library_dirs = /nasa/intel/Compiler/2015.3.187/composer_xe_2015.3.187/mkl/lib/intel64/
include_dirs = /nasa/intel/Compiler/2015.3.187/composer_xe_2015.3.187/mkl/include
mkl_libs = mkl_rt
lapack_libs =
```

These are based on intels instructions for compiling numpy with ifort and they seem to work so far.

Then proceed with:

```
python3 setup.py config --compiler=intelem build_clib --compiler=intelem build_ext --
↪compiler=intelem install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_test_full
chmod +x numpy_test_full
./numpy_test_full
```

We succesfully link against fast BLAS and the test results look normal.

Python library stack

After `numpy` has been built we will proceed with the rest of our python stack.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Dong a pip install fails, so we'll keep doing it the old fashioned way:

```
wget http://sourceforge.net/projects/scipy/files/scipy/$LOCAL_SCIPY_VERSION/scipy-
↪$LOCAL_SCIPY_VERSION.tar.gz
tar -xvf scipy-$LOCAL_SCIPY_VERSION.tar.gz
cd scipy-$LOCAL_SCIPY_VERSION
python3 setup.py config --compiler=intelem --fcompiler=intelem build_clib \
                                        --compiler=intelem --fcompiler=intelem build_
↪ext \
                                        --compiler=intelem --fcompiler=intelem install
```

Note: We do not have umfpack; we should address this moving forward, but for now I will defer that to a later day.

Installing matplotlib

This should just be pip installed. In versions of matplotlib>1.3.1, Qhull has a compile error if the C compiler is used rather than C++, so we force the C complier to be icpc

```
export CC=icpc
pip3 install matplotlib
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O. Intel compilers are failing on this when done with mpi-sgi, and on NASA's recommendation we're falling back to gcc for this library:

```
export MPICC_CC=
export MPICXX_CXX=
wget http://www.hdfgroup.org/ftp/HDF5/releases/hdf5-$LOCAL_HDF5_VERSION/src/hdf5-
↪$LOCAL_HDF5_VERSION.tar.gz
tar xzvf hdf5-$LOCAL_HDF5_VERSION.tar.gz
cd hdf5-$LOCAL_HDF5_VERSION
./configure --prefix=$BUILD_HOME CC=mpicc CXX=mpicxx F77=mpif90 \
                    --enable-shared --enable-parallel
make
make install
```

H5PY via pip

This can now just be pip installed (>=2.6.0):

pip3 install h5py

For now we drop our former instructions on attempting to install parallel h5py with collectives. See the repo history for those notes.

Installing Mercurial

On NASA Pleiades, we need to install mercurial itself. I can't get mercurial to build properly on intel compilers, so for now use gcc:

```
cd $BUILD_HOME
wget http://mercurial.selenic.com/release/mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
tar xvf mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
cd mercurial-$LOCAL_MERCURIAL_VERSION
module load gcc
export CC=gcc
make install PREFIX=$BUILD_HOME
```

I suggest you add the following to your `~/.hgrc`:

```
[ui]
username = <your bitbucket username/e-mail address here>
editor = emacs

[web]
cacerts = /etc/ssl/certs/ca-bundle.crt

[extensions]
graphlog =
color =
convert =
mq =
```

Dedalus

Preliminaries

Then do the following:

```
cd $BUILD_HOME
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
pip3 install -r requirements.txt
python3 setup.py build_ext --inplace
```

Running Dedalus on Pleiades

Our scratch disk system on Pleiades is `/nobackup/user-name`. On this and other systems, I suggest soft-linking your scratch directory to a local working directory in home; I uniformly call mine `workdir`:

```
ln -s /nobackup/bpbrown workdir
```

Long-term mass storage is on LOU.

Install notes for NASA/Pleiades: gcc stack

Note: Warning. These instructions for a gcc stack are quite outdated and have not been tested in well over a year. A lot has shifted in the stack since then (e.g., h5py, matplotlib) and using these is at your own risk. We have been using the intel compilers exclusively on Pleiades, so please see those instructions. These gcc instructions are kept for posterity and future use.

Old instructions

An initial Pleiades environment is pretty bare-bones. There are no modules, and your shell is likely a csh varient. To switch shells, send an e-mail to support@nas.nasa.gov; I'll be using `bash`.

Then add the following to your `.profile`:

```
# Add your commands here to extend your PATH, etc.

module load gcc
module load git
module load openssl

export BUILD_HOME=$HOME/build

export PATH=$BUILD_HOME/bin:$BUILD_HOME:/$PATH  # Add private commands to PATH

export LD_LIBRARY_PATH=$BUILD_HOME/lib:$LD_LIBRARY_PATH

export CC=mpicc

#pathing for Dedalus2
export MPI_ROOT=$BUILD_HOME/openmpi-1.8
export PYTHONPATH=$BUILD_HOME/dedalus2:$PYTHONPATH
export MPI_PATH=$MPI_ROOT
export FFTW_PATH=$BUILD_HOME
```

Note: We are moving here to a python 3.4 build. Also, it looks like scipy-0.14 and numpy 1.9 are going to have happier sparse matrix performance.

Doing the entire build took about 1 hour. This was with several (4) open ssh connections to Pleaides to do poor-mans-parallel building (of openBLAS, hdf5, fftw, etc.), and one was on a dev node for the openmpi and openblas compile.

Python stack

Interesting update. Pleiades now appears to have a python3 module. Fascinating. It comes with matplotlib (1.3.1), scipy (0.12), numpy (1.8.0) and cython (0.20.1) and a few others. Very interesting. For now we'll proceed with our usual build-it-from-scratch approach, but this should be kept in mind for the future. No clear mpi4py, and the `mpi4py` install was a hangup below for some time.

Building Openmpi

The suggested `mpi-sgi/mpt` MPI stack breaks with mpi4py; existing versions of openmpi on Pleiades are outdated and suffer from a previously identified bug (v1.6.5), so we'll roll our own. This needs to be built on a compute node so that the right memory space is identified.:

```
# do this on a main node (where you can access the outside internet):
cd $BUILD_HOME
wget http://www.open-mpi.org/software/ompi/v1.8/downloads/openmpi-1.8.tar.gz
tar xvf openmpi-1.7.3.tar.gz

# get ivy-bridge compute node
qsub -I -q devel -l select=1:ncpus=20:mpiprocs=20:model=ivy -l walltime=02:00:00

# once node exists
cd $BUILD_HOME
cd openmpi-1.7.3
./configure \
    --prefix=$BUILD_HOME \
    --enable-mpi-interface-warning \
    --without-slurm \
    --with-tm=/PBS \
    --without-loadleveler \
    --without-portals \
    --enable-mpirun-prefix-by-default \
    CC=gcc

make
make install
```

These compilation options are based on `/nasa/openmpi/1.6.5/NAS_config.sh`, and are thanks to advice from Daniel Kokron at NAS.

We're using openmpi 1.7.3 here because something substantial changes in 1.7.4 and from that point onwards instances of mpirun hang on Pleiades, when used on more than 1 node worth of cores. I've tested this extensively with a simple hello world program (http://www.dartmouth.edu/~rc/classes/intro_mpi/hello_world_ex.html) and for now suggest we move forward until this is resolved.

Building Python3

Create `$BUILD_HOME` and then proceed with downloading and installing Python-3.4:

```
cd $BUILD_HOME
wget https://www.python.org/ftp/python/3.4.0/Python-3.4.0.tgz --no-check-certificate
tar xzf Python-3.4.0.tgz
cd Python-3.4.0

./configure --prefix=$BUILD_HOME \
                    CC=mpicc \
                    CXX=mpicxx \
                    F90=mpif90 \
                    --enable-shared LDFLAGS="-lpthread" \
                    --with-cxx-main=mpicxx --with-system-ffi

make
make install
```

All of the intel patches, etc. are unnecessary in the gcc stack.

Note: We're getting a problem on `_curses_panel` and on `_sqlite3`; ignoring for now.

Installing pip

Python 3.4 now automatically includes pip.

On Pleiades, you'll need to edit `.pip/pip.conf`:

```
[global]
cert = /etc/ssl/certs/ca-bundle.crt
```

You will now have `pip3` installed in `$BUILD_HOME/bin`. You might try doing `pip3 -V` to confirm that `pip3` is built against python 3.4. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

Installing mpi4py

This should be pip installed:

```
pip3 install mpi4py
```

Note: Test that this works by doing a:

from mpi4py import MPI

This will segfault on sgi-mpi, but appears to work fine on openmpi-1.8, 1.7.3, etc.

Installing FFTW3

We need to build our own FFTW3, under intel 14 and mvapich2/2.0b:

```
 wget http://www.fftw.org/fftw-3.3.4.tar.gz
 tar -xzf fftw-3.3.4.tar.gz
 cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=mpicc \
                      CXX=mpicxx \
                      F77=mpif90 \
                      MPICC=mpicc MPICXX=mpicxx \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads
 make
 make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Installing cython

This should just be pip installed:

```
pip3 install cython
```

The Feb 11, 2014 update to cython (0.20.1) seems to work with gcc.

Numpy and BLAS libraries

Numpy will be built against a specific BLAS library. On Pleiades we will build against the OpenBLAS libraries.

All of the intel patches, etc. are unnecessary in the gcc stack.

Building OpenBLAS

From Stampede instructions:

```
# this needs to be done on a frontend
cd $BUILD_HOME
git clone git://github.com/xianyi/OpenBLAS

# suggest doing this build on a compute node, so we get the
# right number of openmp threads and architecture
cd $BUILD_HOME
cd OpenBLAS
make
make PREFIX=$BUILD_HOME install
```

Here's the build report before the `make install`:

```
OpenBLAS build complete. (BLAS CBLAS LAPACK LAPACKE)

OS               ... Linux
Architecture     ... x86_64
BINARY           ... 64bit
C compiler       ... GCC  (command line : mpicc)
Fortran compiler ... GFORTRAN  (command line : gfortran)
Library Name     ... libopenblas_sandybridgep-r0.2.9.rc2.a (Multi threaded; Max num-
↪threads is 40)
```

Building numpy against OpenBLAS

Now, acquire `numpy` (1.8.1):

```
wget http://sourceforge.net/projects/numpy/files/NumPy/1.8.1/numpy-1.8.1.tar.gz
tar xvf numpy-1.8.1.tar.gz
cd numpy-1.8.1
```

Create `site.cfg` with information for the OpenBLAS library directory

Next, make a site specific config file:

```
cp site.cfg.example site.cfg
emacs -nw site.cfg
```

Edit `site.cfg` to uncomment the `[openblas]` section; modify the library and include directories so that they correctly point to your `~/build/lib` and `~/build/include` (note, you may need to do fully expanded paths). With my account settings, this looks like:

```
[openblas]
libraries = openblas
library_dirs = /u/bpbrown/build/lib
include_dirs = /u/bpbrown/build/include
```

where `$BUILD_HOME=/u/bpbrown/build`. We may in time want to consider adding fftw as well. Now build:

```
python3 setup.py config build_clib build_ext install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_test_full
chmod +x numpy_test_full
./numpy_test_full
```

We succesfully link against fast BLAS and the test results look normal.

Python library stack

After `numpy` has been built we will proceed with the rest of our python stack.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Dong a pip install fails, so we'll keep doing it the old fashioned way:

```
wget http://sourceforge.net/projects/scipy/files/scipy/0.13.3/scipy-0.13.3.tar.gz
tar -xvf scipy-0.13.3.tar.gz
cd scipy-0.13.3
python3 setup.py config build_clib build_ext install
```

Note: We do not have umfpack; we should address this moving forward, but for now I will defer that to a later day.

Installing matplotlib

This should just be pip installed:

```
pip3 install matplotlib
```

Installing sympy

This should just be pip installed:

```
pip3 install sympy
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O:

```
wget http://www.hdfgroup.org/ftp/HDF5/current/src/hdf5-1.8.12.tar
tar xvf hdf5-1.8.12.tar
cd hdf5-1.8.12
./configure --prefix=$BUILD_HOME \
                    CC=mpicc \
                    CXX=mpicxx \
                    F77=mpif90 \
                    MPICC=mpicc MPICXX=mpicxx \
                    --enable-shared --enable-parallel
make
make install
```

Next, install h5py. For reasons that are currently unclear to me, this cannot be done via pip install.

Installing h5py with collectives

We've been exploring the use of collectives for faster parallel file writing.

git is having some problems, especially with it's SSL version. I suggest adding the following to `~/.gitconfig`:

```
[http]
sslCAinfo = /etc/ssl/certs/ca-bundle.crt
```

This is still not working, owing (most likely) to git being built on an outdated SSL version. Here's a short-term hack:

```
export GIT_SSL_NO_VERIFY=true
```

To build that version of the h5py library:

```
git clone git://github.com/andrewcollette/h5py
cd h5py
git checkout mpi_collective
export CC=mpicc
export HDF5_DIR=$BUILD_HOME
python3 setup.py configure --mpi
```

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```
python3 setup.py build
python3 setup.py install
```

Here's the original h5py repository:

```
git clone git://github.com/h5py/h5py
cd h5py
export CC=mpicc
export HDF5_DIR=$BUILD_HOME
python3 setup.py configure --mpi
python3 setup.py build
python3 setup.py install
```

Note: This is ugly. We're getting a "-R" error at link, triggered by distutils not recognizing that mpicc is gcc or something like that. Looks like we're failing `if self._is_gcc(compiler)` For now, I've hand-edited unixccompiler.py in `lib/python3.3/distutils` and changed this line:

> **def _is_gcc(self, compiler_name):** return "gcc" in compiler_name or "g++" in compiler_name

to:

> **def _is_gcc(self, compiler_name):** return "gcc" in compiler_name or "g++" in compiler_name or "mpicc" in compiler_name

This is a hack, but it get's us running and alive!

Note: Ahh... I understand what's happening here. We built with `mpicc`, and the test `_is_gcc` looks for whether gcc appears anywhere in the compiler name. It doesn't in `mpicc`, so the `gcc` checks get missed. This is only ever used in the `runtime_library_dir_option()` call. So we'd need to either rename the mpicc wrapper something like `mpicc-gcc` or do a test on `compiler --version` or something. Oh boy. Serious upstream problem for mpicc wrapped builds that cythonize and go to link. Hmm...

Installing Mercurial

On NASA Pleiades, we need to install mercurial itself:

```
wget http://mercurial.selenic.com/release/mercurial-2.9.tar.gz
tar xvf mercurial-2.9.tar.gz
cd mercurial-2.9
make install PREFIX=$BUILD_HOME
```

I suggest you add the following to your `~/.hgrc`:

```
[ui]
username = <your bitbucket username/e-mail address here>
editor = emacs

[web]
cacerts = /etc/ssl/certs/ca-bundle.crt

[extensions]
```

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```
graphlog =
color =
convert =
mq =
```

Dedalus2

Preliminaries

With the modules set as above, set:

```
export BUILD_HOME=$BUILD_HOME
export FFTW_PATH=$BUILD_HOME
export MPI_PATH=$BUILD_HOME/openmpi-1.8
```

Then change into your root dedalus directory and run:

```
python setup.py build_ext --inplace
```

further packages needed for Keaton's branch:

```
pip3 install tqdm
pip3 install pathlib
```

Running Dedalus on Pleiades

Our scratch disk system on Pleiades is `/nobackup/user-name`. On this and other systems, I suggest soft-linking your scratch directory to a local working directory in home; I uniformly call mine `workdir`:

```
ln -s /nobackup/bpbrown workdir
```

Long-term mass storage is on LOU.

Install notes for NASA/Discover

This installation is fairly straightforward because most of the work has already been done by the NASA/Discover staff, namely Jules Kouatchou.

First, add the following lines to your `~/.bashrc` file and source it:

```
module purge
module load other/comp/gcc-4.9.1
module load lib/mkl-15.0.0.090
module load other/Py3Dist/py-3.4.1_gcc-4.9.1_mkl-15.0.0.090
module load other/mpi/openmpi/1.8.2-gcc-4.9.1

export BUILD_HOME=$HOME/build
export PYTHONPATH=$HOME/dedalus2
```

This loads the gcc compiler, MKL linear algebra package, openmpi version 1.8.2, and crucially various python3 libraries. To see the list of python libraries,

```
listPyPackages
```

We actually have all the python libraries we need for Dedalus. However, we still need fftw. To install fftw,

```
mkdir build

cd $BUILD_HOME
wget http://www.fftw.org/fftw-3.3.4.tar.gz
tar -xzf fftw-3.3.4.tar.gz
cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=mpicc \
                      CXX=mpicxx \
                      F77=mpif90 \
                      MPICC=mpicc MPICXX=mpicxx \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads

make
make install
```

All that remains is to pull Dedalus down from Bitbucket and install it.

```
cd $HOME
hg clone https://bitbucket.org/dedalus-project/dedalus2

export FFTW_PATH=$BUILD_HOME
export HDF5_DIR=$BUILD_HOME
export MPI_DIR=/usr/local/other/SLES11.1/openMpi/1.8.2/gcc-4.9.1
cd $HOME/dedalus2
python3 setup.py build_ext --inplace
```

Install notes for PSC/Bridges: Intel stack

Here we build using the recommended Intel compilers. Bridges comes with python 3.4 at present, but for now we'll maintain a boutique build to keep access to python >=3.5 and to tune numpy performance by hand (though the value proposition of this should be tested).

Then add the following to your `.bash_profile`:

```
# Add your commands here to extend your PATH, etc.

export BUILD_HOME=$HOME/build

export PATH=$BUILD_HOME/bin:$BUILD_HOME:/$PATH  # Add private commands to PATH
export LD_LIBRARY_PATH=$BUILD_HOME/lib:$LD_LIBRARY_PATH

export CC=mpiicc

export I_MPI_CC=icc

#pathing for Dedalus
export LOCAL_PYTHON_VERSION=3.5.1
export LOCAL_NUMPY_VERSION=1.11.0
export LOCAL_SCIPY_VERSION=0.17.0
```

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```
export LOCAL_HDF5_VERSION=1.8.16
export LOCAL_MERCURIAL_VERSION=3.7.3

export PYTHONPATH=$BUILD_HOME/dedalus:$PYTHONPATH
export MPI_PATH=$MPI_ROOT
export FFTW_PATH=$BUILD_HOME
export HDF5_DIR=$BUILD_HOME
```

Python stack

Here we use the recommended Intel mpi compilers, rather than our own openmpi.

Building Python3

Create `$BUILD_HOME` and then proceed with downloading and installing Python-3:

```
cd $BUILD_HOME
wget https://www.python.org/ftp/python/$LOCAL_PYTHON_VERSION/Python-$LOCAL_PYTHON_
↪VERSION.tgz --no-check-certificate
tar xzf Python-$LOCAL_PYTHON_VERSION.tgz
cd Python-$LOCAL_PYTHON_VERSION
./configure --prefix=$BUILD_HOME \
                    OPT="-w -vec-report0 -opt-report0" \
                    FOPT="-w -vec-report0 -opt-report0" \
                    CFLAGS="-mkl -O3 -ipo -xCORE-AVX2 -fPIC" \
                    CPPFLAGS="-mkl -O3 -ipo -xCORE-AVX2 -fPIC" \
                    F90FLAGS="-mkl -O3 -ipo -xCORE-AVX2 -fPIC" \
                    CC=mpiicc  CXX=mpiicpc F90=mpiifort  \
                    LDFLAGS="-lpthread"
make -j
make install
```

The previous intel patch is no longer required.

Installing pip

Python 3.4+ now automatically includes pip.

You will now have `pip3` installed in `$BUILD_HOME/bin`. You might try doing `pip3 -V` to confirm that `pip3` is built against python 3.4. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

We suggest doing the following immediately to suppress version warning messages:

```
pip3 install --upgrade pip
```

Installing mpi4py

This should be pip installed:

```
pip3 install mpi4py
```

This required setting the `I_MPI_CC=icc` envirnoment variable above; otherwise we keep hitting gcc.

Installing FFTW3

We build our own FFTW3:

```
 wget http://www.fftw.org/fftw-3.3.4.tar.gz
 tar -xzf fftw-3.3.4.tar.gz
 cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=mpiicc        CFLAGS="-O3 -xCORE-AVX2" \
                      CXX=mpiicpc CPPFLAGS="-O3 -xCORE-AVX2" \
                      F77=mpiifort  F90FLAGS="-O3 -xCORE-AVX2" \
                      MPICC=mpiicc MPICXX=mpiicpc \
                      LDFLAGS="-lmpi" \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads
 make -j
 make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Installing cython

This should just be pip installed:

```
pip3 install cython
```

Numpy and BLAS libraries

Numpy will be built against a specific BLAS library.

Building numpy against MKL

Now, acquire `numpy`. The login nodes for Bridges are 14-core Haswell chips, just like the compute nodes, so let's try doing it with the normal numpy settings (no patching to adjust the compiler commands in distutils for cross-compiling). Ah shoots. Nope. The numpy distutils only employs xSSE4.2 and none of the AVX2 arch flags, nor a basic xhost. Well. On we go. Change `-xSSE4.2` to `-xCORE-AVX2` in `numpy/distutils/intelccompiler.py` and `numpy/distutils/fcompiler/intel.py`. We should really put in a PR and an ability to pass flags via `site.cfg` or other approach.

Here's an automated way to do this, using `numpy_intel.patch`.:

```
cd $BUILD_HOME
wget http://sourceforge.net/projects/numpy/files/NumPy/$LOCAL_NUMPY_VERSION/numpy-
↪$LOCAL_NUMPY_VERSION.tar.gz
tar -xvf numpy-$LOCAL_NUMPY_VERSION.tar.gz
cd numpy-$LOCAL_NUMPY_VERSION
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_intel.patch
patch -p1 < numpy_intel.patch
```

We'll now need to make sure that `numpy` is building against the MKL libraries. Start by making a `site.cfg` file:

```
cat >> site.cfg << EOF
[mkl]
library_dirs = /opt/packages/intel/compilers_and_libraries/linux/mkl/lib/intel64
include_dirs = /opt/packages/intel/compilers_and_libraries/linux/mkl/include
mkl_libs = mkl_rt
lapack_libs =
EOF
```

Then proceed with:

```
python3 setup.py config --compiler=intelem build_clib --compiler=intelem build_ext --
↪compiler=intelem install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_test_full
chmod +x numpy_test_full
./numpy_test_full
```

Numpy has changed the location of _dotblas, so our old test doesn't work. From the dot product speed, it looks like we have succesfully linked against fast BLAS and the test results look relatively normal, but this needs to be looked in to.

Python library stack

After `numpy` has been built we will proceed with the rest of our python stack.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Scipy now is no longer hosted at sourceforge for anything past v0.16, so lets try git:

```
git clone git://github.com/scipy/scipy.git scipy
cd scipy
# fall back to stable version
git checkout tags/v$LOCAL_SCIPY_VERSION
python3 setup.py config --compiler=intelem --fcompiler=intelem build_clib \
```

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```
                                        --compiler=intelem --fcompiler=intelem build_
↪ext \
                                        --compiler=intelem --fcompiler=intelem install
```

Note: We do not have umfpack; we should address this moving forward, but for now I will defer that to a later day. Again. Still.

Installing matplotlib

This should just be pip installed. In versions of matplotlib>1.3.1, Qhull has a compile error if the C compiler is used rather than C++, so we force the C complier to be icpc

```
export CC=icpc
pip3 install matplotlib
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O. Intel compilers are failing on this when done with mpi-sgi, and on NASA's recommendation we're falling back to gcc for this library:

```
wget http://www.hdfgroup.org/ftp/HDF5/releases/hdf5-$LOCAL_HDF5_VERSION/src/hdf5-
↪$LOCAL_HDF5_VERSION.tar.gz
tar xzvf hdf5-$LOCAL_HDF5_VERSION.tar.gz
cd hdf5-$LOCAL_HDF5_VERSION
./configure --prefix=$BUILD_HOME CC=mpiicc CXX=mpiicpc F77=mpiifort \
                    --enable-shared --enable-parallel
make
make install
```

H5PY via pip

This can now just be pip installed (>=2.6.0):

```
pip3 install h5py
```

For now we drop our former instructions on attempting to install parallel h5py with collectives. See the NASA/Pleiades repo history for those notes.

Installing Mercurial

Here we install mercurial itself. Following NASA/Pleiades approaches, we will use gcc. I haven't checked whether the default bridges install has mercurial:

```
cd $BUILD_HOME
wget http://mercurial.selenic.com/release/mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
tar xvf mercurial-$LOCAL_MERCURIAL_VERSION.tar.gz
```

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```
cd mercurial-$LOCAL_MERCURIAL_VERSION
module load gcc
export CC=gcc
make install PREFIX=$BUILD_HOME
```

I suggest you add the following to your ~/.hgrc:: cat >> ~/.hgrc << EOF [ui] username = <your bitbucket username/e-mail address here> editor = emacs

[extensions] graphlog = color = convert = mq = EOF

Dedalus

Preliminaries

Then do the following:

```
cd $BUILD_HOME
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
# this has some issues with mpi4py versioning --v
pip3 install -r requirements.txt
python3 setup.py build_ext --inplace
```

Running Dedalus on Bridges

Our scratch disk system on Bridges is `/pylon1/group-name/user-name`. On this and other systems, I suggest soft-linking your scratch directory to a local working directory in home; I uniformly call mine `workdir`:

```
ln -s /pylon1/group-name/user-name workdir
```

Long-term spinning storage is on `/pylon2` and is provided by allocation request.

Install notes for Trestles

Note: These are a very old set of installation instructions. They likely no longer work.

Make sure to do

$ module purge

first.

Modules

This is a minimalist list for now:

- gnu/4.8.2 (this is now the default gnu module)
- openmpi_ib
- fftw/3.3.3 (make sure to do this one last, as it's compiler/MPI dependent)

Building Python3

I usually build everything in *~/build*, but you can do it whereever. Download Python-3.3. Once loading the above modules, in the Python-3.3 source directory, do

$ ./configure –prefix=$HOME/build

followed by the usual *make -j4; make install* (the *-j4* tells make to use 4 cores). You may get something like this:

```
Python build finished, but the necessary bits to build these modules were not found:
_dbm               _gdbm              _lzma
_sqlite3
To find the necessary bits, look in setup.py in detect_modules() for the module's␣
↪name.
```

I think this should be totally fine.

At this point, make sure the python3 you installed is in your path!

Installing virtualenv

In order to test multiple numpys and scipys (and really, their underlying BLAS libraries), I am using virtualenv. In order install virtulenv, once Python-3.3 is installed, you first need to install pip manuall. Follow the steps here http://www.pip-installer.org/en/latest/installing.html for "Install or Upgrade Setuptools" and then "Install or Upgrade pip". Briefly, you need to download and run ez_setup.py and then get-pip.py. This should run without incident. Once *pip* is installed, do

$ pip install virtualenv

Building OpenBLAS

To build openBLAS, first do *$ git clone https://github.com/xianyi/OpenBLAS.git* to get OpenBLAS. Then, with the modules loaded, do *make -j4*; and *make PREFIX=path/to/build/dir install*

Building numpy

First construct a virtualenv to hold all of your python modules. I like to do this right in my home directory. For example,

$ mkdir ~/venv (assuming you don't already have *~/venv*) *$ cd ~/venv $ virtualenv openblas*

will create an *openblas* directory, with a *bin* subdirectory. You "activate" the virtual env by doing *$ source path/to/virtualenv/bin/activate*. This will change all of your environment variables so that the active python will see whatever modules are in that directory. **Note that this messes with modules!** To be safe, I'd recommend *$ module purge; module load gnu openmpi_ib* afterwards.

- *$ cp site.cfg.example site.cfg*

edit *site.cfg* to uncomment the [openblas] section and fill in the include and library dirs to whereever you installed openblas.

- *$ python setup.py config*

to make sure that the numpy build has FOUND your openblas install. If it did, you should see something like this:

```
(openblas)trestles-login1:/home/../numpy-1.8.0 [10:15]$ python setup.py config
Running from numpy source directory.
F2PY Version 2
blas_opt_info:
blas_mkl_info:
  libraries mkl,vml,guide not found in ['/home/joishi/venv/openblas/lib', '/usr/local/
↪lib64', '/usr/local/lib', '/usr/lib64', '/usr/lib', '/usr/lib/']
  NOT AVAILABLE

openblas_info:
  FOUND:
    language = f77
    library_dirs = ['/home/joishi/build/lib']
    libraries = ['openblas', 'openblas']

  FOUND:
    language = f77
    library_dirs = ['/home/joishi/build/lib']
    libraries = ['openblas', 'openblas']

non-existing path in 'numpy/lib': 'benchmarks'
lapack_opt_info:
  FOUND:
    language = f77
    library_dirs = ['/home/joishi/build/lib']
    libraries = ['openblas', 'openblas']

/home/joishi/build/lib/python3.3/distutils/dist.py:257: UserWarning: Unknown␣
↪distribution option: 'define_macros'
  warnings.warn(msg)
running config
```

- *$ python setup.py build*

if successful,

- *$ python setup.py install*

Installing Scipy

Scipy is easier, because it just gets its config from numpy.

- *$ python setup.py config*

This notes a lack of UMFPACK. . . will that make a speed difference? Nevertheless, it works ok.

Do

- *$ python setup.py build*

if successful,

- *$ python setup.py install*

Installing mpi4py

This should just be pip installed, *$ pip install mpi4py*

Installing cython

This should just be pip installed, *$ pip install cython*

Installing matplotlib

This should just be pip installed, *$ pip install matplotlib*

UMFPACK

Requires AMD (another package by the same group, not processor) and SuiteSparse_config, too.

Dedalus2

With the modules set as above (for NOW), set *$ export FFTW_PATH=/opt/fftw/3.3.3/gnu/openmpi/ib* and *$ export MPI_PATH=/opt/openmpi/gnu/ib*. Then do *$ python setup.py build_ext –inplace*.

Install notes for CU/Janus

As with NASA/Pleiades, an initial Janus environment is pretty bare-bones. There are no modules, and your shell is likely a bash varient. Here we'll do a full build of our stack, using only the prebuilt openmpi compilers. Later we'll try a module heavy stack to see if we can avoid this.

Add the following to your `.my.bash_profile`:

```
# Add your commands here to extend your PATH, etc.

module load intel

export BUILD_HOME=$HOME/build

export PATH=$BUILD_HOME/bin:$BUILD_HOME:/$PATH  # Add private commands to PATH

export LD_LIBRARY_PATH=$BUILD_HOME/lib:$LD_LIBRARY_PATH

export CC=mpicc

#pathing for Dedalus
export LOCAL_MPI_VERSION=openmpi-1.8.5
export LOCAL_MPI_SHORT=v1.8
export LOCAL_PYTHON_VERSION=3.4.3
export LOCAL_NUMPY_VERSION=1.9.2
export LOCAL_SCIPY_VERSION=0.15.1
export LOCAL_HDF5_VERSION=1.8.15


export MPI_ROOT=$BUILD_HOME/$LOCAL_MPI_VERSION
export PYTHONPATH=$BUILD_HOME/dedalus:$PYTHONPATH
export MPI_PATH=$MPI_ROOT
export FFTW_PATH=$BUILD_HOME
export HDF5_DIR=$BUILD_HOME
```

Do your builds on the janus compile nodes (see MOTD). As a positive note, Janus compile nodes have access to the internet (e.g., wget), so you can download and compile on-node. For now we're using stock Pleiades compile flags and patch files. With intel 15.0.1 the cython install is now working well, as does h5py.

Building Openmpi

Tim Dunn has pointed out that we may (may) be able to get some speed improvements by building our own openmpi. Why not give it a try! Compiling on the janus-compile nodes seems to do a fine job, and unlike Pleiades we can grab software from the internet on the compile nodes too. This streamlines the process.:

```
cd $BUILD_HOME
wget http://www.open-mpi.org/software/ompi/$LOCAL_MPI_SHORT/downloads/$LOCAL_MPI_
↪VERSION.tar.gz
tar xvf $LOCAL_MPI_VERSION.tar.gz
cd $LOCAL_MPI_VERSION
./configure \
    --prefix=$BUILD_HOME \
    --with-slurm \
    --with-threads=posix \
    --enable-mpi-thread-multiple \
    CC=icc CXX=icpc FC=ifort

make -j
make install
```

Config flags thanks to Tim Dunn; the CFLAGS etc are from Pleiades and should be general.

Building Python3

Create `$BUILD_HOME` and then proceed with downloading and installing Python-3.4:

```
cd $BUILD_HOME
wget https://www.python.org/ftp/python/$LOCAL_PYTHON_VERSION/Python-$LOCAL_PYTHON_
↪VERSION.tgz
tar xzf Python-$LOCAL_PYTHON_VERSION.tgz
cd Python-$LOCAL_PYTHON_VERSION

./configure --prefix=$BUILD_HOME \
                    CC=mpicc         CFLAGS="-mkl -O3 -axAVX -xSSE4.1 -fPIC -ipo" \
                    CXX=mpicxx CPPFLAGS="-mkl -O3 -axAVX -xSSE4.1 -fPIC -ipo" \
                    F90=mpif90  F90FLAGS="-mkl -O3 -axAVX -xSSE4.1 -fPIC -ipo" \
                    --enable-shared LDFLAGS="-lpthread" \
                    --with-cxx-main=mpicxx --with-system-ffi

make -j
make install
```

The former patch for Intel compilers to handle ctypes is no longer necessary.

Installing pip

Python 3.4 now automatically includes pip.

You will now have `pip3` installed in `$BUILD_HOME/bin`. You might try doing `pip3 -V` to confirm that `pip3` is built against python 3.4. We will use `pip3` throughout this documentation to remain compatible with systems (e.g., Mac OS) where multiple versions of python coexist.

Installing mpi4py

This should be pip installed:

```
pip3 install mpi4py
```

Installing FFTW3

We need to build our own FFTW3, under intel 14 and mvapich2/2.0b, or under openmpi:

```
 cd $BUILD_HOME
 wget http://www.fftw.org/fftw-3.3.4.tar.gz
 tar xvzf fftw-3.3.4.tar.gz
 cd fftw-3.3.4

./configure --prefix=$BUILD_HOME \
                      CC=mpicc        CFLAGS="-O3 -axAVX -xSSE4.1" \
                      CXX=mpicxx CPPFLAGS="-O3 -axAVX -xSSE4.1" \
                      F77=mpif90  F90FLAGS="-O3 -axAVX -xSSE4.1" \
                      MPICC=mpicc MPICXX=mpicxx \
                      --enable-shared \
                      --enable-mpi --enable-openmp --enable-threads

 make -j
 make install
```

It's critical that you use `mpicc` as the C-compiler, etc. Otherwise the libmpich libraries are not being correctly linked into `libfftw3_mpi.so` and dedalus failes on fftw import.

Installing nose

Nose is useful for unit testing, especially in checking our numpy build:

```
pip3 install nose
```

Installing cython

This should just be pip installed:

```
pip3 install cython
```

Cython is now working (intel 15.0/openmpi-1.8.5).

Numpy and BLAS libraries

Numpy will be built against a specific BLAS library. On Pleiades we will build against the OpenBLAS libraries.

All of the intel patches, etc. are unnecessary in the gcc stack.

Building numpy against MKL

Now, acquire `numpy` (1.9.0):

```
cd $BUILD_HOME
wget http://sourceforge.net/projects/numpy/files/NumPy/$LOCAL_NUMPY_VERSION/numpy-
↪$LOCAL_NUMPY_VERSION.tar.gz
tar -xvf numpy-$LOCAL_NUMPY_VERSION.tar.gz
cd numpy-$LOCAL_NUMPY_VERSION
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_janus_intel_
↪patch.tar
tar xvf numpy_janus_intel_patch.tar
```

This last step saves you from needing to hand edit two files in `numpy/distutils`; these are `intelccompiler.py` and `fcompiler/intel.py`. I've built a crude patch, `numpy_janus_intel_patch.tar` which is auto-deployed within the `numpy-$LOCAL_NUMPY_VERSION` directory by the instructions above. This will unpack and overwrite:

```
numpy/distutils/intelccompiler.py
numpy/distutils/fcompiler/intel.py
```

This differs from prior versions in that "-xhost" is replaced with "-axAVX -xSSE4.1".

We'll now need to make sure that `numpy` is building against the MKL libraries. Start by making a `site.cfg` file:

```
cp site.cfg.example site.cfg
emacs -nw site.cfg
```

Edit `site.cfg` in the `[mkl]` section; modify the library directory so that it correctly point to TACC's `$MKLROOT/lib/intel64/`. With the modules loaded above, this looks like:

```
[mkl]
library_dirs = /curc/tools/x_86_64/rh6/intel/15.0.1/composer_xe_2015.1.133/mkl/lib/
↪intel64
include_dirs = /curc/tools/x_86_64/rh6/intel/15.0.1/composer_xe_2015.1.133/mkl/include
mkl_libs = mkl_rt
lapack_libs =
```

These are based on intels instructions for compiling numpy with ifort and they seem to work so far.

Then proceed with:

```
python3 setup.py config --compiler=intelem build_clib --compiler=intelem build_ext --
↪compiler=intelem install
```

This will config, build and install numpy.

Test numpy install

Test that things worked with this executable script `numpy_test_full`. You can do this full-auto by doing:

```
wget http://dedalus-project.readthedocs.org/en/latest/_downloads/numpy_test_full
chmod +x numpy_test_full
./numpy_test_full
```

We succesfully link against fast BLAS and the test results look normal.

Python library stack

After `numpy` has been built we will proceed with the rest of our python stack.

Installing Scipy

Scipy is easier, because it just gets its config from numpy. Dong a pip install fails, so we'll keep doing it the old fashioned way:

```
wget http://sourceforge.net/projects/scipy/files/scipy/$LOCAL_SCIPY_VERSION/scipy-
↪$LOCAL_SCIPY_VERSION.tar.gz
tar -xvf scipy-$LOCAL_SCIPY_VERSION.tar.gz
cd scipy-$LOCAL_SCIPY_VERSION
python3 setup.py config --compiler=intelem --fcompiler=intelem build_clib \
                                          --compiler=intelem --fcompiler=intelem build_
↪ext \
                                          --compiler=intelem --fcompiler=intelem install
```

Note: We do not have umfpack; we should address this moving forward, but for now I will defer that to a later day.

Installing matplotlib

This should just be pip installed. In versions of matplotlib>1.3.1, Qhull has a compile error if the C compiler is used rather than C++, so we force the C complier to be icpc

```
export CC=icpc
pip3 install matplotlib
```

Installing HDF5 with parallel support

The new analysis package brings HDF5 file writing capbaility. This needs to be compiled with support for parallel (mpi) I/O:

```
wget http://www.hdfgroup.org/ftp/HDF5/releases/hdf5-$LOCAL_HDF5_VERSION/src/hdf5-
↪$LOCAL_HDF5_VERSION.tar.gz

tar xvzf hdf5-$LOCAL_HDF5_VERSION.tar.gz
cd hdf5-$LOCAL_HDF5_VERSION
./configure --prefix=$BUILD_HOME \
                    CC=mpicc         CFLAGS="-O3 -axAVX -xSSE4.1" \
                    CXX=mpicxx CPPFLAGS="-O3 -axAVX -xSSE4.1" \
                    F77=mpif90  F90FLAGS="-O3 -axAVX -xSSE4.1" \
                    MPICC=mpicc MPICXX=mpicxx \
                    --enable-shared --enable-parallel

make -j
make install
```

Installing h5py

This now can be pip installed:

```
pip3 install hypy
```

Installing Mercurial

On Janus, we need to install mercurial itself. I can't get mercurial to build properly on intel compilers, so for now use gcc. Ah, and we also need python2 for the mercurial build (only):

```
module unload openmpi intel
module load gcc/gcc-4.9.1
module load python/anaconda-2.0.0
wget http://mercurial.selenic.com/release/mercurial-3.4.tar.gz
tar xvf mercurial-3.4.tar.gz
cd mercurial-3.4
export CC=gcc
make install PREFIX=$BUILD_HOME
```

I suggest you add the following to your `~/.hgrc`:

```
[ui]
username = <your bitbucket username/e-mail address here>
editor = emacs

[extensions]
graphlog =
color =
convert =
mq =
```

Dedalus

Preliminaries

With the modules set as above, set:

```
export BUILD_HOME=$BUILD_HOME
export FFTW_PATH=$BUILD_HOME
export MPI_PATH=$BUILD_HOME/$LOCAL_MPI_VERSION
```

Pull the dedalus repository::

```
hg clone https://bitbucket.org/dedalus-project/dedalus
```

Then change into your root dedalus directory and run:

```
pip3 install -r requirements.txt
python3 setup.py build_ext --inplace
```

Running Dedalus on Janus

Our scratch disk system on Pleiades is `/lustre/janus_scratch/user-name`. On this and other systems, I suggest soft-linking your scratch directory to a local working directory in home; I uniformly call mine `workdir`:

```
ln -s /lustre/janus_scratch/bpbrown workdir
```

I also suggest you move your stack to the `projects` directory, `/projects/user-name`. There, I bring back a symbolic link:

ln -s /projects/bpbrown projects ln -s projects/build build

Install notes for BRC HPC SAVIO cluster

Installing on the SAVIO cluster is pretty straightforward, as many things can be loaded via modules. First, load the following modules.

```
module purge
module load intel
module load openmpi
module load fftw/3.3.4-intel
module load python/3.2.3
module load nose
module load numpy/1.8.1
module load scipy/0.14.0
module load mpi4py
module load pip
module load virtualenv/1.7.2
module load mercurial/2.0.2
module load hdf5/1.8.13-intel-p
```

We next need to make a virtual environment in which to build the rest of the Dedalus depencencies.

```
virtualenv python_build
source python_build/bin/activate
```

The rest of the depencies will be pip-installed. However, because we are using intel compilers, we need to specify the compiler and some how to link things properly.

```
export CC=icc
export LDFLAGS="-lirc -limf"
```

Now we can use pip to install most of the remaining dependencies.

```
pip-3.2 install cython
pip-3.2 install h5py
pip-3.2 install matplotlib==1.3.1
```

Dedalus itself can be pulled down from Bitbucket.

```
hg clone https://bitbucket.org/dedalus-project/dedalus
cd dedalus
pip-3.2 install -r requirements.txt
```

To build Dedalus, you must specify the locations of FFTW and MPI.

```
export FFTW_PATH=/global/software/sl-6.x86_64/modules/intel/2013_sp1.4.211/fftw/3.3.4-
↪intel
export MPI_PATH=/global/software/sl-6.x86_64/modules/intel/2013_sp1.2.144/openmpi/1.6.
↪5-intel
python3 setup.py build_ext --inplace
```

Using Dedalus

To use Dedalus, put the following in your `~/.bashrc` file:

```
module purge
module load intel
module load openmpi
module load fftw/3.3.4-intel
module load python/3.2.3
module load numpy/1.8.1
module load scipy/0.14.0
module load mpi4py
module load mercurial/2.0.2
module load hdf5/1.8.13-intel-p
source python_build/bin/activate
export PYTHONPATH=$PYTHONPATH:~/dedalus
```

Install notes for MIT Engaging Cluster

This installation uses the Python, BLAS, and MPI modules available on Engaging, while manually building HDF5 and FFTW. Be sure to login to Engaging through the `eofe7` head-node.

Modules and paths

The following commands should be added to your `~/.bashrc` file to setup the correct modules and paths. Modify the `HDF5_DIR`, `FFTW_PATH`, and `DEDALUS_REPO` environment variables as desired to change the build locations of these packages.

```
# Basic modules
module load gcc
module load slurm

# Python from modules
module load engaging/python/2.7.10
module load engaging/python/3.6.0
export PATH=~/.local/bin:${PATH}

# BLAS from modules
module load engaging/OpenBLAS/0.2.14
export BLAS=/cm/shared/engaging/OpenBLAS/0.2.14/lib/libopenblas.so

# MPI from modules
module load engaging/openmpi/2.0.3
export MPI_PATH=/cm/shared/engaging/openmpi/2.0.3

# HDF5 built from source
```

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```
export HDF5_DIR=~/software/hdf5
export HDF5_VERSION=1.10.1
export HDF5_MPI="ON"
export PATH=${HDF5_DIR}/bin:${PATH}
export LD_LIBRARY_PATH=${HDF5_DIR}/lib:${LD_LIBRARY_PATH}

# FFTW built from source
export FFTW_PATH=~/software/fftw
export FFTW_VERSION=3.3.6-pl2
export PATH=${FFTW_PATH}/bin:${PATH}
export LD_LIBRARY_PATH=${FFTW_PATH}/lib:${LD_LIBRARY_PATH}

# Dedalus from mercurial
export DEDALUS_REPO=~/software/dedalus
export PYTHONPATH=${DEDALUS_REPO}:${PYTHONPATH}
```

Build procedure

Source your `~/.bashrc` to activate the above changes, or re-login to the cluster, before running the following build procedure.

```
# Python basics
/cm/shared/engaging/python/2.7.10/bin/pip install --ignore-installed --user pip
/cm/shared/engaging/python/3.6.0/bin/pip3 install --ignore-installed --user pip
pip2 install --user --upgrade setuptools
pip2 install --user mercurial
pip3 install --user --upgrade setuptools
pip3 install --user nose cython

# Python packages
pip3 install --user --no-use-wheel numpy
pip3 install --user --no-use-wheel scipy
pip3 install --user mpi4py

# HDF5 built from source
mkdir -p ${HDF5_DIR}
cd ${HDF5_DIR}
wget https://support.hdfgroup.org/ftp/HDF5/current/src/hdf5-${HDF5_VERSION}.tar
tar -xvf hdf5-${HDF5_VERSION}.tar
cd hdf5-${HDF5_VERSION}
./configure --prefix=${HDF5_DIR} \
    CC=mpicc \
    CXX=mpicxx \
    F77=mpif90 \
    MPICC=mpicc \
    MPICXX=mpicxx \
    --enable-shared \
    --enable-parallel
make
make install
pip3 install --user --no-binary=h5py h5py

# FFTW built from source
mkdir -p ${FFTW_PATH}
cd ${FFTW_PATH}
```

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```
wget http://www.fftw.org/fftw-${FFTW_VERSION}.tar.gz
tar -xvzf fftw-${FFTW_VERSION}.tar.gz
cd fftw-${FFTW_VERSION}
./configure --prefix=${FFTW_PATH} \
    CC=mpicc \
    CXX=mpicxx \
    F77=mpif90 \
    MPICC=mpicc \
    MPICXX=mpicxx \
    --enable-shared \
    --enable-mpi \
    --enable-openmp \
    --enable-threads
make
make install

# Dedalus from mercurial
hg clone https://bitbucket.org/dedalus-project/dedalus ${DEDALUS_REPO}
cd ${DEDALUS_REPO}
pip3 install --user -r requirements.txt
python3 setup.py build_ext --inplace
```

Notes

Last updated on 2017/09/18 by Keaton Burns.

Once the dependency stack has been installed, Dedalus can be installed *as described above*.

2.2 Getting started with Dedalus

2.2.1 Tutorial Notebooks

This tutorial on using Dedalus consists of three short IPython notebooks, which can be downloaded and ran interactively, or viewed on-line through the links below.

The notebooks cover the basics of setting up and interacting with the primary facets of the code, culminating in the setup and simulation of the 1D KdV-Burgers equation.

Tutorial 1: Bases and Domains

This tutorial covers the basics of setting up and interacting with basis and domain objects in Dedalus.

First, we'll import the public interface and suppress some of the logging messages:

```
In [1]: from dedalus import public as de
        import numpy as np
        import matplotlib.pyplot as plt

        de.logging_setup.rootlogger.setLevel('ERROR')
        %matplotlib inline
```

1.1: Bases

Creating a basis

Each basis is represented by a separate class, e.g. `Chebyshev`, `SinCos`, and `Fourier`. When instantiating a basis, you provide a name for the basis, the number of modes, and the endpoints of the basis interval as a `(left, right)` tuple.

Optionally, you can specify a dealiasing scaling factor, indicating how much to pad the tracked modes when transforming to grid space. To properly dealias quadratic nonlinearities, for instance, you would need a scaling factor $\geq 3/2$.

```
In [2]: xbasis = de.Chebyshev('x', 32, interval=(0,5), dealias=3/2)
```

Basis methods & attributes

Basis objects have associated methods for transforming and operating on fields, and defining the sparse matrices used to solve the linear portions of PDEs in Dedalus. However, these features are not typically directly accessed through the basis objects, but rather through field methods and operators, which we'll cover in later notebooks.

Basis grids and scale factors

The global grid of a basis can be easily accessed using the basis object's `grid` method, where you'll have to pass a scale factor determining the number of points in the grid, relative to the number of basis modes. Here we'll show the Chebyshev grids with scaling factors of 1 and $3/2$.

```
In [3]: grid_normal = xbasis.grid(scale=1)
        grid_dealias = xbasis.grid(scale=3/2)

        plt.figure(figsize=(10, 1))
        plt.plot(grid_normal, np.zeros_like(grid_normal)+1, 'o', markersize=5)
        plt.plot(grid_dealias, np.zeros_like(grid_dealias)-1, 'o', markersize=5)
        plt.ylim([-2, 2])
        plt.gca().yaxis.set_ticks([]);
```

Compound bases

A compound basis consisting of stacked Chebyshev segments can be constructed simply by grouping a set of individual Chebyshev bases defined over adjacent intervals.

```
In [4]: xb1 = de.Chebyshev('x1', 16, interval=(0,2))
        xb2 = de.Chebyshev('x2', 32, interval=(2,8))
        xb3 = de.Chebyshev('x3', 16, interval=(8,10))
        xbasis = de.Compound('x', (xb1, xb2, xb3))
```

Since we use the interior roots grid for the Chebyshev polynomials, the grid of the compound bases is simply the union of the subbasis grids. When solving a problem with Dedalus, the continuity of fields across the subbasis interfaces is internally enforced.

```
In [5]: compound_grid = xbasis.grid(scale=1)

        plt.figure(figsize=(10, 1))
        plt.plot(compound_grid, np.zeros_like(compound_grid), 'o', markersize=5)
        plt.gca().yaxis.set_ticks([]);
```

1.2: Domains

Creating a domain

Domain objects represent physical domains, spanned by the direct product of a set of orthogonal bases. To build a domain, we pass a list of the composite bases, specify the (grid-space) datatype, and optionally specify the process mesh for parallelization. Let's construct a real 3D domain using Fourier and Chebyshev bases.

```
In [6]: xbasis = de.Fourier('x', 8, interval=(0,2), dealias=3/2)
        ybasis = de.Fourier('y', 8, interval=(0,2), dealias=3/2)
        zbasis = de.Chebyshev('z', 8, interval=(0,1), dealias=3/2)
        domain = de.Domain([xbasis, ybasis, zbasis], grid_dtype=np.float64, mesh=[1]);
```

Parallelization & process mesh

Dedalus currently supports N-dimensional domains where the first (N-1) dimensions are separable, meaning that the linear parts of the transformed differential equations are uncoupled between modes in this subspace. The currently implemented separable bases are the `Fourier` basis for periodic intervals, and the `SinCos` (parity) basis for problems where the variables exhibit definite parity about the interval endpoints.

Problems can be easily parallelized over the separable dimensions, and Dedalus supports distribution over arbitrary (N-1)-dimensional process meshes. The current MPI environment must have the same number of processes as the product of the mesh shape. By default, problems are distributed across a 1-dimensional mesh of all the available MPI processes, but specifying a higher-dimensional mesh when possible will typically improve performance.

Layouts

The primary function of the domain object is to build the machinery necessary for the parallelized allocation and transformation of fields. This is done by creating `layout` objects describing the necessary transform/distribution states of the data between coefficient space and grid space. Subsequent layouts are connected by basis transforms, which must be performed locally, and global transposes (rearrangements of the data distribution across the process mesh) to achieve the required locality.

The general algorithm starts from coefficient space, with the last axis local (non-distributed). It proceeds to grid space by transforming the last axis into grid space, globally transposing the data such that the preceding axis is local, transforming that axis into grid space, etc.

Let's examine the layouts for the domain we just constructed:

```
In [7]: for layout in domain.distributor.layouts:
            print('Layout {}:  Grid space: {}  Local: {}'.format(layout.index, layout.grid_space, lay
```

```
Layout 0:  Grid space: [False False False]  Local: [ True  True  True]
Layout 1:  Grid space: [False False  True]  Local: [ True  True  True]
Layout 2:  Grid space: [False  True  True]  Local: [ True  True  True]
Layout 3:  Grid space: [ True  True  True]  Local: [ True  True  True]
```

Since this is being performed serially, no global transposes are necessary (all axes are local), and the paths between layouts consist of coefficient-to-grid transforms, backwards from the last axis.

To see how things work for a distributed simulation, we'll change the process mesh and rebuild the layout objects, circumventing the internal checks on the number of available processes, etc.

Note this is for demonstration only... messing with these attributes will generally break things.

```
In [8]: # Don't do this.
        domain.distributor.mesh = np.array([4, 2])
        domain.distributor.coords = np.array([0, 0])
        domain.distributor._build_layouts(domain, dry_run=True)
```

```
In [9]: for layout in domain.distributor.layouts:
            print('Layout {}:  Grid space: {}  Local: {}'.format(layout.index, layout.grid_space, lay
```

```
Layout 0:  Grid space: [False False False]  Local: [False False  True]
Layout 1:  Grid space: [False False  True]  Local: [False False  True]
Layout 2:  Grid space: [False False  True]  Local: [False  True False]
Layout 3:  Grid space: [False  True  True]  Local: [False  True False]
Layout 4:  Grid space: [False  True  True]  Local: [ True False False]
Layout 5:  Grid space: [ True  True  True]  Local: [ True False False]
```

We can see that there are two additional layouts, corresponding to the transposed states of the mixed-transform layouts. Two global transposes are necessary in order for the y and x axes to be stored locally, which is required in order to perform the respective basis transforms.

Interacting with the layout objects directly is typically not necessary, but being aware of this system for controlling the distribution and tranformation state of data is important for interacting with field objects, as we'll see in future notebooks.

Distributed grids

Domain objects construct properly oriented arrays representing the local portions of the basis grids, for use in creating field data, setting initial conditions, etc.

The axis 0 grid is the full x-basis Fourier grid, since the first axis is local in grid space (i.e. the last `layout`). The axis 1 and 2 grids are the local portions of the y and z basis Fourier and Chebyshev grids, distributed across the specified process mesh (4 and 2 processes, respectively).

Scale factors for the grids can be specified as a tuple (one scale for each dimension), or as a scalar to apply the same scaling to each dimension.

```
In [10]: print('Grid 0 shape:', domain.grid(0, scales=1).shape)
         print('Grid 1 shape:', domain.grid(1, scales=1).shape)
         print('Grid 2 shape:', domain.grid(2, scales=1).shape)
```

```
Grid 0 shape: (8, 1, 1)
Grid 1 shape: (1, 2, 1)
Grid 2 shape: (1, 1, 4)
```

Tutorial 2: Fields and Operators

This tutorials covers the basics of setting up and interacting with field and operator objects in Dedalus.

First, we'll import the public interface and suppress some of the logging messages:

```
In [1]: from dedalus import public as de
        import numpy as np
        import matplotlib.pyplot as plt

        de.logging_setup.rootlogger.setLevel('ERROR')
        %matplotlib inline
```

2.1: Fields

Creating a field

Field objects represent scalar fields defined over a domain. A field can be directly instantiated from the `Field` class by passing a domain object, or using the `domain.new_field` method. Let's set up a 2D domain and build a field:

```
In [2]: xbasis = de.Fourier('x', 64, interval=(0,2*np.pi), dealias=3/2)
        ybasis = de.Chebyshev('y', 64, interval=(-1,1), dealias=3/2)
        domain = de.Domain([xbasis, ybasis], grid_dtype=np.float64, mesh=[1])
        f = domain.new_field(name='f')
```

We also gave the field a name – something which is automatically done for the state fields when solving a problem in Dedalus (we'll see more about this in the next notebook), but we've just done it manually, for now.

Manipulating field data

The `layout` attribute of each field is a reference to the layout object (discussed in tutorial 1) describing the current transform/distribution state of that field's data.

```
In [3]: f.layout.grid_space
```

```
Out[3]: array([False, False])
```

Field data can be written and retrieved in any layout by indexing a field a layout object. In most cases it's just the full grid and full coefficient data that's most useful to interact with, and these layouts can be easily accessed using `'g'` and `'c'` keys as shortcuts. Field objects also have several methods that can be used to convert the data between layouts.

Remember that when accessing field data, you're manipulating just the local data of the globally distributed dataset. Details about the data distribution are available through methods on the layout objects.

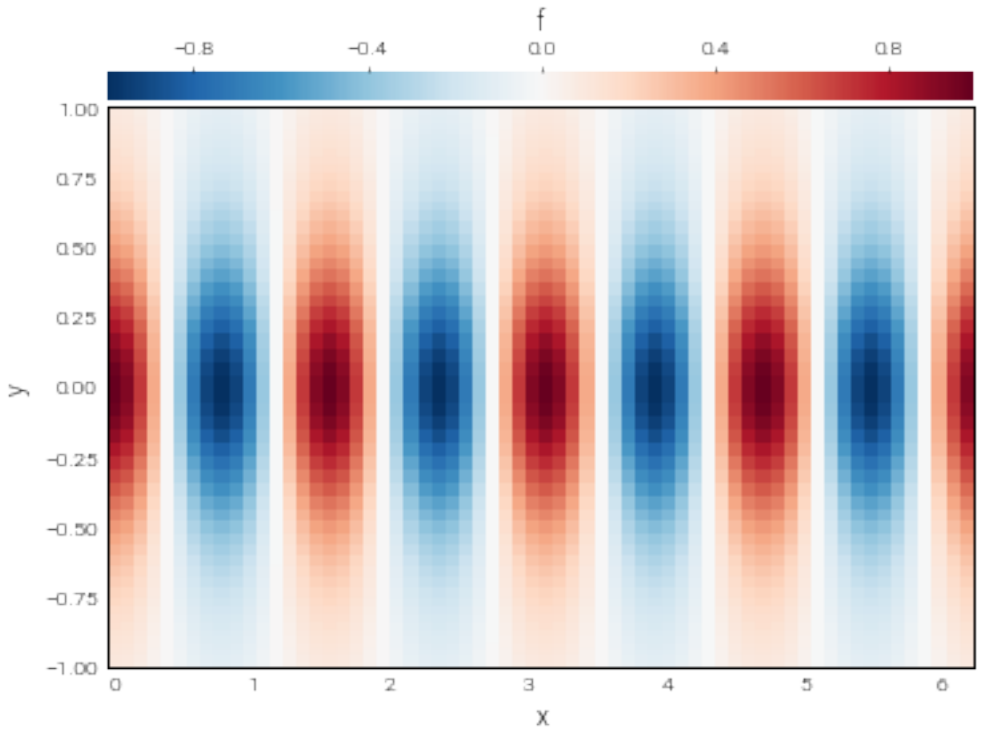
Let's assign our field some data using the local domain grids.

```
In [4]: x, y = domain.grids(scales=1)
        # Set data in grid space using 'g' key
        f['g'] = np.cos(4*x) / np.cosh(3*y)
```

And let's take a look at this data using some helper functions from the `plot_tools` module.

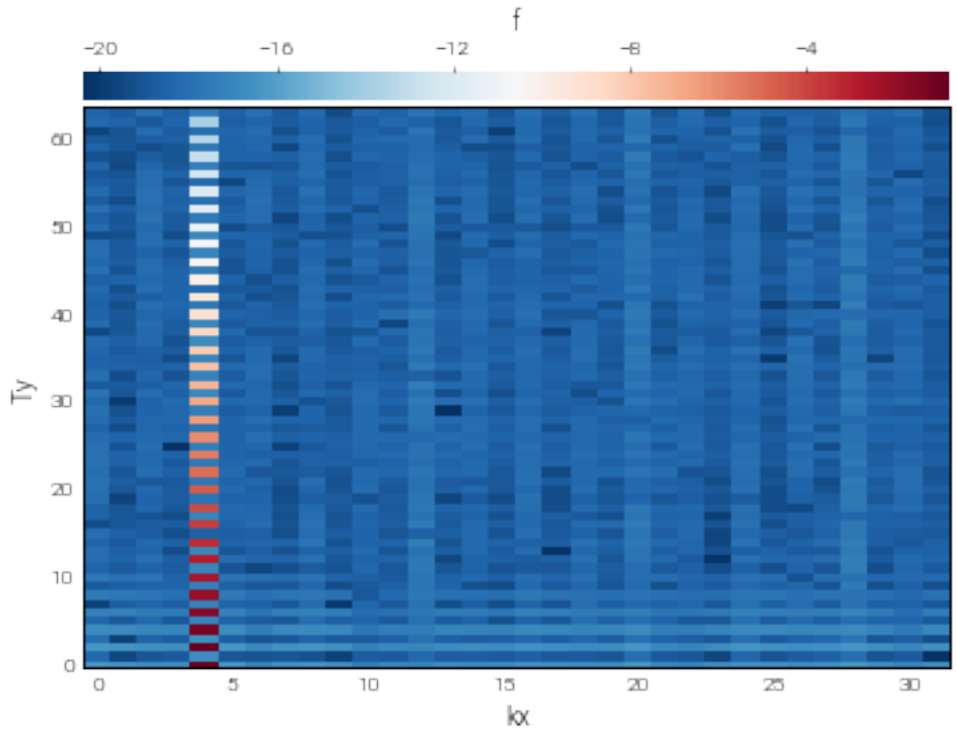
```
In [5]: from dedalus.extras.plot_tools import plot_bot_2d
```

```
In [6]: plot_bot_2d(f);
```



Now let's take a look at the magnitude of the coefficients:

```
In [7]: # Convert data to coefficient space by indexing with 'c' key
        f['c']
        # Plot log of magnitude of data
        def log_magnitude(xmesh, ymesh, data):
            return xmesh, ymesh, np.log10(np.abs(data))
        plot_bot_2d(f, func=log_magnitude);
```



We can see that the specified function is pretty well-resolved.

In addition to the key interface, we can change the layout of a field using the `require_coeff_space`, `require_grid_space`, `require_layout`, and `require_local` methods.

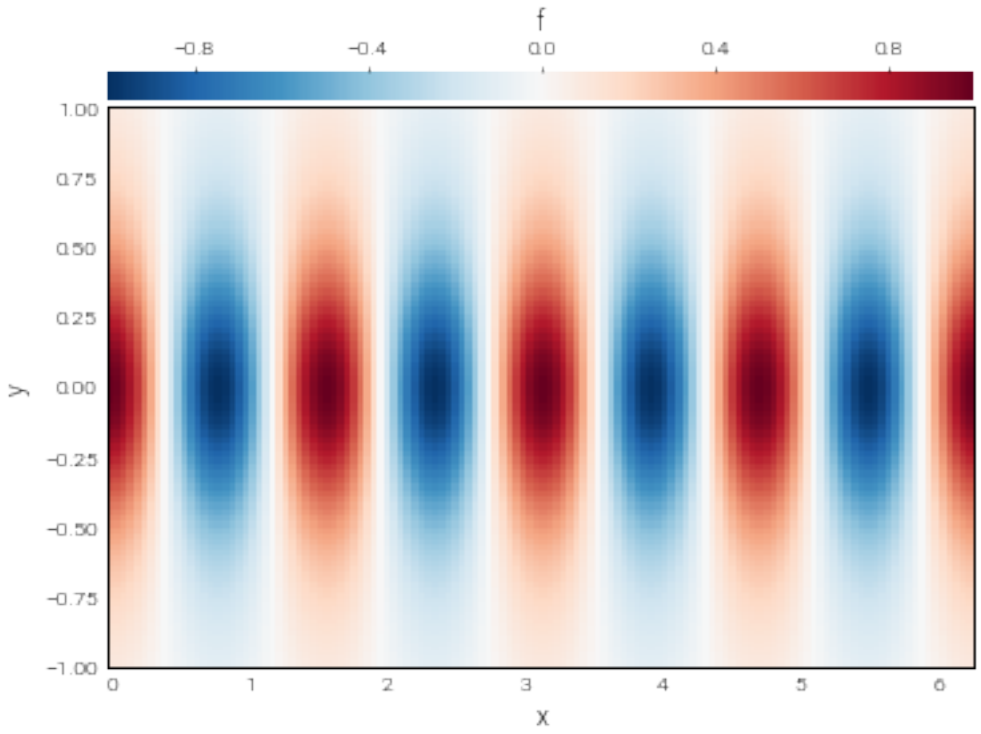
Field scale factors

The `set_scales` method is used to change the scaling factors used when transforming field data into grid space. When setting a field's data using grid arrays, shape errors will result if there is a mismatch between the field and grid's scale factors.

Large scale factors can be used to interpolate the field data onto a high-resolution grid, while small scale factors can be used to view a lower-resolution grid representation of a field. *Beware: using scale factors less than 1 will result in a loss of data when transforming to grid space.*

Let's take a look at a high-resolution sampling of our field, by increasing the scales.

```
In [8]: f.set_scales(2)
        f['g']
        plot_bot_2d(f);
```



2.2: Operators

Arithmetic with fields

Mathematical operations on fields, such as arithmetic, differentiation, integration, and interpolation, are represented by `operator` classes. An instance of an operator class represents a specific mathematical operation, and provides an interface for the deferred evaluation of that operation with respect to it's potentially evolving arguments.

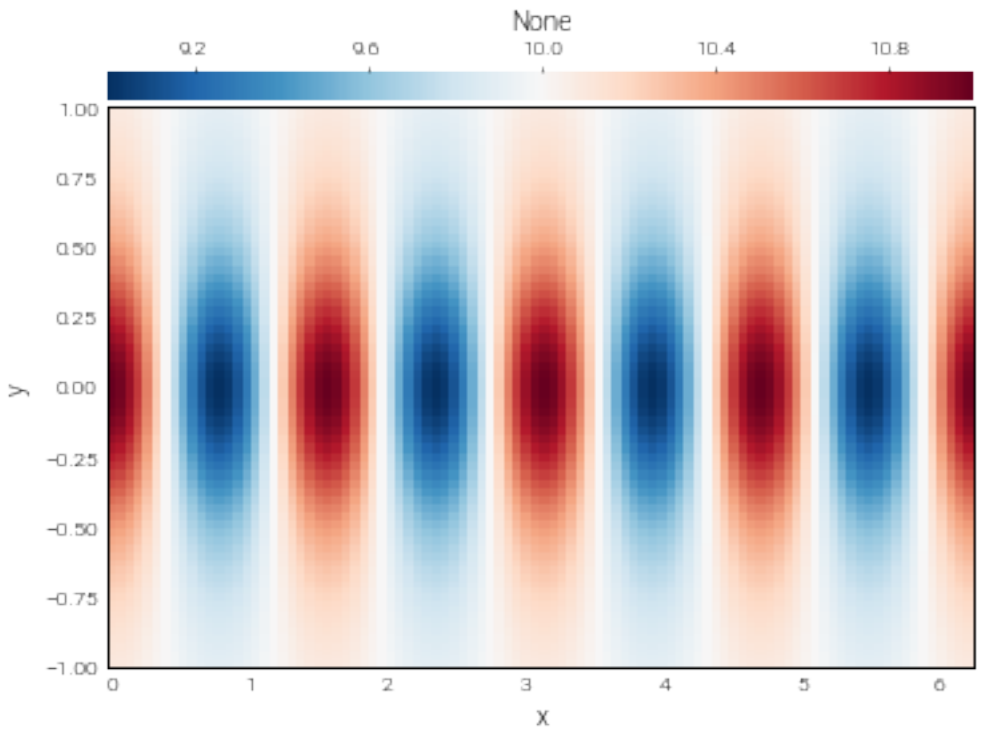
Arithmetic operations between fields, or fields and scalars, are produced simply using Python's infix operators for arithmetic. Let's start with a very simple example of adding a scalar to the field we previously defined.

```
In [9]: add_op = 10 + f
        add_op
```

```
Out[9]: Add(<Scalar 4644516864>, <Field 4603650344>)
```

The object we get is not another field, but an operator object representing the addition of 10 and our field. To actually compute this operation, we use the `evaluate` method, which returns a new field with the result. The dealias scale factors set during basis instantiation are used for the evaluation of all operators.

```
In [10]: add_result = add_op.evaluate()
         add_result.require_grid_space()
         plot_bot_2d(add_result);
```



Building expressions

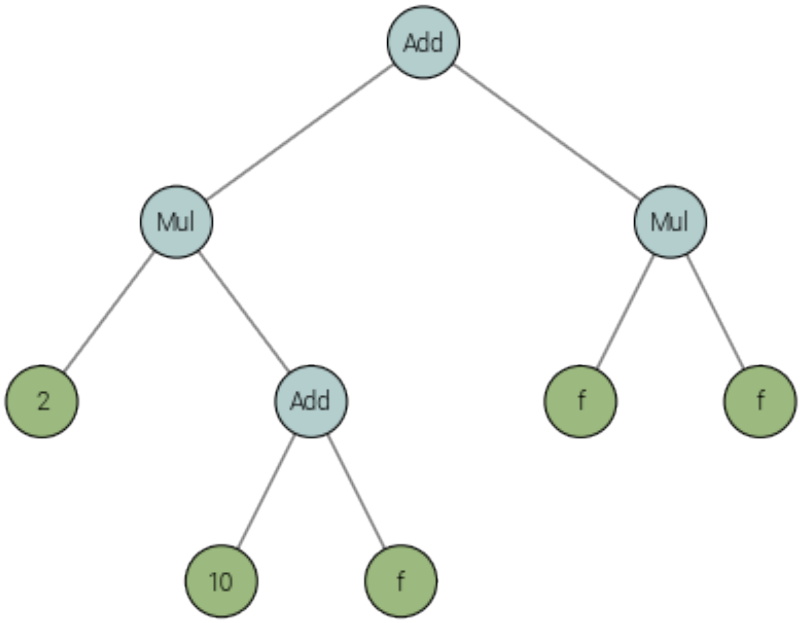
Operator instances can be passed as arguments to other operators, building trees that represent more complicated expressions:

```
In [11]: tree_op = 2*add_op + f*f
         tree_op
```

```
Out[11]: Add(Mul(<Scalar 4645745944>, Add(<Scalar 4644516864>, <Field 4603650344>)), Mul(<Field 4603
```

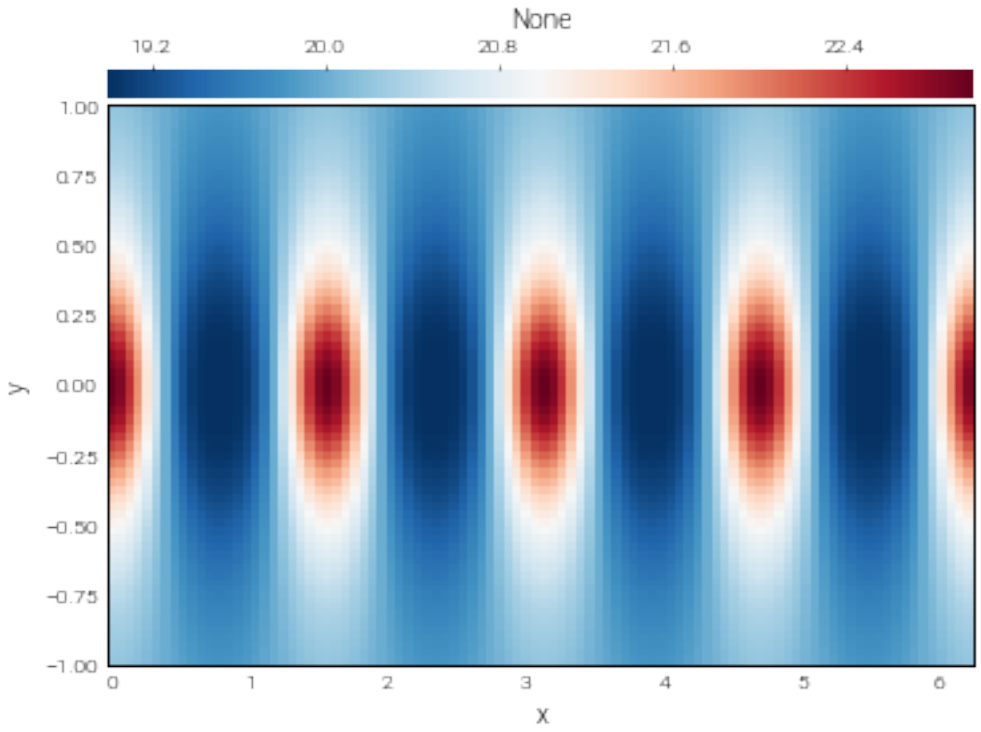
Reading these signatures can be a little cumbersome, but we can plot the operator's structure using a helper from dedalus.tools:

```
In [12]: from dedalus.tools.plot_op import plot_operator
         plot_operator(tree_op, figsize=8, fontsize=12)
```



And evaluating it:

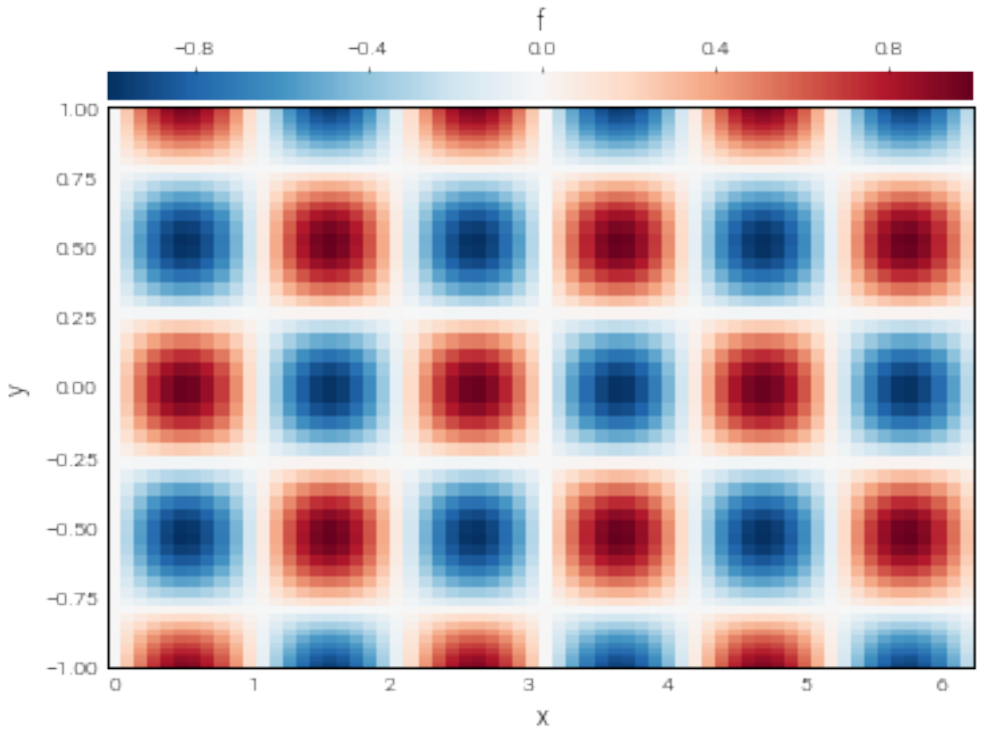
```
In [13]: tree_result = tree_op.evaluate()
         tree_result.require_grid_space
         plot_bot_2d(tree_result);
```



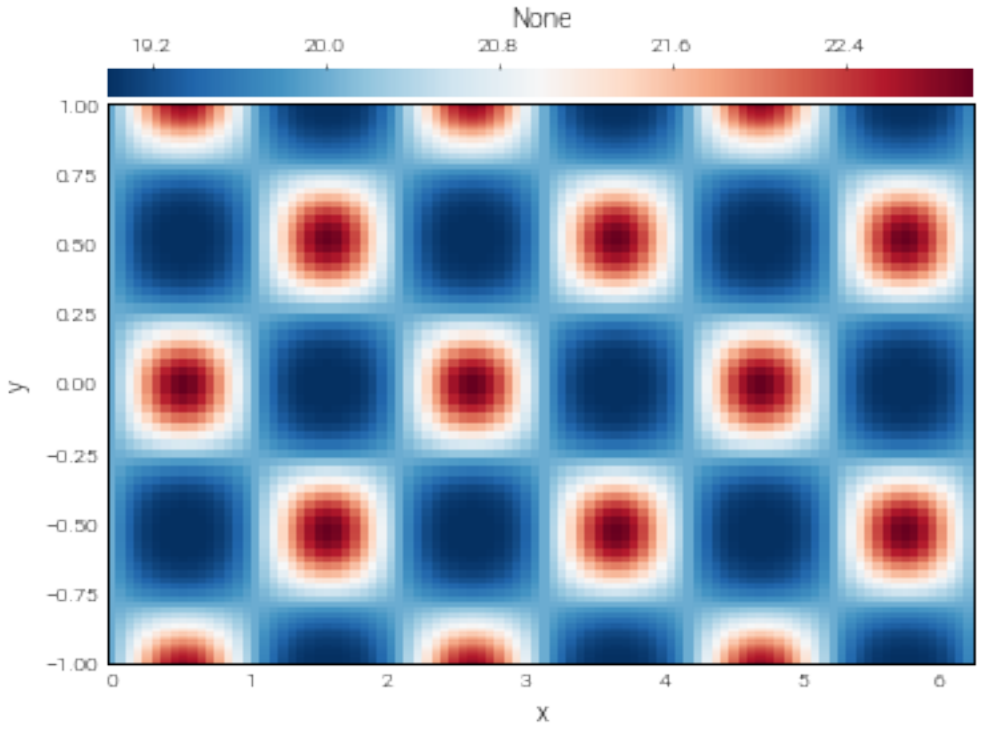
Deferred evaluation

A key point is that the operator objects symbolically represent an operation on the field arguments, and are evaluated using deferred evaluation. If we change the data of the field arguments and re-evaluate an operator, we get a new result.

```
In [14]: # Set scales back to 1 to build new grid data
         f.set_scales('1', keep_data=False)
         f['g'] = np.sin(3*x) * np.cos(6*y)
         plot_bot_2d(f);
```



In [15]:
```
tree_result = tree_op.evaluate()
tree_result.require_grid_space
plot_bot_2d(tree_result);
```



Differentiation, integration, interpolation

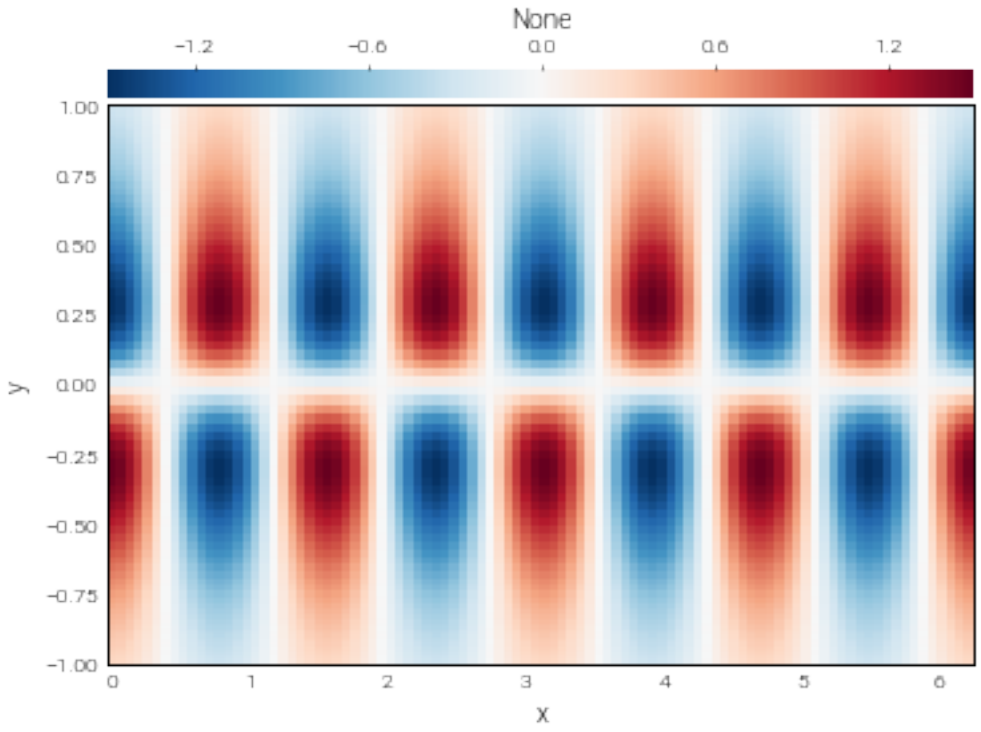
In addition to arithmetic, operators are used for differentiation, integration, and interpolation. There are three ways to apply these operators to a field.

First, the operators performing these operations along a given dimension of the data can be accessed through the `basis.Differentiate`, `basis.Integrate`, and `basis.Interpolate` methods of the corresponding basis object.

```
In [16]: # Let's change the data back to our first example, with a constant offset
         f.set_scales('1', keep_data=False)
         f['g'] = np.cos(4*x) / np.cosh(3*y) + 1

         # Let's setup some operations using the basis operators
         fx_op = ybasis.Differentiate(f)
         int_f_op = ybasis.Integrate(f)
         f0_op = ybasis.Interpolate(f, position=0)

         # And we'll just evaluate and plot one of them
         fx = fx_op.evaluate()
         fx.require_grid_space()
         plot_bot_2d(fx);
```



Second, more general interfaces taking bases as arguments are available through the `operators` module. The `operators.differentiate` factory allows us to easily construct higher-order and mixed derivatives involving different bases. The `operators.integrate` and `operators.interpolate` factories allow us to integrate/interpolate along multiple axes, as well.

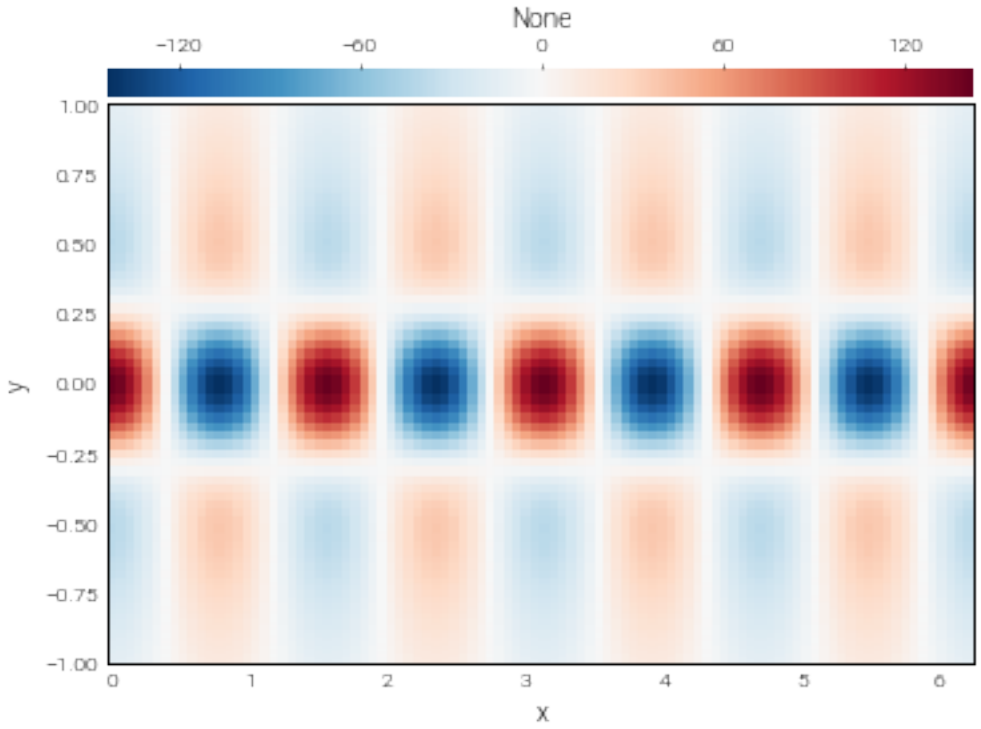
```
In [17]: # Some examples using the constructors from the operators module
         fxxyy_op = de.operators.differentiate(f, x=2, y=2)
         total_int_f_op = de.operators.integrate(f, 'x', 'y')
         f00_op = de.operators.interpolate(f, x=0, y=0)
```

```
fxxyy = fxxyy_op.evaluate()
total_int_f = total_int_f_op.evaluate()
f00 = f00_op.evaluate()

print('Total integral:', total_int_f['g'][0,0])
print('f at (x,y)=(0,0):', f00['g'][0,0])

fxxyy.require_grid_space()
plot_bot_2d(fxxyy);
```

```
Total integral: 12.566370614359172
f at (x,y)=(0,0): 1.9999999999999727
```



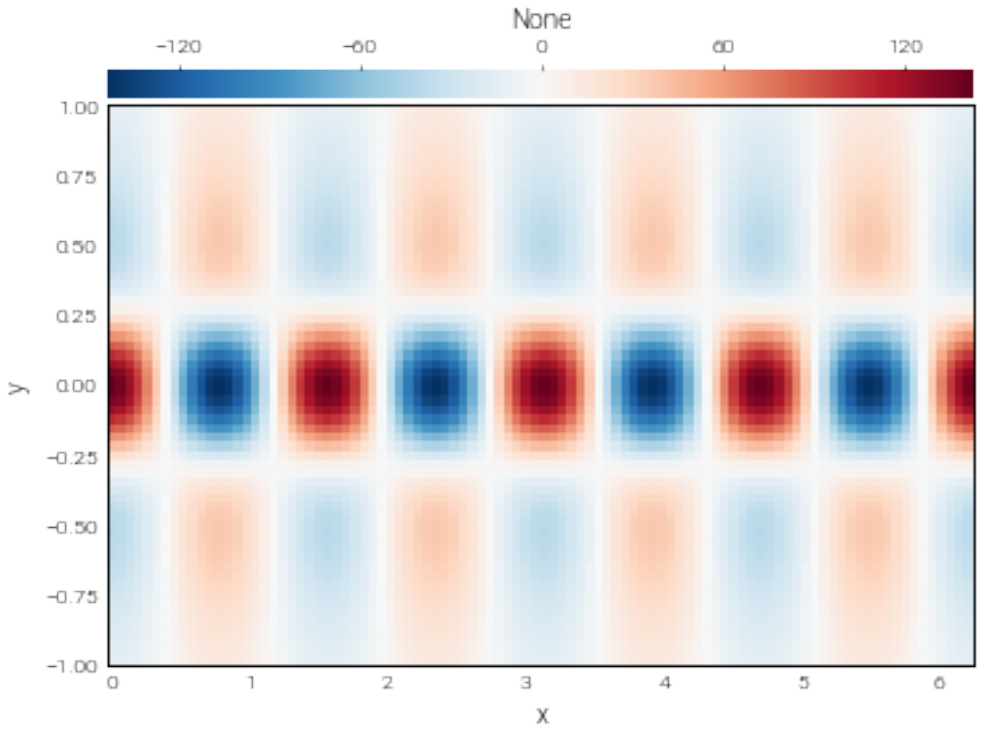
Third, the `differentiate`, `integrate`, and `interpolate` field methods provide short-cuts for building and evaluating these operations, directly returning the resulting fields.

```
In [18]: # The same results, directly from field methods
         fxxyy = f.differentiate(x=2, y=2)
         total_int_f = f.integrate('x', 'y')
         f00 = f.interpolate(x=0, y=0)

         print('Total integral:', total_int_f['g'][0,0])
         print('f at (x,y)=(0,0):', f00['g'][0,0])

         fxxyy.require_grid_space()
         plot_bot_2d(fxxyy);
```

```
Total integral: 12.566370614359172
f at (x,y)=(0,0): 1.9999999999999727
```



Tutorial 3: Problems and Solvers

This notebook covers the basics of setting up and solving problems using Dedalus.

First, we'll import the public interface and suppress some of the logging messages:

```
In [1]: from dedalus import public as de
        import numpy as np
        import matplotlib.pyplot as plt

        de.logging_setup.rootlogger.setLevel('ERROR')
        %matplotlib inline
```

3.1: Problems

Problem formulations

Systems of differential equations in Dedalus are represented in the form:

$$\mathcal{M} \cdot \partial_t \mathcal{X} + \mathcal{L} \cdot \mathcal{X} = \mathcal{F}$$

where $\mathcal{X}$ is a state-vector of fields, $\mathcal{F}$ is a set of generally nonlinear expressions represented by operator trees, and $\mathcal{M}$ and $\mathcal{L}$ are matrices of linear differential operators. This generalized form accomodates prognostic equations, diagnostic constraints, and boundary conditions using the tau method.

Dedalus includes a symbolic parser that takes equations and boundary conditions specified in plain text, and manipulates them into the above matrix form. This form requires the equations to be first-order in time and coupled (Chebyshev) derivatives, and must only contain linear terms on the left-hand-side. The entire RHS is parsed into an operator tree, and generally contains non-linear terms and linear terms that would couple different Fourier/parity modes, such as non-constant coefficients changing in these directions.

To create a problem object, you must provide a domain object and the names of the variables that appear in the equations. Let's start setting up the KdV-Burgers equation on a finite interval:

$$\partial_t u + u\partial_x u = a\partial_{xx} u + b\partial_{xxx} u$$

The KdV-Burgers equation only has one primative field but is third-order in it's derivatives, so we'll have to introduce two extra fields to reduce the equation to first-order. This problem will use the `IVP` class for initial value problems. Separate classes are available for linear and nonlinear boundary value problems, and generalized eigenvalue problems.

```
In [2]: # Create basis and domain
        x_basis = de.Chebyshev('x', 1024, interval=(-2, 6), dealias=3/2)
        domain = de.Domain([x_basis], np.float64)

        # Create problem
        problem = de.IVP(domain, variables=['u', 'ux', 'uxx'])
```

Meta-data and preconditioning

Metadata for the problem variables can be specified through the `meta` attribute of the problem object, and indexing by variable name, axis, and property, respectively.

The most common metadata to set here is the `dirichlet` option for Chebyshev bases, which performs a Dirichlet preconditioning / basis-recombination that sparsifies Dirichlet boundary conditions (interpolation at the Chebyshev interval endpoints), at the expense of a slightly increased problem bandwidth. This can drastically improve performance for problems formulated with only Dirichlet boundary conditions. Note that because the formulation is first-order in Chebyshev derivatives, this often includes what would be e.g. Neumann boundary conditions in a higher-order formulation.

Here we'll apply a Dirichlet preconditioning to all of our variables, for simplicity.

```
In [3]: problem.meta[:]['x']['dirichlet'] = True
```

Parameters and non-constant coefficients

Before adding the equations to the problem, we first add any parameters, defined as fields or scalars used in the equations but not part of the state vector of problem variables, to the `problem.parameters` dictionary.

For constant/scalar parameters, like we have here, we simply add the desired numerical values to the parameters dictionary.

```
In [4]: problem.parameters['a'] = 2e-4
        problem.parameters['b'] = 1e-4
```

For non-constant coefficients, we pass a field object with the desired data. For linear terms, Dedalus currently only accepts NCCs that couple the Chebyshev direction, i.e. are constant along the Fourier/Parity directions, so that those directions remain linearly uncoupled. To inform the parser that a NCC will not couple these directions, you must explicitly add some metadata to the NCC fields indiciating that they are constant along the Fourier/Parity directions.

We don't have NCCs or separable dimensions here, but we'll sketch the process here anyways. Consider a 3D problem on a Fourier (x), SinCos (y), Chebyshev (z) domain. Here's how we would add a simple non-constant coefficient in z to a problem.

```
In [5]: # ncc = domain.new_field(name='c')
        # ncc['g'] = z**2
        # ncc.meta['x', 'y']['constant'] = True
        # problem.paramters['c'] = ncc
```

Substitutions

To simplify equation entry, you can define substitution rules, which effectively act as string-replacement rules that will be applied during the parsing process.

Substitutions can be used to provide short aliases to quantities computed from the problem variables, and to define shortcut functions similart to python lambda functions, but with normal mathematical-function syntax. Here's a sketch of how you might define some substitutions that could be useful for a fluid simulation.

```
In [6]: ## Substitution defining the kinetic energy density for a 3D fluid simulation.
        ## Here rho, u, v, and w would be variables in the simulation.

        # problem.substitutions['KE_density'] = "rho * (u*u + v*v + w*w) / 2"

        ## Substitution defining the cartesian Laplacian of a field.
        ## Here A and Az are dummy variables that would be replaced by simulation variables in the eq

        # problem.substitutions['Lap(A, Az)'] = 'dx(dx(A)) + dy(dy(A)) + dz(Az)'
```

Equation entry

Equations and boundary conditions are then entered in plain text, optionally with conditions specifying which separable modes (indexed by `nx` and `ny` for separable axes named `x` and `y`, etc.) that equation applies to.

The parsing namespace basically consists of: * The variables, parameters, and substitutions defined in the problem * The axis names (`'x'` here), representing the individual basis grids * The differential operators for each basis, named as e.g. `'dx'` * The `differentiate`, `integrate`, and `interpolate` factories aliased as `'d'`, `'integ'`, and `'interp'` * `'left'` and `'right'` as aliases to interpolation at the endpoints of the Chebyshev direction, if present * Time and temporal derivatives as `'t'` and `'dt'`, by default (can be modified at IVP instantiation) * Simple mathematical functions (logarithmic and trigonometric), e.g. `'sin'`, `'exp'`, ...

Let's see how to enter the equations and boundary conditions for our problem.

```
In [7]: # Main equation, with linear terms on the LHS and nonlinear terms on the RHS
        problem.add_equation("dt(u) - a*dx(ux) - b*dx(uxx) = -u*ux")
        # Auxiliary equations defining the first-order reduction
        problem.add_equation("ux - dx(u) = 0")
        problem.add_equation("uxx - dx(ux) = 0")
        # Boundary conditions
        problem.add_bc('left(u) = 0')
        problem.add_bc('left(ux) = 0')
        problem.add_bc('right(ux) = 0')
```

3.2: Solvers

Building a solver

Each problem type (initial value, linear and nonlinear boundary value, and eigenvalue) has a corresponding solver class that actually performs the solution or iterations for a corresponding problem. Solvers are simply build using the `problem.build_solver` method.

For IVPs, we select a timestepping method when building the solver. Several multistep and Runge-Kutta IMEX schemes are available.

```
In [8]: solver = problem.build_solver(de.timesteppers.RK443)
```

Setting initial conditions

The fields representing the problem variables can be accessed with a dictionary-like interface through the `solver.state` system. For IVPs and nonlinear BVPs, initial conditions are set by directly modifying the state variable data before running a simulation.

```
In [9]: # Reference local grid and state fields
        x = domain.grid(0)
        u = solver.state['u']
        ux = solver.state['ux']
        uxx = solver.state['uxx']

        # Setup smooth triangle with support in (-1, 1)
        n = 20
        u['g'] = np.log(1 + np.cosh(n)**2/np.cosh(n*x)**2) / (2*n)
        u.differentiate('x', out=ux)
        ux.differentiate('x', out=uxx)
```

```
Out[9]: <Field 4786238072>
```

Setting stop criteria

For IVPs, stop criteria for halting time evolution are specified by setting setting the `stop_iteration`, `stop_wall_time` (seconds since solver instantiation), and/or `stop_sim_time` attributes on the solver.

Let's stop after 5000 iterations:

```
In [10]: # Stop stopping criteria
         solver.stop_sim_time = np.inf
         solver.stop_wall_time = np.inf
         solver.stop_iteration = 1000
```

Solving/iterating a problem

Linear BVPs and EVPs are solved using the `solver.solve` method, nonlinear BVPs are iterated using the `solver.newton_iteration` method, and IVPs are iterated using the `solver.step` method with a provided timestep.

The logic controlling the main-loop of a Dedalus simulation occurs explicitly in the simulation script. The `solver.ok` property can be used to halt an evolution loop once any of the specified stopping criteria have been met. Let's timestep our problem until a halting condition is reached, copying the grid values of `u` every few iterations. This should take less than a minute on most machines.

```
In [11]: import time

         # Setup storage
         u_list = [np.copy(u['g'])]
         t_list = [solver.sim_time]

         # Main loop
         dt = 1e-2
         start_time = time.time()
         while solver.ok:
             solver.step(dt)
             if solver.iteration % 5 == 0:
                 u_list.append(np.copy(u['g']))
                 t_list.append(solver.sim_time)
```

```
            if solver.iteration % 100 == 0:
                print('Completed iteration {}'.format(solver.iteration))
        end_time = time.time()
        print('Runtime:', end_time-start_time)
```

```
Completed iteration 100
Completed iteration 200
Completed iteration 300
Completed iteration 400
Completed iteration 500
Completed iteration 600
Completed iteration 700
Completed iteration 800
Completed iteration 900
Completed iteration 1000
Runtime: 4.605678081512451
```

Now let's make a space-time plot of the solution on the full dealiased grid:

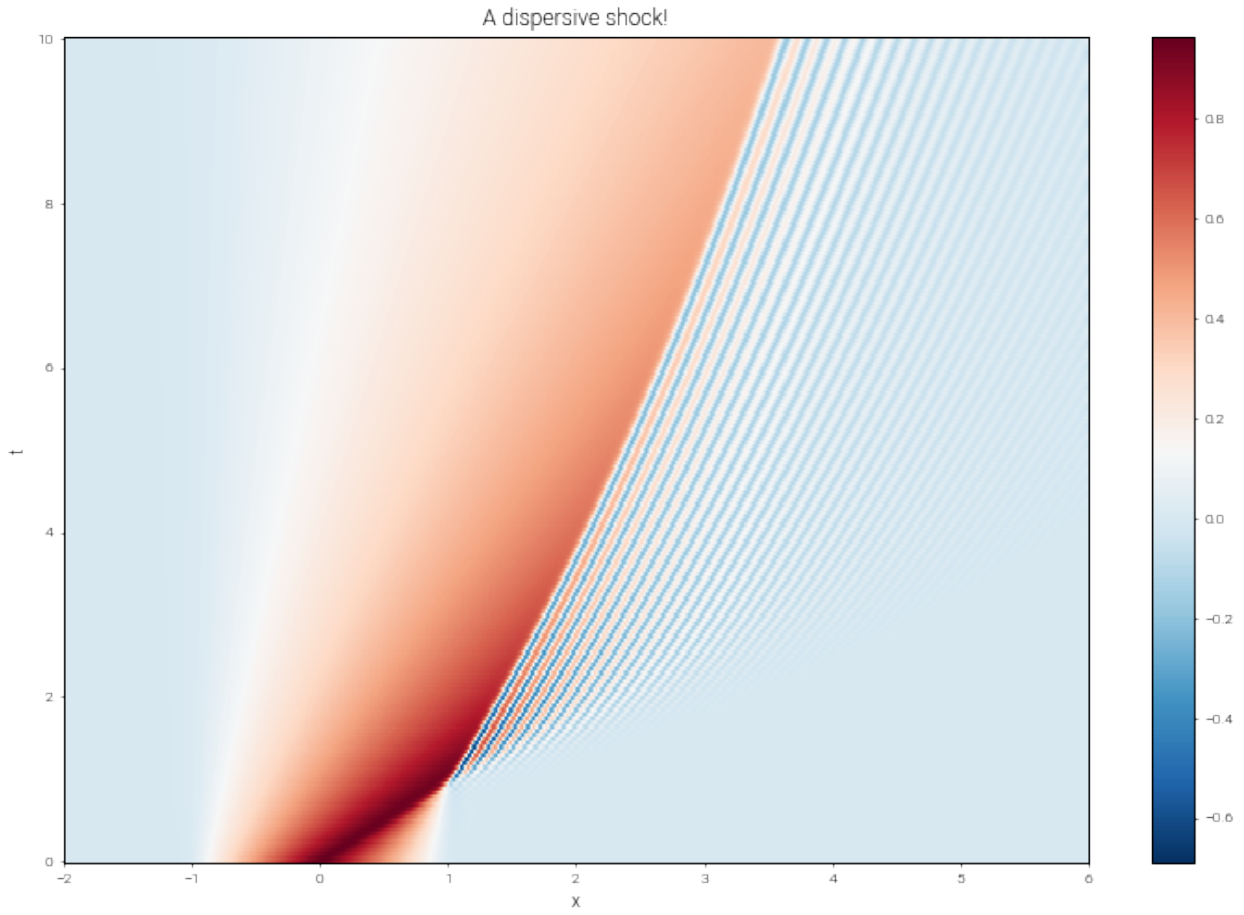
```
In [12]: from dedalus.extras import plot_tools

         # Convert storage to arrays
         u_array = np.array(u_list)
         t_array = np.array(t_list)

         # Build space and time meshes
         x_da = domain.grid(0, scales=domain.dealias)
         xmesh, ymesh = plot_tools.quad_mesh(x=x_da, y=t_array)

         # Plot
         plt.figure(figsize=(12, 8))
         plt.pcolormesh(xmesh, ymesh, u_array, cmap='RdBu_r')
         plt.axis(plot_tools.pad_limits(xmesh, ymesh))
         plt.colorbar()
         plt.xlabel('x')
         plt.ylabel('t')
         plt.title('A dispersive shock!')
```

```
Out[12]: Text(0.5,1,'A dispersive shock!')
```



Tutorial 4: Analysis and Post-processing

This notebook covers the basics of data analysis and post-processing using Dedalus.

First, we'll import the public interface and suppress some of the logging messages:

```
In [1]: from dedalus import public as de
        import numpy as np
        import matplotlib.pyplot as plt

        de.logging_setup.rootlogger.setLevel('ERROR')
        %matplotlib inline
```

4.1: Analysis

Dedalus includes a framework for evaluating and saving arbitrary analysis tasks while an initial value problem is running. To get started, let's setup the KdV-Burgers problem from the previous tutorial.

```
In [2]: # Create basis and domain
        x_basis = de.Chebyshev('x', 1024, interval=(-2, 6), dealias=3/2)
        domain = de.Domain([x_basis], np.float64)

        # Create problem
        problem = de.IVP(domain, variables=['u', 'ux', 'uxx'])
```

```
problem.meta[:]['x']['dirichlet'] = True
problem.parameters['a'] = 2e-4
problem.parameters['b'] = 1e-4
problem.add_equation("dt(u) - a*dx(ux) - b*dx(uxx) = -u*ux")
problem.add_equation("ux - dx(u) = 0")
problem.add_equation("uxx - dx(ux) = 0")
problem.add_bc('left(u) = 0')
problem.add_bc('left(ux) = 0')
problem.add_bc('right(ux) = 0')

# Build solver
solver = problem.build_solver(de.timesteppers.RK443)
solver.stop_sim_time = np.inf
solver.stop_wall_time = np.inf
solver.stop_iteration = 1000

# Reference local grid and state fields
x = domain.grid(0)
u = solver.state['u']
ux = solver.state['ux']
uxx = solver.state['uxx']

# Setup smooth triangle with support in (-1, 1)
n = 20
u['g'] = np.log(1 + np.cosh(n)**2/np.cosh(n*x)**2) / (2*n)
u.differentiate('x', out=ux)
ux.differentiate('x', out=uxx)
```

```
Out[2]: <Field 4732662728>
```

Analysis handlers

The explicit evaluation of analysis tasks during timestepping is controlled by the `solver.evaluator` object. Various handler objects are attached to the evaluator, and control when the evaluator computes their own set of tasks and what happens to the resulting data.

For example, an internal `SystemHandler` object directs the evaluator to evaluate the RHS expressions on every iteration, and uses the data for the explicit part of the timestepping algorithm.

For simulation analysis, the most useful handler is the `FileHandler`, which regularly computes tasks and writes the data to HDF5 files. When setting up a file handler, you specify the name/path for the output directory/files, as well as the cadence at which you want the handler's tasks to be evaluated. This cadence can be in terms of any combination of * simulation time, specified with `sim_dt` * wall time, specified with `wall_dt` * iteration number, specified with `iter`

To limit file sizes, the output from a file handler is split up into different sets over time, each containing some number of writes that can be limited with the `max_writes` keyword when the file handler is constructed.

Let's setup a file handler to be evaluated every few iterations.

```
In [3]: analysis = solver.evaluator.add_file_handler('analysis', iter=5, max_writes=100)
```

You can add an arbitrary number of file handlers to save different sets of tasks at different cadences and to different files.

Analysis tasks

Analysis tasks are added to a given handler using the `add_task` method. Tasks are entered in plain text, and parsed using the same namespace that is used for equation entry. For each task, you can additionally specify the output layout and scaling factors.

Let's add tasks for tracking the first and second moments of the solution.

```
In [4]: analysis.add_task("integ(u,'x')", layout='g', name='<u>')
        analysis.add_task("integ(u**2,'x')", layout='g', name='<uu>')
```

For checkpointing, you can also simply specify that all of the state variables should be saved.

```
In [5]: analysis.add_system(solver.state, layout='g')
```

We can now run the simulation just as in the previous tutorial, but without needing to manually save any data during the main loop.

```
In [6]: import time

        # Main loop
        dt = 1e-2
        start_time = time.time()
        while solver.ok:
            solver.step(dt)
            if solver.iteration % 100 == 0:
                print('Completed iteration {}'.format(solver.iteration))
        end_time = time.time()
        print('Runtime:', end_time-start_time)
```

```
Completed iteration 100
Completed iteration 200
Completed iteration 300
Completed iteration 400
Completed iteration 500
Completed iteration 600
Completed iteration 700
Completed iteration 800
Completed iteration 900
Completed iteration 1000
Runtime: 7.432521104812622
```

4.2: Post-processing

File arrangement

By default, the output files for each file handler are arranged as follows: 1. A base folder taking the name that was specified when the file handler was constructed, e.g. `analysis/`. 2. Within the base folder are subfolders for each set of outputs, with the same name plus a set number, e.g. `analysis_s0/`. 3. Within each set subfolder are HDF5 files for each process, with the same name plus a process number, e.g. `analysis_s0_p1.h5`.

Let's take a look at the output files from our example problem. We should see two sets (1000 total iterations, 5 iteration cadence, 100 writes per file) and data from one process.

```
In [7]: import subprocess
        print(subprocess.check_output("find analysis", shell=True).decode())
```

```
analysis
analysis/analysis_s1
analysis/analysis_s1/analysis_s1_p0.h5
```

```
analysis/analysis_s2
analysis/analysis_s2/analysis_s2_p0.h5
```

Merging output files

By default, each process writes its local portion of the analysis tasks to its own file, but often it is substantially easier to deal with the global dataset. The distributed process files can be easily merged into a global file for each set using the `merge_process_files` function from the `dedalus.tools.post` module.

Since we ran this problem serially, here this will essentially just perform a copy of the root process file, but we'll do the merge for illustrative purposes, anyways.

```
In [8]: from dedalus.tools import post
        post.merge_process_files("analysis", cleanup=True)
```

After the merge, we see that instead of a subfolder and process files for each output set, we have a single global set file for each output set.

```
In [9]: import subprocess
        print(subprocess.check_output("find analysis", shell=True).decode())
```

```
analysis
analysis/analysis_s1.h5
analysis/analysis_s2.h5
```

For some types of analysis, it's additionally convenient to merge the output sets together into a single file that's global in space and time, which can be done with the `merge_sets` function.

Note: this can generate very large files, so it's not recommended for analysis that is simply slicing over time, e.g. plotting snapshots of an analysis task at different times. However, if you want to explicitly plot a quantity versus time, instead of slicing over time, it can be useful.

```
In [10]: import pathlib
         set_paths = list(pathlib.Path("analysis").glob("analysis_s*.h5"))
         post.merge_sets("analysis/analysis.h5", set_paths, cleanup=True)
```

Now we see that the two sets have been merged into a single file.

```
In [11]: import subprocess
         print(subprocess.check_output("find analysis", shell=True).decode())
```

```
analysis
analysis/analysis.h5
```

Handling data

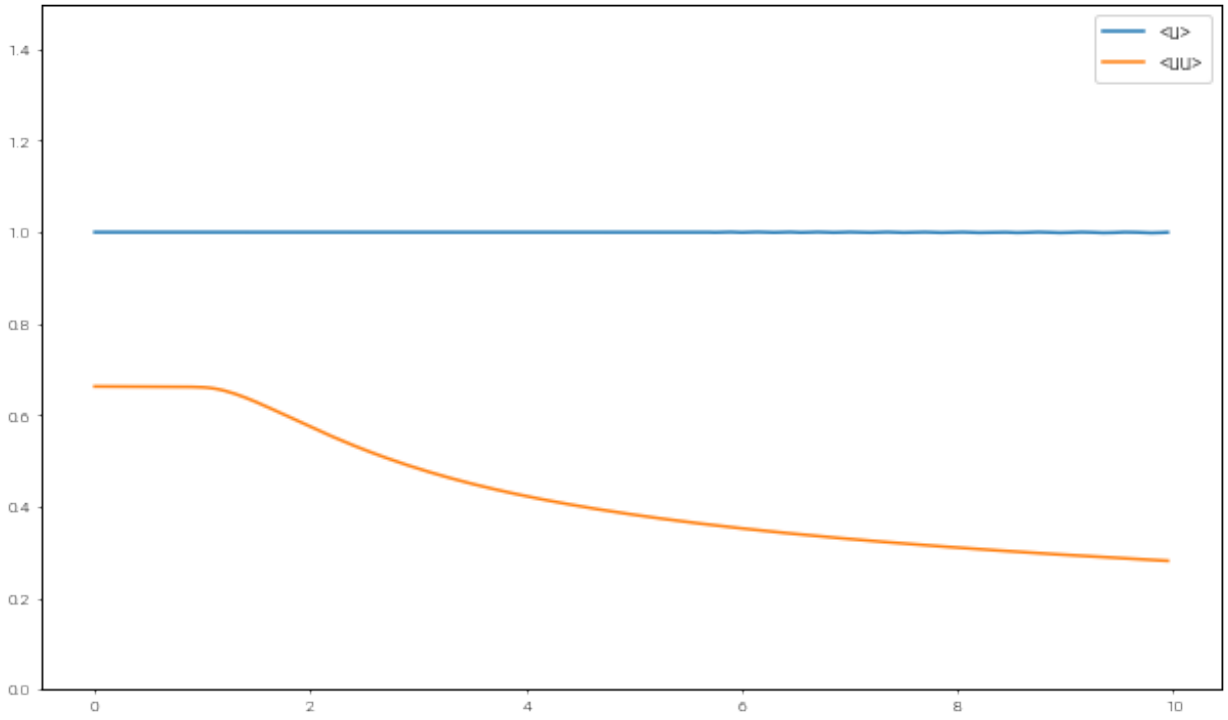
Each HDF5 file contains a "tasks" group containing a dataset for each task assigned to the file handler. The first dimension of the dataset is time, and the subsequent dimensions are the spatial dimensions of the output field.

The HDF5 datasets are self-describing, with dimensional scales attached to each axis. For the first axis, these include the simulation time, wall time, iteration, and write number. The scales indicate grid points or mode numbers for the spatial axes, based on the task layout. See the h5py docs for more details.

Let's open up the merged analysis file and plot time series of the moments. We expect the first moment (momentum) to be conserved through the simulation, while the second moment (kinetic energy) should decay due to dissipation in the shock.

```
In [12]: import h5py

         fig = plt.figure(figsize=(10, 6))
         with h5py.File("analysis/analysis.h5", mode='r') as file:
             u1 = file['tasks']['<u>']
             u2 = file['tasks']['<uu>']
             t = file['scales']['sim_time']
             plt.plot(t, u1, label="<u>")
             plt.plot(t, u2, label="<uu>")
             plt.ylim(0, 1.5)
             plt.legend(loc='upper right', fontsize=10)
```

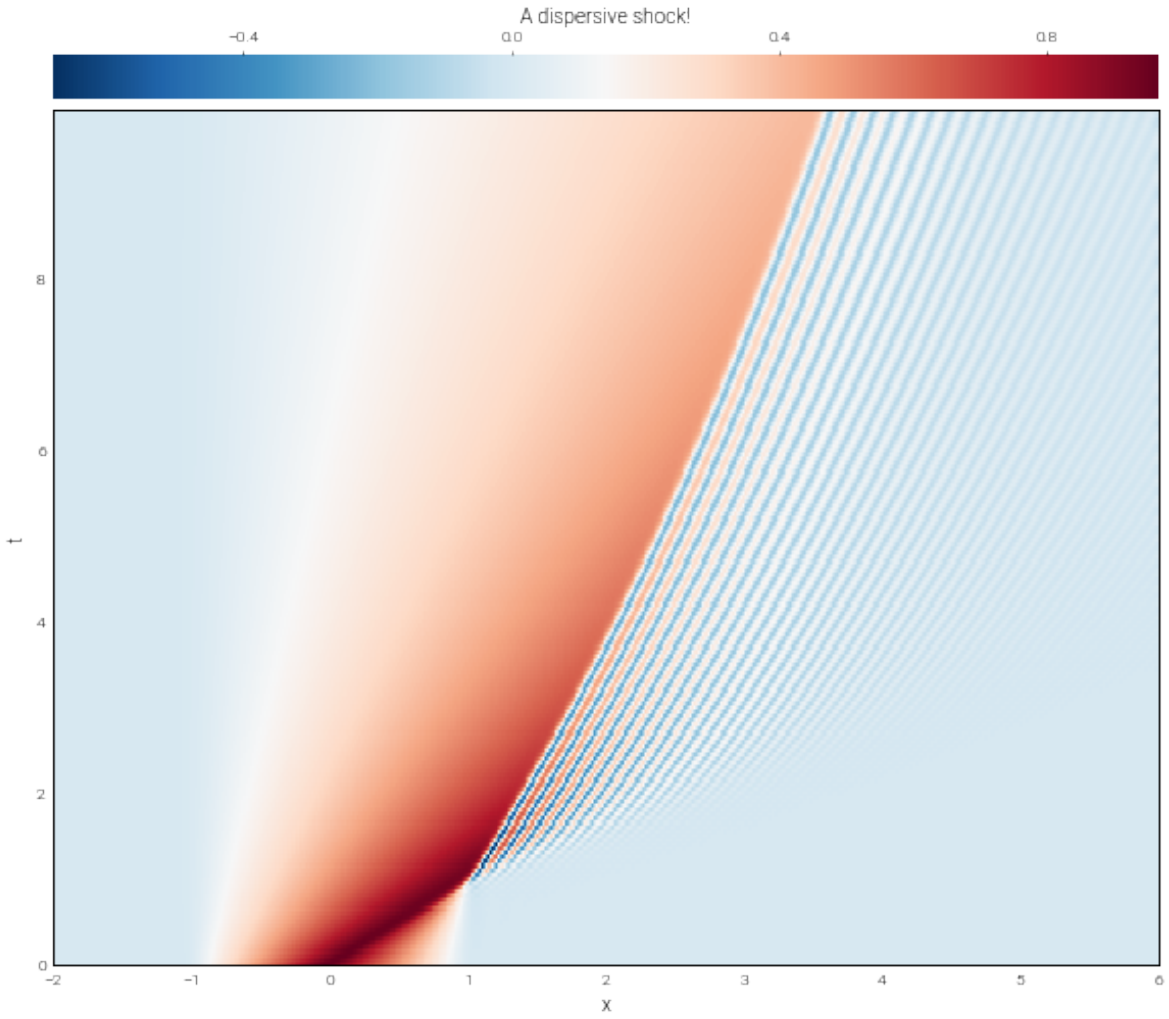


We can also pass datasets, like fields, to the plotting helper functions in the `plot_tools` module.

```
In [13]: from dedalus.extras import plot_tools

         fig = plt.figure(figsize=(10, 8))
         ax = fig.add_subplot(111)

         with h5py.File("analysis/analysis.h5", mode='r') as file:
             u = file['tasks']['u']
             plot_tools.plot_bot_2d(u, title="A dispersive shock!", transpose=True, axes=ax)
```



Finally, let's cleanup the analysis files we created.

```
In [14]: import shutil
         shutil.rmtree('analysis')
```

2.2.2 Example Notebooks

Below are several notebooks that walk through the setup and execution of more complicated multidimensional example problems.

Kelvin-Helmholtz Instability

(image: Chuck Doswell)

We will simulate the incompressible Kelvin-Helmholtz problem. We non-dimensionalize the problem by taking the box height to be one and the jump in velocity to be one. Then the Reynolds number is given by

$$\mathrm{Re} = \frac{UH}{\nu} = \frac{1}{\nu}.$$

We use no slip boundary conditions, and a box with aspect ratio $L/H = 2$. The initial velocity profile is given by a hyperbolic tangent, and only a single mode is initially excited. We will also track a passive scalar which will help us visualize the instability.

First, we import the necessary modules.

```
In [1]: %matplotlib inline
```

```
In [2]: import numpy as np
        import matplotlib.pyplot as plt
        import h5py
        from dedalus import public as de
        from dedalus.extras import flow_tools
        import time
        from IPython import display
```

Here, we set logging to `INFO` level. Currently, by default, Dedalus sets its logging output to `DEBUG`, which produces more info than we need here.

```
In [3]: import logging
        root = logging.root
        for h in root.handlers:
            h.setLevel("INFO")

        logger = logging.getLogger(__name__)
```

To perform an initial value problem (IVP) in Dedalus, you need three things:

1. A domain to solve the problem on
2. Equations to solve
3. A timestepping scheme

Problem Domain

First, we will specify the domain. Domains are built by taking the direct product of bases. Here we are running a 2D simulation, so we will define x and y bases. From these, we build the domain.

```
In [4]: #Aspect ratio 2
        Lx, Ly = (2., 1.)
        nx, ny = (192, 96)

        # Create bases and domain
        x_basis = de.Fourier('x', nx, interval=(0, Lx), dealias=3/2)
        y_basis = de.Chebyshev('y',ny, interval=(-Ly/2, Ly/2), dealias=3/2)
        domain = de.Domain([x_basis, y_basis], grid_dtype=np.float64)
```

The last basis (z direction) is represented in Chebyshev polynomials. This will allow us to apply interesting boundary conditions in the z direction. We call the other directions (in this case just x) the "horizontal" directions. The horizontal directions must be "easy" in the sense that taking derivatives cannot couple different horizontal modes. Right now, we have Fourier and Sin/Cos series implemented for the horizontal directions, and are working on implementing spherical harmonics.

Equations

Next we will define the equations that will be solved on this domain. The equations are

$$\partial_t u + \boldsymbol{u} \cdot \boldsymbol{\nabla} u + \partial_x p = \frac{1}{\mathrm{Re}} \nabla^2 u$$

$$\partial_t v + \boldsymbol{u}\cdot\boldsymbol{\nabla} v + \partial_y p = \frac{1}{\mathrm{Re}}\nabla^2 v$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$$

$$\partial_t s + \boldsymbol{u}\cdot\boldsymbol{\nabla} s = \frac{1}{\mathrm{ReSc}}\nabla^2 s$$

The equations are written such that the left-hand side (LHS) is treated implicitly, and the right-hand side (RHS) is treated explicitly. The LHS is limited to only linear terms, though linear terms can also be placed on the RHS. Since y is our special direction in this example, we also restrict the LHS to be at most first order in derivatives with respect to y.

We also set the parameters, the Reynolds and Schmidt numbers.

```
In [5]: Reynolds = 1e4
        Schmidt = 1.

        problem = de.IVP(domain, variables=['p','u','v','uy','vy','s','sy'])
        problem.meta[:]['y']['dirichlet'] = True
        problem.parameters['Re'] = Reynolds
        problem.parameters['Sc'] = Schmidt
        problem.add_equation("dt(u) + dx(p) - 1/Re*(dx(dx(u)) + dy(uy)) = - u*dx(u) - v*uy")
        problem.add_equation("dt(v) + dy(p) - 1/Re*(dx(dx(v)) + dy(vy)) = - u*dx(v) - v*vy")
        problem.add_equation("dx(u) + vy = 0")
        problem.add_equation("dt(s) - 1/(Re*Sc)*(dx(dx(s)) + dy(sy)) = - u*dx(s) - v*sy")
        problem.add_equation("uy - dy(u) = 0")
        problem.add_equation("vy - dy(v) = 0")
        problem.add_equation("sy - dy(s) = 0")
```

Because we are using this first-order formalism, we define auxiliary variables `uy`, `vy`, and `sy` to be the y-derivative of `u`, `v`, and `s` respectively.

Next, we set our boundary conditions. "Left" boundary conditions are applied at $y = -Ly/2$ and "right" boundary conditions are applied at $y = +Ly/2$.

```
In [6]: problem.add_bc("left(u) = 0.5")
        problem.add_bc("right(u) = -0.5")
        problem.add_bc("left(v) = 0")
        problem.add_bc("right(v) = 0", condition="(nx != 0)")
        problem.add_bc("left(p) = 0", condition="(nx == 0)")
        problem.add_bc("left(s) = 0")
        problem.add_bc("right(s) = 1")
```

Note that we have a special boundary condition for the $k_x = 0$ mode (singled out by `condition="(dx==0)"`). This is because the continuity equation implies $\partial_y v = 0$ if $k_x = 0$; thus, $v = 0$ on the top and bottom are redundant boundary conditions. We replace one of these with a gauge choice for the pressure.

Timestepping

We have implemented about twenty implicit-explicit timesteppers in Dedalus. This contains both multi-stage and multi-step methods. For this problem, we will use a four-stage, fourth order Runge-Kutta integrator. Changing the timestepping algorithm is as easy as changing one line of code.

```
In [7]: ts = de.timesteppers.RK443
```

Initial Value Problem

We now have the three ingredients necessary to set up our IVP:

```
In [8]: solver =  problem.build_solver(ts)
```

```
2018-10-14 09:03:10,921 pencil 0/1 INFO :: Building pencil matrix 1/96 (~1%) Elapsed: 0s, Remaining:
2018-10-14 09:03:11,228 pencil 0/1 INFO :: Building pencil matrix 10/96 (~10%) Elapsed: 0s, Remaining
2018-10-14 09:03:11,551 pencil 0/1 INFO :: Building pencil matrix 20/96 (~21%) Elapsed: 1s, Remaining
2018-10-14 09:03:11,896 pencil 0/1 INFO :: Building pencil matrix 30/96 (~31%) Elapsed: 1s, Remaining
2018-10-14 09:03:12,223 pencil 0/1 INFO :: Building pencil matrix 40/96 (~42%) Elapsed: 1s, Remaining
2018-10-14 09:03:12,566 pencil 0/1 INFO :: Building pencil matrix 50/96 (~52%) Elapsed: 2s, Remaining
2018-10-14 09:03:12,902 pencil 0/1 INFO :: Building pencil matrix 60/96 (~62%) Elapsed: 2s, Remaining
2018-10-14 09:03:13,219 pencil 0/1 INFO :: Building pencil matrix 70/96 (~73%) Elapsed: 2s, Remaining
2018-10-14 09:03:13,526 pencil 0/1 INFO :: Building pencil matrix 80/96 (~83%) Elapsed: 3s, Remaining
2018-10-14 09:03:13,833 pencil 0/1 INFO :: Building pencil matrix 90/96 (~94%) Elapsed: 3s, Remaining
2018-10-14 09:03:14,031 pencil 0/1 INFO :: Building pencil matrix 96/96 (~100%) Elapsed: 3s, Remainir
```

Now we set our initial conditions. We set the horizontal velocity and scalar field to tanh profiles, and using a single-mode initial perturbation in v.

```
In [9]: x = domain.grid(0)
        y = domain.grid(1)
        u = solver.state['u']
        uy = solver.state['uy']
        v = solver.state['v']
        vy = solver.state['vy']
        s = solver.state['s']
        sy = solver.state['sy']

        a = 0.05
        sigma = 0.2
        flow = -0.5
        amp = -0.2
        u['g'] = flow*np.tanh(y/a)
        v['g'] = amp*np.sin(2.0*np.pi*x/Lx)*np.exp(-(y*y)/(sigma*sigma))
        s['g'] = 0.5*(1+np.tanh(y/a))
        u.differentiate('y',out=uy)
        v.differentiate('y',out=vy)
        s.differentiate('y',out=sy)
```

```
Out[9]: <Field 4730968776>
```

Now we set integration parameters and the CFL.

```
In [10]: solver.stop_sim_time = 2.01
         solver.stop_wall_time = np.inf
         solver.stop_iteration = np.inf

         initial_dt = 0.2*Lx/nx
         cfl = flow_tools.CFL(solver,initial_dt,safety=0.8)
         cfl.add_velocities(('u','v'))
```

Analysis

We have a sophisticated analysis framework in which the user specifies analysis tasks as strings. Users can output full data cubes, slices, volume averages, and more. Here we will only output a few 2D slices, and a 1D profile of the horizontally averaged concentration field. Data is output in the hdf5 file format.

```
In [11]: analysis = solver.evaluator.add_file_handler('analysis_tasks', sim_dt=0.1, max_writes=50)
         analysis.add_task('s')
         analysis.add_task('u')
         solver.evaluator.vars['Lx'] = Lx
         analysis.add_task("integ(s,'x')/Lx", name='s profile')
```

Main Loop

We now have everything set up for our simulation. In Dedalus, the user writes their own main loop.

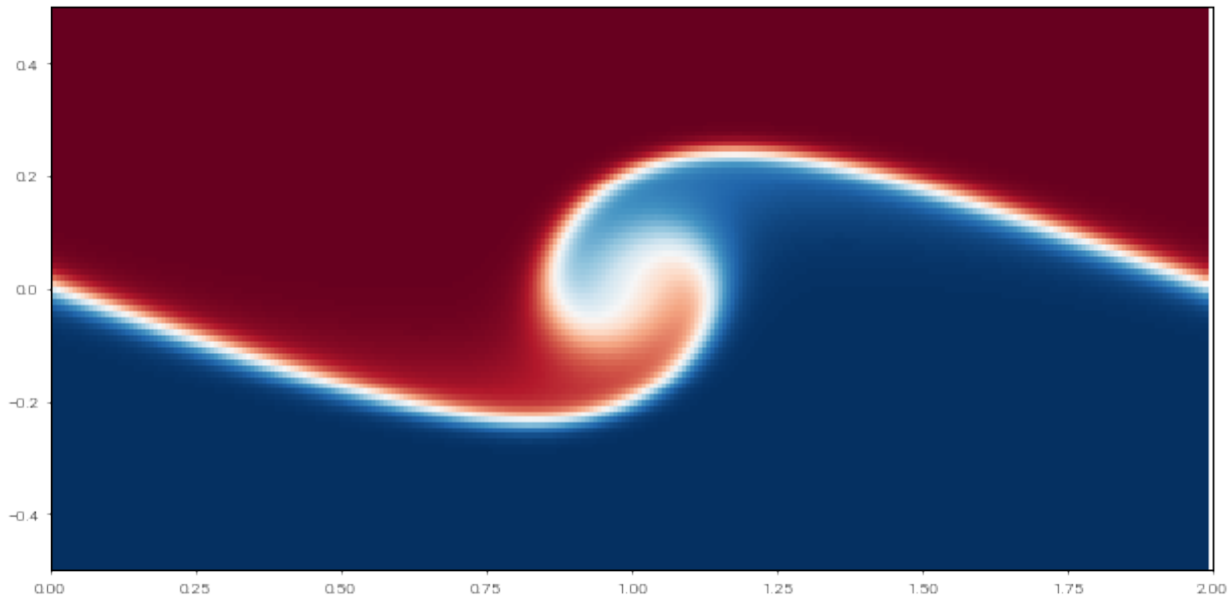
```
In [12]: # Make plot of scalar field
         x = domain.grid(0,scales=domain.dealias)
         y = domain.grid(1,scales=domain.dealias)
         xm, ym = np.meshgrid(x,y)
         fig, axis = plt.subplots(figsize=(10,5))
         p = axis.pcolormesh(xm, ym, s['g'].T, cmap='RdBu_r');
         axis.set_xlim([0,2.])
         axis.set_ylim([-0.5,0.5])

         logger.info('Starting loop')
         start_time = time.time()
         while solver.ok:
             dt = cfl.compute_dt()
             solver.step(dt)
             if solver.iteration % 10 == 0:
                 # Update plot of scalar field
                 p.set_array(np.ravel(s['g'][:-1,:-1].T))
                 display.clear_output()
                 display.display(plt.gcf())
                 logger.info('Iteration: %i, Time: %e, dt: %e' %(solver.iteration, solver.sim_time, c

         end_time = time.time()

         p.set_array(np.ravel(s['g'][:-1,:-1].T))
         display.clear_output()
         # Print statistics
         logger.info('Run time: %f' %(end_time-start_time))
         logger.info('Iterations: %i' %solver.iteration)
```

```
2018-10-14 09:05:29,228 __main__ 0/1 INFO :: Run time: 135.040192
2018-10-14 09:05:29,228 __main__ 0/1 INFO :: Iterations: 269
```



Analysis

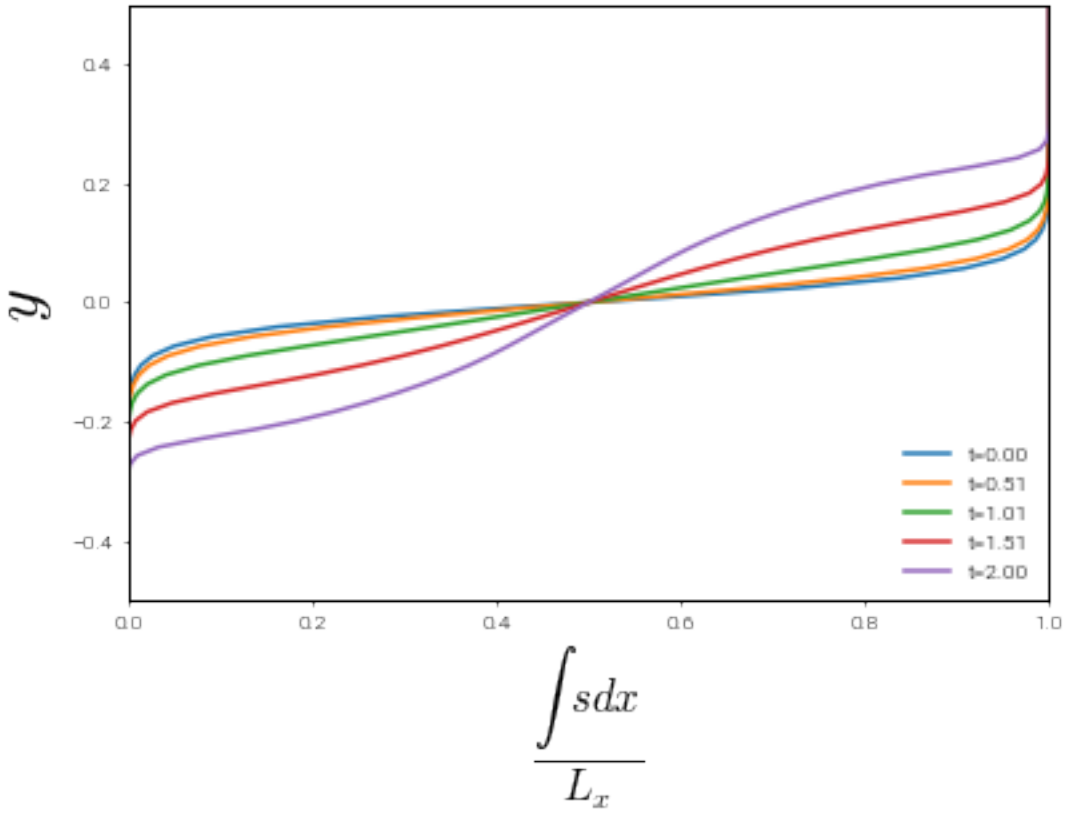
As an example of doing some analysis, we will load in the horizontally averaged profiles of the scalar field s and plot them.

```
In [21]: # Read in the data
         f = h5py.File('analysis_tasks/analysis_tasks_s0/analysis_tasks_s0_p0.h5','r')
         y = f['/scales/y/1.0'][:]
         t = f['scales']['sim_time'][:]
         s_ave = f['tasks']['s profile'][:]
         f.close()

         s_ave = s_ave[:,0,:] # remove length-one x dimension
```

```
In [23]: for i in range(0,21,5):
           plt.plot(s_ave[i,:],y,label='t=%4.2f' %t[i])

         plt.ylim([-0.5,0.5])
         plt.xlim([0,1])
         plt.xlabel(r'$\frac{\int \ s dx}{L_x}$',fontsize=24)
         plt.ylabel(r'$y$',fontsize=24)
         plt.legend(loc='lower right').draw_frame(False)
```




```
In [ ]:
```

Axisymmetric Taylor-Couette flow in Dedalus

(image: wikipedia)

Taylor-Couette flow is characterized by three dimensionless numbers:

$\eta = R1/R2$, the ratio of the inner cylidner radius R_1 to the outer cylinder radius R_2

$\mu = \Omega_2/\Omega_1$, the ratio of the OUTER cylinder rotation rate Ω_2 to the inner rate Ω_1

$\mathrm{Re} = \Omega_1 R_1 \delta/\nu$, the Reynolds numbers, where $\delta = R_2 - R_1$, the gap width between the cylinders

We non dimensionalize the flow in terms of

$[\mathrm{L}] = \delta = R_2 - R_1$

$[\mathrm{V}] = R_1\Omega_1$

$[\mathrm{M}] = \rho\delta^3$

And choose $\delta = 1$, $R_1\Omega_1 = 1$, and $\rho = 1$.

```
In [1]: %pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

```
In [2]: import numpy as np
        import time
        import h5py

        import dedalus.public as de
        from dedalus.extras import flow_tools
```

Here, we set logging to `INFO` level. Currently, by default, the parsing in Dedalus sets its logging output to `DEBUG` in notebooks, which produces more info than we need here.

```
In [3]: import logging
        root = logging.root
        for h in root.handlers:
            h.setLevel("INFO")

        logger = logging.getLogger(__name__)
```

Input parameters

These parameters are taken from Barenghi (1991) J. Comp. Phys. After running, we'll compare it compute the growth rate and compare it to the value $\gamma_{analytic} = 0.430108693$

```
In [4]: # input parameters from Barenghi (1991)
        eta = 1./1.444 # R1/R2
        alpha = 3.13   # vertical wavenumber
        Re = 80.       # in units of R1*Omega1*delta/nu
        mu = 0.        # Omega2/Omega1

        # computed quantitites
        omega_in = 1.
        omega_out = mu * omega_in
        r_in = eta/(1. - eta)
        r_out = 1./(1. - eta)
        height = 2.*np.pi/alpha
        v_l = 1. # by default, we set v_l to 1.
        v_r = omega_out*r_out
```

Problem Domain

Every PDE takes place somewhere, so we define a *domain*, which in this case is the z and r directions. Because the r direction has walls, we use a `Chebyshev` basis, but the z direction is periodic, so we use a `Fourier` basis. The `Domain` object combines these.

```
In [5]: # bases
        r_basis = de.Chebyshev('r', 32, interval=(r_in, r_out), dealias=3/2)
        z_basis = de.Fourier('z', 32, interval=(0., height), dealias=3/2)
        domain = de.Domain([z_basis, r_basis], grid_dtype=np.float64)
```

Equations

We use the `IVP` object, which can parse a set of equations in plain text and combine them into an initial value problem.

Here, we code up the equations for the "primative" variables, $\mathbf{v} = u\hat{\mathbf{r}} + v\hat{\theta} + w\hat{\mathbf{z}}$ and p, along with their first derivatives.

The equations are the incompressible, axisymmetric Navier-Stokes equations in cylindrical coordinates

The axes will be called z and r, and we will expand the non-constant r^2 terms, to a cutoff precision of 10^{-8}. These non-constant coefficients (called "NCC" in Dedalus) are geometric here, but they could be background states in convection, or position dependent diffusion coefficients, or whatever.

We also add the parameters to the object, so we can use their names in the equations below.

```
In [6]: TC = de.IVP(domain, variables=['p', 'u', 'v', 'w', 'ur', 'vr', 'wr'], ncc_cutoff=1e-8)
        TC.meta[:]['r']['dirichlet'] = True
        TC.parameters['nu'] = 1./Re
        TC.parameters['v_l'] = v_l
        TC.parameters['v_r'] = v_r
        mu = TC.parameters['v_r']/TC.parameters['v_l'] * eta
```

The equations are multiplied through by r^2, so that there are no $1/r$ terms, which require more coefficients in the expansion

```
In [7]: TC.add_equation("r*ur + u + r*dz(w) = 0")
        TC.add_equation("r*r*dt(u) - r*r*nu*dr(ur) - r*nu*ur - r*r*nu*dz(dz(u)) + nu*u + r*r*dr(p) =
        TC.add_equation("r*r*dt(v) - r*r*nu*dr(vr) - r*nu*vr - r*r*nu*dz(dz(v)) + nu*v  = -r*r*u*vr -
        TC.add_equation("r*dt(w) - r*nu*dr(wr) - nu*wr - r*nu*dz(dz(w)) + r*dz(p) = -r*u*wr - r*w*dz
        TC.add_equation("ur - dr(u) = 0")
        TC.add_equation("vr - dr(v) = 0")
        TC.add_equation("wr - dr(w) = 0")
```

Initial and Boundary Conditions

First we create some aliases to the r and z grids, so we can quickly compute the analytic Couette flow solution for unperturbed, unstable axisymmetric flow.

```
In [8]: r = domain.grid(1, scales=domain.dealias)
        z = domain.grid(0, scales=domain.dealias)

        p_analytic = (eta/(1-eta**2))**2 * (-1./(2*r**2*(1-eta)**2) -2*np.log(r) +0.5*r**2 * (1.-eta)
        v_analytic = eta/(1-eta**2) * ((1. - mu)/(r*(1-eta)) - r * (1.-eta) * (1 - mu/eta**2))
```

And now we add boundary conditions, simply by typing them in plain text, just like the equations.

```
In [9]: # boundary conditions
        TC.add_bc("left(u) = 0")
        TC.add_bc("left(v) = v_l")
```

```
TC.add_bc("left(w) = 0")
TC.add_bc("right(u) = 0", condition="nz != 0")
TC.add_bc("right(v) = v_r")
TC.add_bc("right(w) = 0")
TC.add_bc("left(p) = 0", condition="nz == 0")
```

We can now set the parameters of the problem, ν, v_l, and v_r, and have the code log μ to the output (which can be `stdout`, a file, or both).

Timestepping

Dedalus comes with a lot of timesteppers, and makes it very easy to add your favorite one. Here we pick `RK443`, an IMEX Runga-Kutta scheme. We set our maximum timestep `max_dt`, and choose the various stopping parameters.

Finally, we've got our full initial value problem (represented by the `IVP`) object: a timestepper, a domain, and a `ParsedProblem` (or equation set)

```
In [10]: dt = max_dt = 1.
         omega1 = TC.parameters['v_l']/r_in
         period = 2*np.pi/omega1

         ts = de.timesteppers.RK443
         IVP = TC.build_solver(ts)
         IVP.stop_sim_time = 15.*period
         IVP.stop_wall_time = np.inf
         IVP.stop_iteration = 10000000
```

```
2018-10-14 08:57:40,080 pencil 0/1 INFO :: Building pencil matrix 1/16 (~6%) Elapsed: 0s, Remaining:
2018-10-14 08:57:40,120 pencil 0/1 INFO :: Building pencil matrix 2/16 (~12%) Elapsed: 0s, Remaining
2018-10-14 08:57:40,196 pencil 0/1 INFO :: Building pencil matrix 4/16 (~25%) Elapsed: 0s, Remaining
2018-10-14 08:57:40,273 pencil 0/1 INFO :: Building pencil matrix 6/16 (~38%) Elapsed: 0s, Remaining
2018-10-14 08:57:40,346 pencil 0/1 INFO :: Building pencil matrix 8/16 (~50%) Elapsed: 0s, Remaining
2018-10-14 08:57:40,420 pencil 0/1 INFO :: Building pencil matrix 10/16 (~62%) Elapsed: 0s, Remainin
2018-10-14 08:57:40,487 pencil 0/1 INFO :: Building pencil matrix 12/16 (~75%) Elapsed: 0s, Remainin
2018-10-14 08:57:40,555 pencil 0/1 INFO :: Building pencil matrix 14/16 (~88%) Elapsed: 1s, Remainin
2018-10-14 08:57:40,624 pencil 0/1 INFO :: Building pencil matrix 16/16 (~100%) Elapsed: 1s, Remainin
```

We initialize the state vector, given by `IVP.state`. To make life a little easier, we set some aliases first:

```
In [11]: p = IVP.state['p']
         u = IVP.state['u']
         v = IVP.state['v']
         w = IVP.state['w']
         ur = IVP.state['ur']
         vr = IVP.state['vr']
         wr = IVP.state['wr']
```

Next, we create a new field, ϕ, defined on the `domain`, which we'll use below to compute incompressible, random velocity perturbations.

```
In [12]: phi = domain.new_field(name='phi')
```

Here, we set all these to their dealiased domains. Dedalus allows you to set the "scale" of your data: this allows you to interpolate your data to a grid of any size at spectral accuracy. Of course, this isn't CSI: Fluid Dynamics, so you won't get any more detail than your highest spectral coefficient.

```
In [13]: for f in [phi,p,u,v,w,ur,vr,wr]:
             f.set_scales(domain.dealias, keep_data=False)
```

Now we set the state vector with our previously computed analytic solution, compute the first derivatives (to make our system first order)

```
In [14]: v['g'] = v_analytic
         #p['g'] = p_analytic

         v.differentiate('r',out=vr)
```

```
Out[14]: <Field 4654371112>
```

And finally, we set some small, incompressible perturbations to the velocity field so we can kick off our linear instability.

First, we initialize ϕ (which we created above) to Gaussian noise and then mask it to only appear in the center of the domain, so we don't violate the boundary conditions. We then take its curl to get the velocity perturbations.

Unfortunately, Gaussian noise on the grid is generally a bad idea: zone-to-zone variations (that is, the highest frequency components) will be amplified arbitrarily by any differentiation. So, let's filter out those high frequency components using this handy little function:

```
In [15]: def filter_field(field,frac=0.5):
             dom = field.domain
             local_slice = dom.dist.coeff_layout.slices(scales=dom.dealias)
             coeff = []
             for i in range(dom.dim)[::-1]:
                 coeff.append(np.linspace(0,1,dom.global_coeff_shape[i],endpoint=False))
             cc = np.meshgrid(*coeff)

             field_filter = np.zeros(dom.local_coeff_shape,dtype='bool')
             for i in range(dom.dim):
                 field_filter = field_filter | (cc[i][local_slice] > frac)
             field['c'][field_filter] = 0j
```

This is not the best filter: it assumes that cutting off above a certain Chebyshev mode n and Fourier mode n will be OK, though this may produce anisotropies in the data (I haven't checked). If you're worrying about the anisotropy of the initial noise of your ICs, you can always replace this filter with something better.

```
In [16]: # incompressible perturbation, arbitrary vorticity
         # u = -dz(phi)
         # w = dr(phi) + phi/r

         phi['g'] = 1e-3* np.random.randn(*v['g'].shape)*np.sin(np.pi*(r - r_in))
         filter_field(phi)
         phi.differentiate('z',out=u)
         u['g'] *= -1
         phi.differentiate('r',out=w)
         w['g'] += phi['g']/r

         u.differentiate('r',out=ur)
         w.differentiate('r',out=wr)
```

```
Out[16]: <Field 4654371168>
```

Now we check that incompressibility is indeed satisfied, first by computing $\nabla \cdot u$,

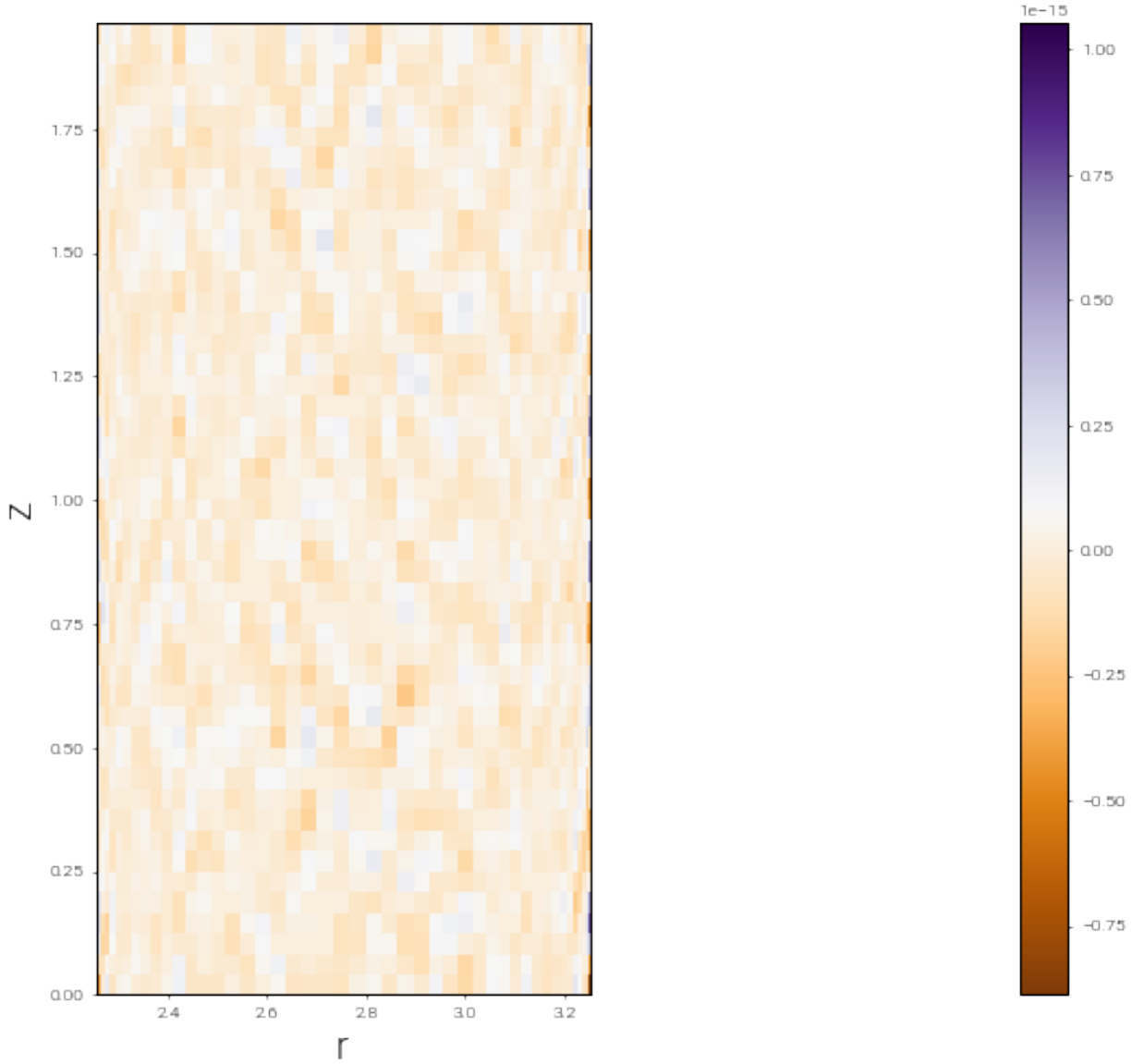
```
In [17]: divu0 = domain.new_field(name='divu0')
         u.differentiate('r',out=divu0)
         divu0['g'] += u['g']/r + w.differentiate('z')['g']
```

and then by plotting it to make sure it's nowhere greater than $\sim 10^{-15}$

```
In [18]: figsize(12,8)
         pcolormesh((r[0]*ones_like(z)).T,(z*ones_like(r)).T,divu0['g'].T,cmap='PuOr')
         colorbar()
         axis('image')
```

```
xlabel('r', fontsize=18)
ylabel('z', fontsize=18)
```

Out[18]: Text(0,0.5,'z')



Time step size and the CFL condition

Here, we use the nice CFL calculator provided by the `flow_tools` package in the `extras` module.

```
In [19]: CFL = flow_tools.CFL(IVP, initial_dt=1e-3, cadence=5, safety=0.3,
                              max_change=1.5, min_change=0.5)
         CFL.add_velocities(('u', 'w'))
```

Analysis

Dedalus has a very powerful inline analysis system, and here we set up a few.

```
In [20]: # Integrated energy every 10 iterations
         analysis1 = IVP.evaluator.add_file_handler("scalar_data", iter=10)
         analysis1.add_task("integ(0.5 * (u*u + v*v + w*w))", name="total kinetic energy")
         analysis1.add_task("integ(0.5 * (u*u + w*w))", name="meridional kinetic energy")
         analysis1.add_task("integ((u*u)**0.5)", name='u_rms')
         analysis1.add_task("integ((w*w)**0.5)", name='w_rms')

         # Snapshots every half an inner rotation period
         analysis2 = IVP.evaluator.add_file_handler('snapshots',sim_dt=0.5*period, max_size=2**30)
         analysis2.add_system(IVP.state, layout='g')

         # radial profiles every 100 timestpes
         analysis3 = IVP.evaluator.add_file_handler("radial_profiles", iter=100)
         analysis3.add_task("integ(r*v, 'z')", name='Angular Momentum')
```

The Main Loop

And here we actually run the simulation!

```
In [21]: dt = CFL.compute_dt()
         # Main loop
         start_time = time.time()

         while IVP.ok:
             IVP.step(dt)
             if IVP.iteration % 10 == 0:
                 logger.info('Iteration: %i, Time: %e, dt: %e' %(IVP.iteration, IVP.sim_time, dt))
             dt = CFL.compute_dt()


         end_time = time.time()

         # Print statistics
         logger.info('Total time: %f' %(end_time-start_time))
         logger.info('Iterations: %i' %IVP.iteration)
         logger.info('Average timestep: %f' %(IVP.sim_time/IVP.iteration))
```

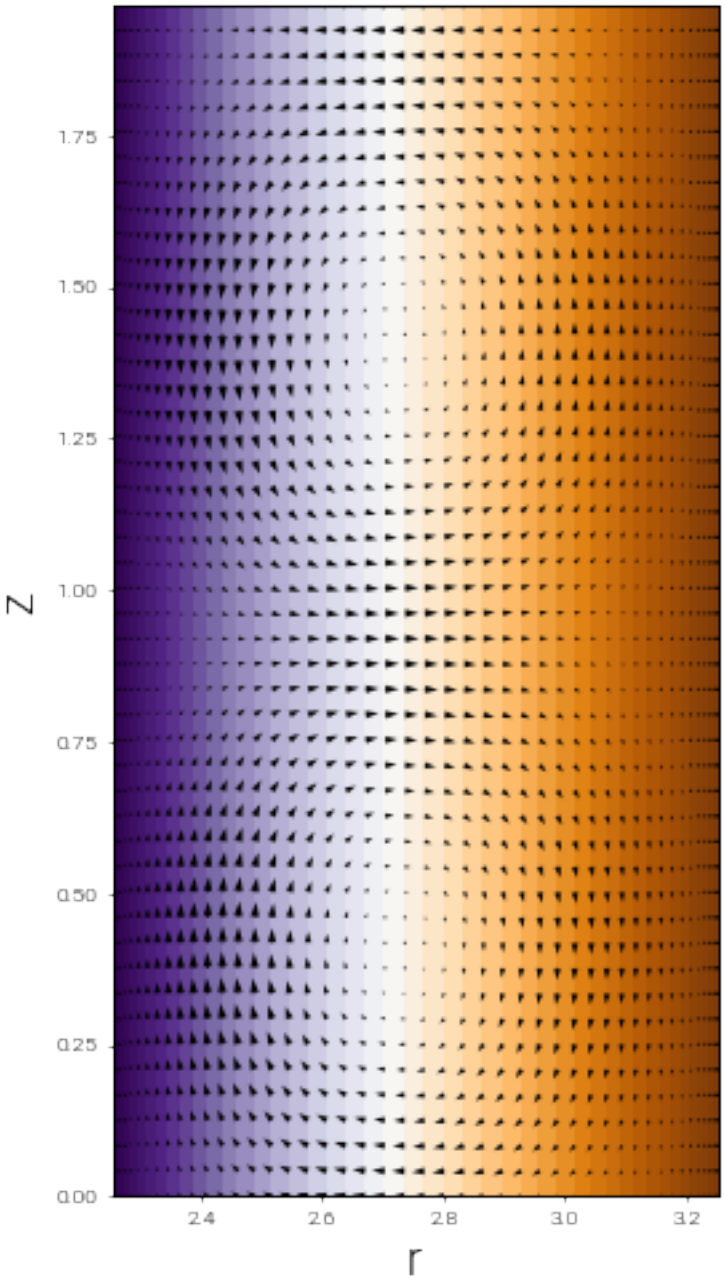
```
2018-10-14 08:57:41,646 __main__ 0/1 INFO :: Iteration: 10, Time: 1.200000e-02, dt: 1.500000e-03
2018-10-14 08:57:42,104 __main__ 0/1 INFO :: Iteration: 20, Time: 3.825000e-02, dt: 3.375000e-03
2018-10-14 08:57:42,564 __main__ 0/1 INFO :: Iteration: 30, Time: 9.731250e-02, dt: 7.593750e-03
2018-10-14 08:57:43,033 __main__ 0/1 INFO :: Iteration: 40, Time: 2.302031e-01, dt: 1.708594e-02
2018-10-14 08:57:43,497 __main__ 0/1 INFO :: Iteration: 50, Time: 5.292070e-01, dt: 3.844336e-02
2018-10-14 08:57:43,970 __main__ 0/1 INFO :: Iteration: 60, Time: 1.201966e+00, dt: 8.649756e-02
2018-10-14 08:57:44,466 __main__ 0/1 INFO :: Iteration: 70, Time: 2.715673e+00, dt: 1.946195e-01
2018-10-14 08:57:44,955 __main__ 0/1 INFO :: Iteration: 80, Time: 6.121514e+00, dt: 4.378939e-01
2018-10-14 08:57:45,478 __main__ 0/1 INFO :: Iteration: 90, Time: 1.378466e+01, dt: 9.852613e-01
2018-10-14 08:57:45,995 __main__ 0/1 INFO :: Iteration: 100, Time: 3.102673e+01, dt: 2.216838e+00
2018-10-14 08:57:46,541 __main__ 0/1 INFO :: Iteration: 110, Time: 6.982139e+01, dt: 4.987885e+00
2018-10-14 08:57:47,206 __main__ 0/1 INFO :: Iteration: 120, Time: 1.571094e+02, dt: 1.122274e+01
2018-10-14 08:57:47,516 solvers 0/1 INFO :: Simulation stop time reached.
2018-10-14 08:57:47,518 __main__ 0/1 INFO :: Total time: 6.484288
2018-10-14 08:57:47,520 __main__ 0/1 INFO :: Iterations: 124
2018-10-14 08:57:47,521 __main__ 0/1 INFO :: Average timestep: 1.764794
```

Analysis

First, let's look at our last time snapshot, plotting the background $v\hat{\theta}$ velocity with arrows representing the meridional flow:

```
In [22]: figsize(12,8)
         pcolormesh((r[0]*ones_like(z)).T,(z*ones_like(r)).T,v['g'].T,cmap='PuOr')
         quiver((r[0]*ones_like(z)).T,(z*ones_like(r)).T,u['g'].T,w['g'].T,width=0.005)
         axis('image')
         xlabel('r', fontsize=18)
         ylabel('z', fontsize=18)
```

```
Out[22]: Text(0,0.5,'z')
```



But we really want some quantitative comparison with the growth rate $\gamma_{analytic}$ from Barenghi (1991). First we construct a small helper function to read our timeseries data, and then we load it out of the self-documented HDF5 file

```
In [23]: def get_timeseries(data, field):
             data_1d = []
             time = data['scales/sim_time'][:]
             data_out = data['tasks/%s'%field][:,0,0]
             return time, data_out
```

```
In [24]: data = h5py.File("scalar_data/scalar_data_s1/scalar_data_s1_p0.h5", "r")
         t, ke = get_timeseries(data, 'total kinetic energy')
         t, kem = get_timeseries(data, 'meridional kinetic energy')
         t, urms = get_timeseries(data, 'u_rms')
         t, wrms = get_timeseries(data, 'w_rms')
```

In order to compare to Barenghi (1991), we scale our results by the Reynolds number, because we have non-dimensionalized slightly differently than he did.

```
In [25]: t_window = (t/period > 2) & (t/period < 14)

         gamma_w, log_w0 = np.polyfit(t[t_window], np.log(wrms[t_window]),1)

         gamma_w_scaled = gamma_w*Re
         gamma_barenghi = 0.430108693
         rel_error_barenghi = (gamma_barenghi - gamma_w_scaled)/gamma_barenghi

         print("gamma_w = %10.8f" % gamma_w_scaled)
         print("relative error = %10.8e" % rel_error_barenghi)
```

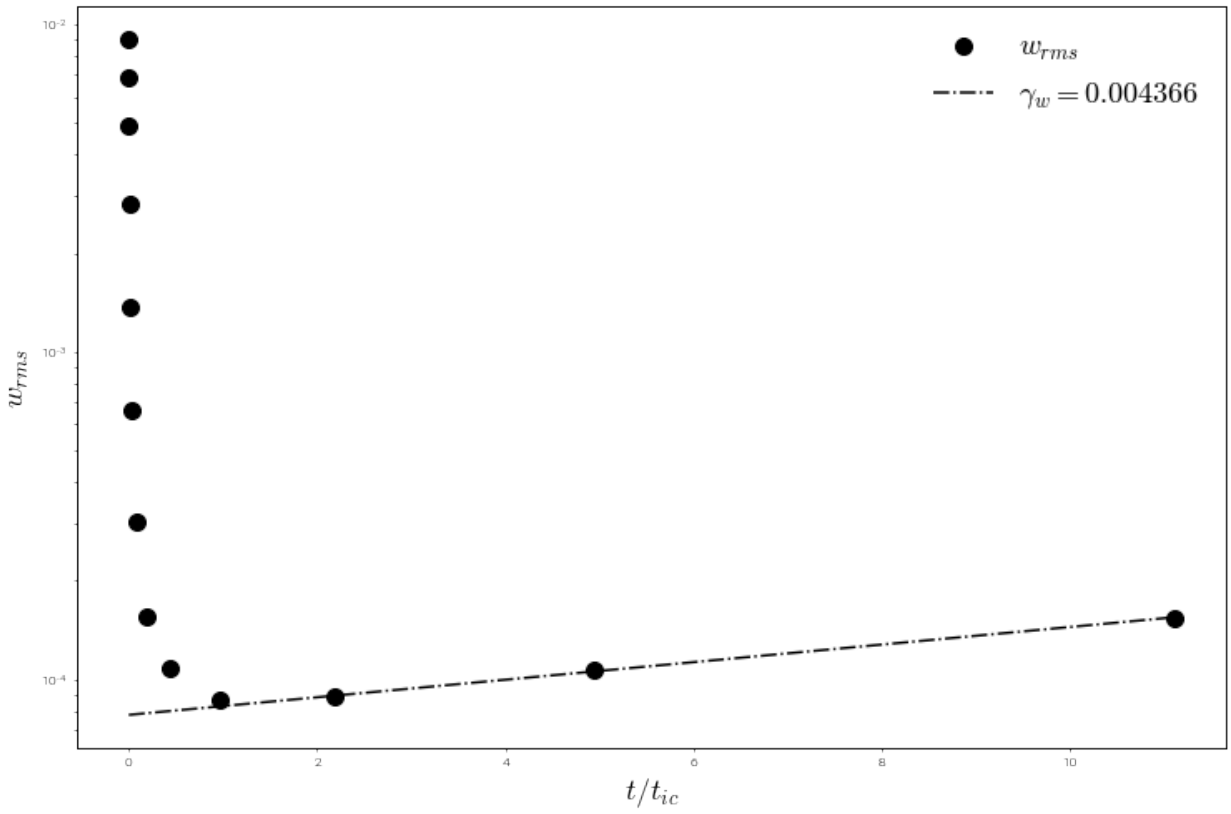
```
gamma_w = 0.34931316
relative error = 1.87849109e-01
```

This looks like a rather high error (order 10% or so), but we know from Barenghi (1991) that the error is dominated by the timestep. Here, we've used a very loose timestep, but if you fix dt (rather than using the CFL calculator), you can get much lower errors at the cost of a longer run.

Finally, we plot the RMS w velocity, and compare it with the fitted exponential solution

```
In [26]: fig = figure()
         ax = fig.add_subplot(111)
         ax.semilogy(t/period, wrms, 'ko', label=r'$w_{rms}$',ms=10)
         ax.semilogy(t/period, np.exp(log_w0)*np.exp(gamma_w*t), 'k-.', label='$\gamma_w = %f$' % gar
         ax.legend(loc='upper right',fontsize=18).draw_frame(False)
         ax.set_xlabel(r"$t/t_{ic}$",fontsize=18)
         ax.set_ylabel(r"$w_{rms}$",fontsize=18)

         fig.savefig('growth_rates.png')
```



In [ ]:

2.2.3 Example Scripts

A wider range of examples are available under the `examples` subdirectory of the main code repository, which you can browse here. These examples cover a wider range of use cases, including larger multidimensional problems designed for parallel execution. Basic post-processing and plotting scripts are also provided with many problems.

These simulation and processing scripts may be useful as a starting point for implementing different problems and equation sets.

2.2.4 Contributions & Suggestions

If you have a script that you'd like to make available as an example, or to request an additional example covering different functionality or use cases, please get in touch on the dev list!

2.3 dedalus

2.3.1 Subpackages

dedalus.core

Submodules

dedalus.core.basis

Abstract and built-in classes for spectral bases.

Module Contents

logger

DEFAULT_LIBRARY

FFTW_RIGOR

class Basis

Base class for spectral bases.

These classes define methods for transforming, differentiating, and integrating corresponding series represented by their spectral coefficients.

Parameters

- **base_grid_size** (*int*) – Number of grid points
- **interval** (*tuple of floats*) – Spatial domain of basis
- **dealias** (*float, optional*) – Fraction of modes to keep after dealiasing (default: 1.)

Variables

- **grid_dtype** (*dtype*) – Grid data type
- **coeff_size** (*int*) – Number of spectral coefficients
- **coeff_embed** (*int*) – Padded number of spectral coefficients for transform
- **coeff_dtype** (*dtype*) – Coefficient data type

library

set_dtype(*self*, *grid_dtype*)
Set transforms based on grid data type.

forward(*self*, *gdata*, *cdata*, *axis*, *meta*)
Grid-to-coefficient transform.

backward(*self*, *cdata*, *gdata*, *axis*, *meta*)
Coefficient-to-grid transform.

differentiate(*self*, *cdata*, *cderiv*, *axis*)
Differentiate using coefficients.

integrate(*self*, *cdata*, *cint*, *axis*)
Integrate over interval using coefficients.

interpolate (*self*, *cdata*, *cint*, *position*, *axis*)
Interpolate in interval using coefficients.

grid_size (*self*, *scale*)
Compute scaled grid size.

check_arrays (*self*, *cdata*, *gdata*, *axis*, *meta=None*)
Verify provided arrays sizes and dtypes are correct. Build compliant arrays if not provided.

class TransverseBasis
Bases: *dedalus.core.basis.Basis*

Base class for bases supporting transverse differentiation.

class ImplicitBasis
Bases: *dedalus.core.basis.Basis*

Base class for bases supporting implicit methods.

These bases define the following matrices encoding the respective linear functions acting on a series represented by its spectral coefficients:

Linear operators (square matrices): Pre : preconditioning (default: identity) Diff : differentiation Mult(p) : multiplication by p-th basis element

Linear functionals (vectors): left_vector : left-endpoint evaluation right_vector : right-endpoint evaluation integ_vector : integration over interval interp_vector : interpolation in interval

Additionally, they define a column vector *bc_vector* indicating which coefficient's Galerkin constraint is to be replaced by the boundary condition on a differential equation (i.e. the order of the tau term).

Multiply (*self*, *p*)
p-element multiplication matrix.

bc_vector (*self*)
Boundary-row column vector.

Precondition (*self*)
Preconditioning matrix.

FilterBoundaryRow (*self*)
Matrix filtering boundary row.

ConstantToBoundary (*self*)
Matrix moving constant coefficient to boundary row.

PrefixBoundary (*self*)
Matrix moving boundary row to first row.

NCC (*self*, *coeffs*, *cutoff*, *max_terms*)
Build NCC multiplication matrix.

class Chebyshev (*name*, *base_grid_size*, *interval=(-1, 1)*, *dealias=1*)
Bases: *dedalus.core.basis.ImplicitBasis*

Chebyshev polynomial basis on the roots grid.

element_label = T

boundary_row

separable = False

coupled = True

default_meta (*self*)

grid(*self*, *scale=1.0*)
Build Chebyshev roots grid.

set_dtype(*self*, *grid_dtype*)
Determine coefficient properties from grid dtype.

Integrate(*self*)
Build integration class.

Interpolate(*self*)
Buld interpolation class.

Differentiate(*self*)
Build differentiation class.

Precondition(*self*)
Preconditioning matrix.

T_n = (U_n - U_(n-2)) / 2 U_(-n) = -U_(n-2)

Dirichlet(*self*)
Dirichlet recombination matrix.

D[0] = T[0] D[1] = T[1] D[n] = T[n] - T[n-2]

<T[i]|D[j]> = <T[i]|T[j]> - <T[i]|T[j-2]> = δ(i,j) - δ(i,j-2)

Multiply(*self*, *p*)
p-element multiplication matrix

T_p * T_n = (T_(n+p) + T_(n-p)) / 2 T_(-n) = T_n

build_mult(*self*, *coeffs*, *order*)

class Fourier(*name*, *base_grid_size*, *interval=(0*, *2 * pi)*, *dealias=1*)
Bases: *dedalus.core.basis.TransverseBasis*

Fourier complex exponential basis.

separable = True

coupled = False

element_label = k

default_meta(*self*)

grid(*self*, *scale=1.0*)
Build evenly spaced Fourier grid.

set_dtype(*self*, *grid_dtype*)
Determine coefficient properties from grid dtype.

Integrate(*self*)
Build integration class.

Interpolate(*self*)
Build interpolation class.

Differentiate(*self*)
Build differentiation class.

HilbertTransform(*self*)
Build Hilbert transform class.

class SinCos(*name*, *base_grid_size*, *interval=(0, pi)*, *dealias=1*)
Bases: *dedalus.core.basis.TransverseBasis*

Sin/Cos series basis.

element_label = k

separable = True

coupled = False

default_meta(*self*)

grid(*self*, *scale=1.0*)
Evenly spaced interior grid: cos(Nx) = 0

set_dtype(*self*, *grid_dtype*)
Determine coefficient properties from grid dtype.

Integrate(*self*)
Build integration class.

Interpolate(*self*)
Build interpolation class.

Differentiate(*self*)
Build differentiation class.

HilbertTransform(*self*)
Build Hilbert transform class.

class Compound(*name*, *subbases*, *dealias=1*)
Bases: *dedalus.core.basis.ImplicitBasis*

Compound basis joining adjascent subbases.

separable = False

coupled = True

library

default_meta(*self*)

grid(*self*, *scale=1.0*)
Build compound grid.

set_dtype(*self*, *grid_dtype*)
Determine coefficient properties from grid dtype.

coeff_start(*self*, *index*)

grid_start(*self*, *index*, *scale*)

sub_gdata(*self*, *gdata*, *index*, *axis*)
Retreive gdata corresponding to one subbasis.

sub_cdata(*self*, *cdata*, *index*, *axis*)
Retrieve cdata corresponding to one subbasis.

forward(*self*, *gdata*, *cdata*, *axis*, *meta*)
Forward transforms.

backward(*self*, *cdata*, *gdata*, *axis*, *meta*)
Backward transforms.

Integrate(*self*)
Build integration class.

Interpolate(*self*)
Buld interpolation class.

Differentiate(*self*)
Build differentiation class.

Precondition(*self*)

Dirichlet(*self*)

Multiply(*self*, *p*, *subindex*)

NCC(*self*, *coeffs*, *cutoff*, *max_terms*)
Build NCC multiplication matrix.

FilterMatchRows(*self*)
Matrix filtering match rows.

Match(*self*)
Matrix matching subbases.

PrefixBoundary(*self*)

dedalus.core.distributor

Classes for available data layouts and the paths between them.

Module Contents

logger

GROUP_TRANSFORMS

TRANSPOSE_LIBRARY

GROUP_TRANSPOSES

SYNC_TRANSPOSES

ALLTOALLV

class Distributor(*domain*, *comm=None*, *mesh=None*)
Directs parallelized distribution and transformation of fields over a domain.

Variables

- **comm** (*MPI communicator*) – Global MPI communicator
- **rank** (*int*) – Internal MPI process number
- **size** (*int*) – Number of MPI processes
- **mesh** (*tuple of ints, optional*) – Process mesh for parallelization (default: 1-D mesh of available processes)
- **comm_cart** (*MPI communicator*) – Cartesian MPI communicator over mesh
- **coords** (*array of ints*) – Coordinates in cartesian communicator (None if outside mesh)

- **layouts** (*list of layout objects*) – Available layouts for domain
- **paths** (*list of path objects*) – Transforms and transposes between layouts

Notes

Computations are parallelized by splitting D-dimensional data fields over an R-dimensional mesh of MPI processes, where R < D. In coefficient space, we take the first R dimensions of the data to be distributed over the mesh, leaving the last (D-R) dimensions local. To transform such a data cube to grid space, we loop backwards over the D dimensions, performing each transform if the corresponding dimension is local, and performing an MPI transpose with the next dimension otherwise. This effectively bubbles the first local dimension up from the (D-R)-th to the first dimension, transforming to grid space along the way. In grid space, then, the first dimensional is local, followed by R dimensions distributed over the mesh, and the last (D-R-1) dimensions local.

The distributor object for a given domain constructs layout objects describing each of the (D+R+1) layouts (sets of transform/distribution states) and the paths between them (D transforms and R transposes).

get_layout_object (*self*, *input*)
Dereference layout identifiers.

buffer_size (*self*, *scales*)
Compute necessary buffer size (bytes) for all layouts.

class Layout (*domain*, *mesh*, *coords*, *local*, *grid_space*, *dtype*)
Object describing the data distribution for a given transform and distribution state.

Variables

- **local** (*array of bools*) – Axis locality flags (True/False for local/distributed)
- **grid_space** (*array of bools*) – Axis grid-space flags (True/False for grid/coeff space)
- **dtype** (*numeric type*) – Data type
- **methods require a tuple of the current transform scales.** (*All*) –

global_shape (*self*, *scales*)
Compute global data shape.

blocks (*self*, *scales*)
Compute block sizes for data distribution.

start (*self*, *scales*)
Compute starting coordinates for local data.

local_shape (*self*, *scales*)
Compute local data shape.

slices (*self*, *scales*)
Compute slices for selecting local portion of global data.

buffer_size (*self*, *scales*)
Compute necessary buffer size (bytes).

class Transform (*layout0*, *layout1*, *axis*, *basis*)
Directs transforms between two layouts.

group_data (*self*, *nfields*, *scales*)

increment_group(*self*, *fields*)

decrement_group(*self*, *fields*)

increment_single(*self*, *field*)
Backward transform.

decrement_single(*self*, *field*)
Forward transform.

increment(*self*, *fields*)
Backward transform.

decrement(*self*, *fields*)
Forward transform.

class Transpose(*layout0*, *layout1*, *axis*, *comm_cart*)
Directs transposes between two layouts.

increment(*self*, *fields*)
Transpose from layout0 to layout1.

decrement(*self*, *fields*)
Transpose from layout1 to layout0.

increment_single(*self*, *field*)
Transpose field from layout0 to layout1.

decrement_single(*self*, *field*)
Transpose field from layout1 to layout0.

increment_group(*self*, **fields*)
Transpose group from layout0 to layout1.

decrement_group(*self*, **fields*)
Transpose group from layout1 to layout0.

dedalus.core.domain

Class for problem domain.

Module Contents

logger

class Domain(*bases*, *grid_dtype=np.complex128*, *comm=None*, *mesh=None*)
Problem domain composed of orthogonal bases.

Parameters

- **bases** (*list of basis objects*) – Bases composing the domain
- **grid_dtype** (*dtype*) – Grid data type
- **mesh** (*tuple of ints, optional*) – Process mesh for parallelization (default: 1-D mesh of available processes)

Variables

- **dim** (*int*) – Dimension of domain, equal to length of bases list
- ***distributor*** (*distributor object*) – Data distribution controller

global_grid_shape(*self*, *scales=None*)

local_grid_shape(*self*, *scales=None*)

get_basis_object(*self*, *basis_like*)
Return basis from a related object.

grids(*self*, *scales=None*)
Return list of local grids along each axis.

grid(*self*, *axis*, *scales=None*)
Return local grid along one axis.

elements(*self*, *axis*)
Return local elements along one axis.

grid_spacing(*self*, *axis*, *scales=None*)
Compute grid spacings along one axis.

new_data(*self*, *type*, ***kw*)

new_field(*self*, ***kw*)

new_fields(*self*, *nfields*, ***kw*)

remedy_scales(*self*, *scales*)

class EmptyDomain(*grid_dtype=np.complex128*)

get_basis_object(*self*, *basis_like*)
Return basis from a related object.

new_data(*self*, *type*, ***kw*)

combine_domains(**domains*)

dedalus.core.evaluator

Class for centralized evaluation of expression trees.

Module Contents

FILEHANDLER_MODE_DEFAULT

FILEHANDLER_PARALLEL_DEFAULT

FILEHANDLER_TOUCH_TMPFILE

logger

class Evaluator(*domain*, *vars*)
Coordinates evaluation of operator trees through various handlers.

Parameters

- **domain** (*domain object*) – Problem domain
- **vars** (*dict*) – Variables for parsing task expression strings

add_dictionary_handler(*self*, ***kw*)
Create a dictionary handler and add to evaluator.

add_system_handler(*self*, ***kw*)
Create a system handler and add to evaluator.

add_file_handler(*self*, *filename*, ***kw*)
Create a file handler and add to evaluator.

add_handler(*self*, *handler*)
Add a handler to evaluator.

evaluate_group(*self*, *group*, ***kw*)
Evaluate all handlers in a group.

evaluate_scheduled(*self*, *wall_time*, *sim_time*, *iteration*, ***kw*)
Evaluate all scheduled handlers.

evaluate_handlers(*self*, *handlers*, *id=None*, ***kw*)
Evaluate a collection of handlers.

require_coeff_space(*self*, *fields*)
Move all fields to coefficient layout.

static get_fields(*tasks*)
Get field set for a collection of tasks.

static attempt_tasks(*tasks*, ***kw*)
Attempt tasks and return the unfinished ones.

class Handler(*domain*, *vars*, *group=None*, *wall_dt=np.inf*, *sim_dt=np.inf*, *iter=np.inf*)
Group of tasks with associated scheduling data.

Parameters

- **domain** (*domain object*) – Problem domain
- **vars** (*dict*) – Variables for parsing task expression strings
- **group** (*str, optional*) – Group name for forcing selected handelrs (default: None)
- **wall_dt** (*float, optional*) – Wall time cadence for evaluating tasks (default: infinite)
- **sim_dt** (*float, optional*) – Simulation time cadence for evaluating tasks (default: infinite)
- **iter** (*int, optional*) – Iteration cadence for evaluating tasks (default: infinite)

add_task(*self*, *task*, *layout='g'*, *name=None*, *scales=None*)
Add task to handler.

add_tasks(*self*, *tasks*, ***kw*)
Add multiple tasks.

add_system(*self*, *system*, ***kw*)
Add fields from a FieldSystem.

class DictionaryHandler(**args*, ***kw*)
Bases: *dedalus.core.evaluator.Handler*

Handler that stores outputs in a dictionary.

process(*self*, ***kw*)
Reference fields from dictionary.

class SystemHandler
Bases: *dedalus.core.evaluator.Handler*

Handler that sets fields in a FieldSystem.

build_system(*self*)
Build FieldSystem and set task outputs.

process(*self*, ***kw*)
Gather fields into system.

class FileHandler(*base_path*, **args*, *max_writes=np.inf*, *max_size=2**30*, *parallel=None*, *mode=None*, ***kw*)
Bases: *dedalus.core.evaluator.Handler*

Handler that writes tasks to an HDF5 file.

Parameters

- **base_path** (*str*) – Base path for analyis output folder
- **max_writes** (*int, optional*) – Maximum number of writes per set (default: infinite)
- **max_size** (*int, optional*) – Maximum file size to write to, in bytes (default: 2**30 = 1 GB). (Note: files may be larger after final write.)
- **parallel** (*bool, optional*) – Perform parallel writes from each process to single file (True), or separately write to individual process files (False). Default behavior set by config option.
- **mode** (*str, optional*) – 'overwrite' to delete any present analysis output with the same base path. 'append' to begin with set number incremented past any present analysis output. Default behavior set by config option.

current_path

check_file_limits(*self*)
Check if write or size limits have been reached.

get_file(*self*)
Return current HDF5 file, creating if necessary.

create_current_file(*self*)
Generate new HDF5 file in current_path.

setup_file(*self*, *file*)

process(*self*, *world_time*, *wall_time*, *sim_time*, *timestep*, *iteration*, ***kw*)
Save task outputs to HDF5 file.

get_write_stats(*self*, *layout*, *scales*, *constant*, *index*)
Determine write parameters for nonconstant subspace of a field.

get_hdf5_spaces(*self*, *layout*, *scales*, *constant*, *index*)
Create HDF5 space objects for writing nonconstant subspace of a field.

dedalus.core.field

Class for data fields.

Module Contents

logger

permc_spec

use_umfpack

class Operand

static parse(*string*, *namespace*, *domain*)
Build operand from a string expression.

static cast(*x*, *domain=None*)

static raw_cast(*x*)

class Data
Bases: *dedalus.core.field.Operand*

set_scales(*self*, *scales*, *keep_data=True*)
Set new transform scales.

atoms(*self*, **types*, ***kw*)

has(*self*, **atoms*)

expand(*self*, **vars*)
Return self.

canonical_linear_form(*self*, **vars*)
Return self.

split(*self*, **vars*)

replace(*self*, *old*, *new*)
Replace an object in the expression tree.

order(*self*, **ops*)

operator_dict(*self*, *index*, *vars*, ***kw*)

sym_diff(*self*, *var*)
Symbolically differentiate with respect to var.

class Scalar(*value=0*, *name=None*, *domain=None*)
Bases: *dedalus.core.field.Data*

class ScalarMeta(*scalar=None*)
Shortcut class to return scalar metadata for any axis.

as_ncc_operator(*self*, ***kw*)
Return self.value.

class Array(*domain*, *name=None*)
Bases: *dedalus.core.field.Data*

from_global_vector(*self*, *data*, *axis*)

from_local_vector(*self*, *data*, *axis*)

as_ncc_operator(*self*, *cacheid=None*, ***kw*)
Cast to field and convert to NCC operator.

class Field(*domain*, *name=None*, *scales=None*)
Bases: *dedalus.core.field.Data*

Scalar field over a domain.

Parameters

- **domain** (*domain object*) – Problem domain
- **name** (*str, optional*) – Field name (default: Python object id)

Variables

- **layout** (*layout object*) – Current layout of field
- **data** (*ndarray*) – View of internal buffer in current layout

layout

create_buffer(*self*, *scales*)
Create buffer for Field data.

set_scales(*self*, *scales*, *keep_data=True*)
Set new transform scales.

require_layout(*self*, *layout*)
Change to specified layout.

towards_grid_space(*self*)
Change to next layout towards grid space.

towards_coeff_space(*self*)
Change to next layout towards coefficient space.

require_grid_space(*self*, *axis=None*)
Require one axis (default: all axes) to be in grid space.

require_coeff_space(*self*, *axis=None*)
Require one axis (default: all axes) to be in coefficient space.

require_local(*self*, *axis*)
Require an axis to be local.

differentiate(*self*, **args*, ***kw*)
Differentiate field.

integrate(*self*, **args*, ***kw*)
Integrate field.

interpolate(*self*, **args*, ***kw*)
Interpolate field.

antidifferentiate(*self*, *basis*, *bc*, *out=None*)
Antidifferentiate field by setting up a simple linear BVP.

Parameters

- **basis** (*basis-like*) – Basis to antidifferentiate along
- **bc** (*(str, object) tuple*) – Boundary conditions as (functional, value) tuple. *functional* is a string, e.g. “left”, “right”, “int” *value* is a field or scalar
- **out** (*field, optional*) – Output field

static cast(*input*, *domain*)

as_ncc_operator(*self*, *cutoff*, *max_terms*, *name=None*, *cacheid=None*)
Convert to operator form representing multiplication as a NCC.

dedalus.core.future

Classes for future evaluation.

Module Contents

logger

PREALLOCATE_OUTPUTS

class Future(**args*, *domain=None*, *out=None*)
Bases: *dedalus.core.field.Operand*

Base class for deferred operations on data.

Parameters

- ***args** (*Operands*) – Operands. Number must match class attribute *arity*, if present.
- **out** (*data, optional*) – Output data object. If not specified, a new object will be used.

Notes

Operators are stacked (i.e. provided as arguments to other operators) to construct trees that represent compound expressions. Nodes are evaluated by first recursively evaluating their subtrees, and then calling the *operate* method.

arity

store_last = False

reset(*self*)
Restore original arguments.

atoms(*self*, **types*, *include_out=False*)

has(*self*, **atoms*)

replace(*self*, *old*, *new*)
Replace an object in the expression tree.

evaluate(*self*, *id=None*, *force=True*)
Recursively evaluate operation.

attempt(*self*, *id=None*)
Recursively attempt to evaluate operation.

meta(*self*)

meta_scale(*self*, *axis*)

meta_dirichlet(*self*, *axis*)

check_conditions(*self*)
Check that all argument fields are in proper layouts.

operate(*self*, *out*)
Perform operation.

as_ncc_operator(*self*, *cacheid=None*, ***kw*)

class FutureScalar
Bases: *dedalus.core.future.Future*

Class for deferred operations producing a Scalar.

future_type

meta

class FutureArray
Bases:*dedalus.core.future.Future*

Class for deferred operations producing an Array.

future_type

class FutureField
Bases:*dedalus.core.future.Future*

Class for deferred operations producing a Field.

future_type

static parse(*string*, *namespace*, *domain*)
Build FutureField from a string expression.

static cast(*input*, *domain*)
Cast an object to a FutureField.

unique_domain(**args*)
Return unique domain from a set of fields.

dedalus.core.metadata

Module Contents

class AliasDict(**args*, ***kw*)
Bases:collections.OrderedDict

class MultiDict
Bases:*dedalus.core.metadata.AliasDict*

class DictGroup(**dicts*)

class Metadata(*domain*)
Bases:*dedalus.core.metadata.MultiDict*

dedalus.core.operators

Abstract and built-in classes defining deferred operations on fields.

Module Contents

parseables

parseable(*op*)

addname(*name*)

is_integer(*x*)

class Operator
Bases:*dedalus.core.future.Future*

base

order(*self*, **ops*)

class FieldCopy(*arg*, ***kw*)
Bases:*dedalus.core.operators.Operator*, *dedalus.core.future.FutureField*

Operator making a new field copy of data.

name = FieldCopy

base

check_conditions(*self*)

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

sym_diff(*self*, *var*)
Symbolically differentiate with respect to var.

split(*self*, **vars*)

class FieldCopyScalar
Bases:*dedalus.core.operators.FieldCopy*

argtypes

operate(*self*, *out*)

class FieldCopyArray
Bases:*dedalus.core.operators.FieldCopy*

argtypes

operate(*self*, *out*)

class FieldCopyField
Bases:*dedalus.core.operators.FieldCopy*

argtypes

operate(*self*, *out*)

class NonlinearOperator
Bases:*dedalus.core.operators.Operator*

expand(*self*, **vars*)
Return self.

canonical_linear_form(*self*, **vars*)
Raise if arguments contain specified variables (default: None)

split(*self*, **vars*)

class GeneralFunction(*domain*, *layout*, *func*, *args=[]*, *kw={}*, *out=None*)
Bases:*dedalus.core.operators.NonlinearOperator*, *dedalus.core.future.FutureField*

Operator wrapping a general python function.

Parameters

- **domain** (*domain object*) – Domain
- **layout** (*layout object or identifier*) – Layout of function output
- **func** (*function*) – Function producing field data
- **args** (*list*) – Arguments to pass to func

- **kw** (*dict*) – Keywords to pass to func
- **out** (*field, optional*) – Output field (default: new field)

Notes

On evaluation, this wrapper evaluates the provided function with the given arguments and keywords, and takes the output to be data in the specified layout, i.e.

out[layout] = func(*args, **kw)

meta_constant (*self*, *axis*)

check_conditions (*self*)

operate (*self*, *out*)

class UnaryGridFunction (*func*, *arg*, ***kw*)

Bases: *dedalus.core.operators.NonlinearOperator*, *dedalus.core.future.Future*

arity = 1

supported

aliased

base

meta_constant (*self*, *axis*)

meta_parity (*self*, *axis*)

sym_diff (*self*, *var*)

Symbolically differentiate with respect to var.

class UnaryGridFunctionScalar

Bases: *dedalus.core.operators.UnaryGridFunction*, *dedalus.core.future.FutureScalar*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class UnaryGridFunctionArray

Bases: *dedalus.core.operators.UnaryGridFunction*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class UnaryGridFunctionField

Bases: *dedalus.core.operators.UnaryGridFunction*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class Arithmetic
Bases: *dedalus.core.future.Future*

arity = 2

order(*self*, **ops*)

class Add
Bases: *dedalus.core.operators.Arithmetic*

name = Add

str_op = +

base

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

expand(*self*, **vars*)
Expand arguments containing specified variables (default: all).

canonical_linear_form(*self*, **vars*)
Ensure arguments have same dependency on specified variables.

split(*self*, **vars*)

operator_dict(*self*, *index*, *vars*, ***kw*)
Produce matrix-operator dictionary over specified variables.

sym_diff(*self*, *var*)
Symbolically differentiate with respect to var.

class AddScalarScalar
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureScalar*

argtypes

check_conditions(*self*)

operate(*self*, *out*)

class AddArrayArray
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureArray*

argtypes

check_conditions(*self*)

operate(*self*, *out*)

class AddFieldField
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureField*

argtypes

check_conditions(*self*)

operate(*self*, *out*)

class AddScalarArray
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureArray*

argtypes

check_conditions(*self*)

operate (*self*, *out*)

class AddArrayScalar
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class AddScalarField
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class AddFieldScalar
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class AddArrayField
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class AddFieldArray
Bases: *dedalus.core.operators.Add*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class Multiply
Bases: *dedalus.core.operators.Arithmetic*

name = Mul

str_op = *

base

meta_constant (*self*, *axis*)

meta_parity (*self*, *axis*)

expand (*self*, **vars*)
Distribute over sums containing specified variables (default: all).

canonical_linear_form (*self*, **vars*)
Eliminate nonlinear multiplications and float specified variables right.

split (*self*, **vars*)

operator_dict (*self*, *index*, *vars*, ***kw*)
Produce matrix-operator dictionary over specified variables.

sym_diff (*self*, *var*)
Symbolically differentiate with respect to var.

class MultiplyScalarScalar
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureScalar*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyArrayArray
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyFieldField
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyScalarArray
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyArrayScalar
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyScalarField
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyFieldScalar
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyArrayField
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class MultiplyFieldArray
Bases: *dedalus.core.operators.Multiply*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class Power
Bases: *dedalus.core.operators.NonlinearOperator*, *dedalus.core.operators.Arithmetic*

name = Pow

str_op = **

base

class PowerDataScalar
Bases: *dedalus.core.operators.Power*

argtypes

meta_constant (*self*, *axis*)

meta_parity (*self*, *axis*)

sym_diff (*self*, *var*)
Symbolically differentiate with respect to var.

class PowerScalarScalar
Bases: *dedalus.core.operators.PowerDataScalar*, *dedalus.core.future.FutureScalar*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class PowerArrayScalar
Bases: *dedalus.core.operators.PowerDataScalar*, *dedalus.core.future.FutureArray*

argtypes

check_conditions (*self*)

operate (*self*, *out*)

class PowerFieldScalar
Bases: *dedalus.core.operators.PowerDataScalar*, *dedalus.core.future.FutureField*

argtypes

check_conditions (*self*)

operate(*self*, *out*)

class LinearOperator

Bases: *dedalus.core.operators.Operator*

kw

expand(*self*, **vars*)

Distribute over sums containing specified variables (default: all).

canonical_linear_form(*self*, **vars*)

Change argument to canonical linear form.

split(*self*, **vars*)

operator_dict(*self*, *index*, *vars*, ***kw*)

Produce matrix-operator dictionary over specified variables.

operator_form(*self*, *index*)

sym_diff(*self*, *var*)

Symbolically differentiate with respect to var.

class TimeDerivative

Bases: *dedalus.core.operators.LinearOperator*, *dedalus.core.future.FutureField*

name = dt

base

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

operator_form(*self*, *index*)

operate(*self*, *out*)

class Separable

Bases: *dedalus.core.operators.LinearOperator*, *dedalus.core.future.FutureField*

operator_form(*self*, *index*)

check_conditions(*self*)

operate(*self*, *out*)

apply_vector_form(*self*, *out*)

explicit_form(*self*, *input*, *output*, *axis*)

vector_form(*self*)

class Coupled

Bases: *dedalus.core.operators.LinearOperator*, *dedalus.core.future.FutureField*

operator_form(*self*, *index*)

check_conditions(*self*)

operate(*self*, *out*)

apply_matrix_form(*self*, *out*)

explicit_form(*self*, *input*, *output*, *axis*)

matrix_form(*self*)

operator_dict(*self*, *index*, *vars*, ***kw*)
Produce matrix-operator dictionary over specified variables.

class Integrate(*arg0*, ***kw*)
Bases:*dedalus.core.operators.LinearOperator*

name = integ

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

integrate(*arg0*, **bases*, *out=None*)

class Interpolate(*arg0*, *position*, *out=None*)
Bases:*dedalus.core.operators.LinearOperator*

name = interp

distribute(*self*)

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

interpolate(*arg0*, *out=None*, ***basis_kw*)

left(*arg0*, *out=None*)
Shortcut for left interpolation along last axis.

right(*arg0*, *out=None*)
Shortcut for right interpolation along last axis.

class Differentiate(*arg0*, ***kw*)
Bases:*dedalus.core.operators.LinearOperator*

name = d

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

expand(*self*, **vars*)
Distribute over sums and apply the product rule to arguments containing specified variables (default: all).

differentiate(*arg0*, **bases*, *out=None*, ***basis_kw*)

class HilbertTransform(*arg0*, ***kw*)
Bases:*dedalus.core.operators.LinearOperator*

name = Hilbert

meta_constant(*self*, *axis*)

meta_parity(*self*, *axis*)

hilberttransform(*arg0*, **bases*, *out=None*, ***basis_kw*)

dedalus.core.pencil

Classes for manipulating pencils.

Module Contents

logger

build_pencils(*domain*)
Create the set of pencils over a domain.

Parameters **domain** (*domain object*) – Problem domain

Returns **pencils** – Pencil objects

Return type list

build_matrices(*pencils*, *problem*, *matrices*)
Build pencil matrices.

class Pencil(*domain*, *local_index*, *global_index*)
Object holding problem matrices for a given transverse wavevector.

Parameters **index** (*tuple of ints*) – Transverse indeces for retrieving pencil from system data

dedalus.core.problems

Classes for representing systems of equations.

Module Contents

logger

class Namespace
Bases:collections.OrderedDict

Class ensuring a conflict-free namespace for parsing.

copy(*self*)
Copy entire namespace.

add_substitutions(*self*, *substitutions*)
Parse substitutions in current namespace before adding to self.

class ProblemBase(*domain*, *variables*, *ncc_cutoff=1e-10*, *max_ncc_terms=None*, *entry_cutoff=0*)
Base class for problems consisting of a system of PDEs, constraints, and boundary conditions.

Parameters

- **domain** (*domain object*) – Problem domain
- **variables** (*list of str*) – List of variable names, e.g. [‘u’, ‘v’, ‘w’]
- **ncc_cutoff** (*float, optional*) – Mode amplitude cutoff for LHS NCC expansions (default: 1e-10)
- **max_ncc_terms** (*int, optional*) – Maximum terms to include in LHS NCC expansions (default: None (no limit))

Variables

- **parameters** (*OrderedDict*) – External parameters used in the equations, and held constant during integration.
- **substitutions** (*OrderedDict*) – String-substitutions to be used in parsing.

Notes

Equations are entered as strings of the form "LHS = RHS", where the left-hand side contains terms that are linear in the dependent variables (and will be parsed into a sparse matrix system), and the right-hand side contains terms that are non-linear (and will be parsed into operator trees).

The specified axes (from domain), variables, parameters, and substitutions are recognized by the parser, along with the built-in operators, which include spatial derivatives (of the form "dx()" for an axis named "x") and basic mathematical operators (trigonometric and logarithmic).

The LHS terms must be linear in the specified variables and first-order in coupled derivatives.

add_equation (*self*, *equation*, *condition='True'*)
Add equation to problem.

add_bc (*self*, *equation*, *condition='True'*)
Add boundary condition to problem.

namespace (*self*)
Build namespace for problem parsing.

build_solver (*self*, **args*, ***kw*)
Build corresponding solver class.

class InitialValueProblem (*domain*, *variables*, *time='t'*, ***kw*)
Bases: *dedalus.core.problems.ProblemBase*

Class for non-linear initial value problems.

Parameters

- **domain** (*domain object*) – Problem domain
- **variables** (*list of str*) – List of variable names, e.g. ['u', 'v', 'w']
- **time** (*str, optional*) – Time label, default: 't'

Notes

This class supports non-linear initial value problems. The LHS terms must be linear in the specified variables, first-order in coupled derivatives, first-order in time derivatives, and contain no explicit time dependence.

M.dt(X) + L.X = F(X, t)

solver_class

namespace_additions (*self*)
Build namespace for problem parsing.

class LinearBoundaryValueProblem
Bases: *dedalus.core.problems.ProblemBase*

Class for inhomogeneous, linear boundary value problems.

Parameters

- **domain** (*domain object*) – Problem domain
- **variables** (*list of str*) – List of variable names, e.g. ['u', 'v', 'w']

Notes

This class supports inhomogeneous, linear boundary value problems. The LHS terms must be linear in the specified variables and first-order in coupled derivatives, and the RHS must be independent of the specified variables.

L.X = F

solver_class

namespace_additions(*self*)

class NonlinearBoundaryValueProblem

Bases: *dedalus.core.problems.ProblemBase*

Class for nonlinear boundary value problems.

Parameters

- **domain** (*domain object*) – Problem domain
- **variables** (*list of str*) – List of variable names, e.g. [‘u’, ‘v’, ‘w’]

Notes

This class supports nonlinear boundary value problems. The LHS terms must be linear in the specified variables and first-order in coupled derivatives.

L.X = F(X)

The problem is reduced into a linear BVP for an update to the solution using the Newton-Kantorovich method and symbolically-computed Frechet derivatives of the RHS.

L.(X0 + X1) = F(X0) + dF(X0).X1 L.X1 - dF(X0).X1 = F(X0) - L.X0

solver_class

namespace_additions(*self*)

Build namespace for problem parsing.

class EigenvalueProblem(*domain*, *variables*, *eigenvalue*, *tolerance=1e-10*, ***kw*)

Bases: *dedalus.core.problems.ProblemBase*

Class for linear eigenvalue problems.

Parameters

- **domain** (*domain object*) – Problem domain
- **variables** (*list of str*) – List of variable names, e.g. [‘u’, ‘v’, ‘w’]
- **eigenvalue** (*str*) – Eigenvalue label, e.g. ‘sigma’ WARNING: ‘lambda’ is a python reserved word. You *cannot* use it as your eigenvalue. Also, note that unicode symbols don’t work on all machines.
- **tolerance** (*float*) – A floating point number (>= 0) which helps ‘define’ zero for the RHS of the equation. If the RHS has nonzero NCCs which add to zero, dedalus will check to make sure that the max of the expression on the RHS normalized by the max of all NCCs going in that expression is smaller than this tolerance (see ProblemBase._check_if_zero())

Notes

This class supports linear eigenvalue problems. The LHS terms must be linear in the specified variables, first-order in coupled derivatives, and linear or independent of the specified eigenvalue. The RHS must be zero.

σM.X + L.X = 0

solver_class

namespace_additions(*self*)
Build namespace for problem parsing.

IVP

LBVP

NLBVP

EVP

dedalus.core.solvers

Classes for solving differential equations.

Module Contents

PERMC_SPEC

USE_UMFPACK

logger

class EigenvalueSolver(*problem*)
Solves linear eigenvalue problems for oscillation frequency omega, (d_t -> -i omega) for a given pencil, and stores the eigenvalues and eigenvectors. The set_state method can be used to set solver.state to the specified eigenmode.

Parameters **problem** (*problem object*) – Problem describing system of differential equations and constraints

Variables

- **state** (*system object*) – System containing solution fields (after solve method is called)
- **eigenvalues** (*numpy array*) – Contains a list of eigenvalues omega
- **eigenvectors** (*numpy array*) – Contains a list of eigenvectors. The eigenvector corresponding to the ith eigenvalue is in eigenvectors[:,i]
- **eigenvalue_pencil** (*pencil*) – The pencil for which the eigenvalue problem has been solved.

solve_dense(*self*, *pencil*, *rebuild_coeffs=False*, ***kw*)
Solve EVP for selected pencil.

Parameters

- **pencil** (*pencil object*) – Pencil for which to solve the EVP
- **rebuild_coeffs** (*bool, optional*) – Flag to rebuild cached coefficient matrices (default: False)

- **Other keyword options passed to scipy.linalg.eig.**

solve_sparse(*self*, *pencil*, *N*, *target*, *rebuild_coeffs=False*, ***kw*)
Perform targeted sparse eigenvalue search for selected pencil.

Parameters

- **pencil** (*pencil object*) – Pencil for which to solve the EVP
- **N** (*int*) – Number of eigenmodes to solver for. Note: the dense method may be more efficient for finding large numbers of eigenmodes.
- **target** (*complex*) – Target eigenvalue for search.
- **rebuild_coeffs** (*bool, optional*) – Flag to rebuild cached coefficient matrices (default: False)
- **Other keyword options passed to scipy.sparse.linalg.eigs.**

set_state(*self*, *index*)
Set state vector to the specified eigenmode.

Parameters **index** (*int*) – Index of desired eigenmode

solve(*self*, **args*, ***kw*)
Deprecated. Use solve_dense instead.

class LinearBoundaryValueSolver(*problem*)
Linear boundary value problem solver.

Parameters **problem** (*problem object*) – Problem describing system of differential equations and constraints

Variables **state** (*system object*) – System containing solution fields (after solve method is called)

solve(*self*, *rebuild_coeffs=False*)
Solve BVP.

class NonlinearBoundaryValueSolver(*problem*)
Nonlinear boundary value problem solver.

Parameters **problem** (*problem object*) – Problem describing system of differential equations and constraints

Variables **state** (*system object*) – System containing solution fields (after solve method is called)

newton_iteration(*self*, *damping=1*)
Update solution with a Newton iteration.

class InitialValueSolver(*problem*, *timestepper*)
Initial value problem solver.

Parameters

- **problem** (*problem object*) – Problem describing system of differential equations and constraints
- **timestepper** (*timestepper class*) – Timestepper to use in evolving initial conditions

Variables

- **state** (*system object*) – System containing current solution fields
- **dt** (*float*) – Timestep

- **stop_sim_time** (*float*) – Simulation stop time, in simulation units
- **stop_wall_time** (*float*) – Wall stop time, in seconds from instantiation
- **stop_iteration** (*int*) – Stop iteration
- **time** (*float*) – Current simulation time
- **iteration** (*int*) – Current iteration

sim_time

ok
Check that current time and iteration pass stop conditions.

get_world_time(*self*)

load_state(*self*, *path*, *index=-1*)
Load state from HDF5 file.

Parameters

- **path** (*str or pathlib.Path*) – Path to Dedalus HDF5 savefile
- **index** (*int, optional*) – Local write index (within file) to load (default: -1)

Returns

- **write** (*int*) – Global write number of loaded write
- **dt** (*float*) – Timestep at loaded write

sim_dt_cadences(*self*)
Build array of finite handler sim_dt cadences.

step(*self*, *dt*, *trim=False*)
Advance system by one iteration/timestep.

evolve(*self*, *timestep_function*)
Advance system until stopping criterion is reached.

evaluate_handlers_now(*self*, *dt*, *handlers=None*)
Evaluate all handlers right now. Useful for writing final outputs.

by default, all handlers are evaluated; if a list is given only those will be evaluated.

dedalus.core.system

Classes for systems of coefficients/fields.

Module Contents

class CoeffSystem(*nfields*, *domain*)
Representation of a collection of fields that don't need to be transformed, and are therefore stored as a contigous set of coefficient data for efficient pencil and group manipulation.

Parameters

- **nfields** (*int*) – Number of fields to represent
- **domain** (*domain object*) – Problem domain

Variables **data** (*ndarray*) – Contiguous buffer for field coefficients

get_pencil (*self*, *pencil*)
Return pencil view from system buffer.

set_pencil (*self*, *pencil*, *data*)
Set pencil data in system buffer.

class FieldSystem (*field_names*, *domain*)
Bases: *dedalus.core.system.CoeffSystem*

Collection of fields alongside a CoeffSystem buffer for efficient pencil and group manipulation.

Parameters

- **field_names** (*list of strings*) – Names of fields to build
- **domain** (*domain object*) – Problem domain

Variables

- **data** (*ndarray*) – Contiguous buffer for field coefficients
- **fields** (*list*) – Field objects
- **nfields** (*int*) – Number of fields in system
- **field_dict** (*dict*) – Dictionary of fields

classmethod from_fields (*cls*, *fields*)

gather (*self*)
Copy fields into system buffer.

scatter (*self*)
Extract fields from system buffer.

dedalus.core.timesteppers

ODE solvers for timestepping.

Module Contents

STORE_LU

PERMC_SPEC

USE_UMFPACK

class MultistepIMEX (*nfields*, *domain*)
Base class for implicit-explicit multistep methods.

Parameters

- **nfields** (*int*) – Number of fields in problem
- **domain** (*domain object*) – Problem domain

Notes

These timesteppers discretize the system M.dt(X) + L.X = F

into the general form aj M.X(n-j) + bj L.X(n-j) = cj F(n-j)

where j runs from {0, 0, 1} to {amax, bmax, cmax}.

The system is then solved as (a0 M + b0 L).X(n) = cj F(n-j) - aj M.X(n-j) - bj L.X(n-j)

where j runs from {1, 1, 1} to {cmax, amax, bmax}.

References

4. Wang and S. J. Ruuth, Journal of Computational Mathematics 26, (2008).*

- **Our coefficients are related to those used by Wang as:** amax = bmax = cmax = s aj = α(s-j) / k(n+s-1) bj = γ(s-j) cj = β(s-j)

step (*self*, *solver*, *dt*)
Advance solver by one timestep.

class CNAB1
Bases: *dedalus.core.timesteppers.MultistepIMEX*

1st-order Crank-Nicolson Adams-Bashforth scheme [Wang 2008 eqn 2.5.3]

Implicit: 2nd-order Crank-Nicolson Explicit: 1st-order Adams-Bashforth (forward Euler)

amax = 1

bmax = 1

cmax = 1

classmethod compute_coefficients (*self*, *timesteps*, *iteration*)

class SBDF1
Bases: *dedalus.core.timesteppers.MultistepIMEX*

1st-order semi-implicit BDF scheme [Wang 2008 eqn 2.6]

Implicit: 1st-order BDF (backward Euler) Explicit: 1st-order extrapolation (forward Euler)

amax = 1

bmax = 1

cmax = 1

classmethod compute_coefficients (*self*, *timesteps*, *iteration*)

class CNAB2
Bases: *dedalus.core.timesteppers.MultistepIMEX*

2nd-order Crank-Nicolson Adams-Bashforth scheme [Wang 2008 eqn 2.9]

Implicit: 2nd-order Crank-Nicolson Explicit: 2nd-order Adams-Bashforth

amax = 2

bmax = 2

cmax = 2

classmethod compute_coefficients (*self*, *timesteps*, *iteration*)

class MCNAB2
Bases: *dedalus.core.timesteppers.MultistepIMEX*

2nd-order modified Crank-Nicolson Adams-Bashforth scheme [Wang 2008 eqn 2.10]

Implicit: 2nd-order modified Crank-Nicolson Explicit: 2nd-order Adams-Bashforth

amax = 2

bmax = 2

cmax = 2

classmethod compute_coefficients(*self*, *timesteps*, *iteration*)

class SBDF2

Bases:*dedalus.core.timesteppers.MultistepIMEX*

2nd-order semi-implicit BDF scheme [Wang 2008 eqn 2.8]

Implicit: 2nd-order BDF Explicit: 2nd-order extrapolation

amax = 2

bmax = 2

cmax = 2

classmethod compute_coefficients(*self*, *timesteps*, *iteration*)

class CNLF2

Bases:*dedalus.core.timesteppers.MultistepIMEX*

2nd-order Crank-Nicolson leap-frog scheme [Wang 2008 eqn 2.11]

Implicit: ?-order wide Crank-Nicolson Explicit: 2nd-order leap-frog

amax = 2

bmax = 2

cmax = 2

classmethod compute_coefficients(*self*, *timesteps*, *iteration*)

class SBDF3

Bases:*dedalus.core.timesteppers.MultistepIMEX*

3rd-order semi-implicit BDF scheme [Wang 2008 eqn 2.14]

Implicit: 3rd-order BDF Explicit: 3rd-order extrapolation

amax = 3

bmax = 3

cmax = 3

classmethod compute_coefficients(*self*, *timesteps*, *iteration*)

class SBDF4

Bases:*dedalus.core.timesteppers.MultistepIMEX*

4th-order semi-implicit BDF scheme [Wang 2008 eqn 2.15]

Implicit: 4th-order BDF Explicit: 4th-order extrapolation

amax = 4

bmax = 4

cmax = 4

classmethod compute_coefficients(*self*, *timesteps*, *iteration*)

class RungeKuttaIMEX (*nfields*, *domain*)
Base class for implicit-explicit multistep methods.

Parameters

- **nfields** (*int*) – Number of fields in problem
- **domain** (*domain object*) – Problem domain

Notes

These timesteppers discretize the system M.dt(X) + L.X = F

by constructing s stages M.X(n,i) - M.X(n,0) + k Hij L.X(n,j) = k Aij F(n,j)

where j runs from {0, 0} to {i, i-1}, and F(n,i) is evaluated at time t(n,i) = t(n,0) + k ci

The s stages are solved as (M + k Hii L).X(n,i) = M.X(n,0) + k Aij F(n,j) - k Hij L.X(n,j)

where j runs from {0, 0} to {i-1, i-1}.

The final stage is used as the advanced solution*: X(n+1,0) = X(n,s) t(n+1,0) = t(n,s) = t(n,0) + k

- **Equivalently the Butcher tableaus must follow** b_im = H[s, :] b_ex = A[s, :] c[s] = 1

References

21. (m) Ascher, S. J. Ruuth, and R. J. Spiteri, Applied Numerical Mathematics (1997).

step (*self*, *solver*, *dt*)
Advance solver by one timestep.

class RK111
Bases: *dedalus.core.timesteppers.RungeKuttaIMEX*

1st-order 1-stage DIRK+ERK scheme [Ascher 1997 sec 2.1]

stages = 1

c

A

H

class RK222
Bases: *dedalus.core.timesteppers.RungeKuttaIMEX*

2nd-order 2-stage DIRK+ERK scheme [Ascher 1997 sec 2.6]

stages = 2

γ

δ

c

A

H

class RK443
Bases: *dedalus.core.timesteppers.RungeKuttaIMEX*

3rd-order 4-stage DIRK+ERK scheme [Ascher 1997 sec 2.8]

stages = 4

c

A

H

class RKSMR
Bases: *dedalus.core.timesteppers.RungeKuttaIMEX*

(3-ϵ)-order 3rd-stage DIRK+ERK scheme [Spalart 1991 Appendix]

stages = 3

c

A

H

dedalus.extras

Submodules

dedalus.extras.atmospheres

Module Contents

class DedalusAtmosphere(*z_basis*, *num_coeffs=20*)

truncate_atmosphere(*self*, *key*)

get_coeffs(*self*, *key*)

get_values(*self*, *key*)

check_spectrum(*self*, *key*, *individual_plots=True*)

check_atmosphere(*self*, *key*, *individual_plots=True*)

class Polytrope(*gamma*, *polytropic_index*, *z0*, *z*, ***args*)
Bases: *dedalus.extras.atmospheres.DedalusAtmosphere*

grad_ln_rho(*self*)

grad_S(*self*)

grad_ln_T(*self*)

rho(*self*)

T(*self*)

P(*self*)

S(*self*)

class ScaledPolytrope(*gamma*, *polytropic_index*, *z0*, *z*, ***args*)
Bases: *dedalus.extras.atmospheres.Polytrope*

grad_ln_rho(*self*)

grad_S(*self*)

grad_ln_T(*self*)

rho(*self*)

T(*self*)

P(*self*)

S(*self*)

Lz = 10

dedalus.extras.flow_tools

Extra tools that are useful in hydrodynamical problems.

Module Contents

logger

class GlobalArrayReducer(*comm*, *dtype=np.float64*)
Directs parallelized reduction of distributed array data.

Parameters

- **comm** (*MPI communicator*) – MPI communicator
- **dtype** (*data type, optional*) – Array data type (default: np.float64)

reduce_scalar(*self*, *local_scalar*, *mpi_reduce_op*)
Compute global reduction of a scalar from each process.

global_min(*self*, *data*, *empty=np.inf*)
Compute global min of all array data.

global_max(*self*, *data*, *empty=-np.inf*)
Compute global max of all array data.

global_mean(*self*, *data*)
Compute global mean of all array data.

class GlobalFlowProperty(*solver*, *cadence=1*)
Directs parallelized determination of a global flow property on the grid.

Parameters

- **solver** (*solver object*) – Problem solver
- **cadence** (*int, optional*) – Iteration cadence for property evaluation (default: 1)

Examples

```
>>> flow = GlobalFlowProperty(solver)
>>> flow.add_property('sqrt(u*u + w*w) * Lz / nu', name='Re')
...
>>> flow.max('Re')
1024.5
```

add_property(*self*, *property*, *name*, *precompute_integral=False*)
Add a property.

min(*self*, *name*)
Compute global min of a property on the grid.

max(*self*, *name*)
Compute global max of a property on the grid.

grid_average(*self*, *name*)
Compute global mean of a property on the grid.

volume_average(*self*, *name*)
Compute volume average of a property.

class CFL(*solver*, *initial_dt*, *cadence=1*, *safety=1.0*, *max_dt=np.inf*, *min_dt=0.0*, *max_change=np.inf*, *min_change=0.0*, *threshold=0.0*)
Computes CFL-limited timestep from a set of frequencies/velocities.

Parameters

- **solver** (*solver object*) – Problem solver
- **initial_dt** (*float*) – Initial timestep
- **cadence** (*int, optional*) – Iteration cadence for computing new timestep (default: 1)
- **safety** (*float, optional*) – Safety factor for scaling computed timestep (default: 1.)
- **max_dt** (*float, optional*) – Maximum allowable timestep (default: inf)
- **min_dt** (*float, optional*) – Minimum allowable timestep (default: 0.)
- **max_change** (*float, optional*) – Maximum fractional change between timesteps (default: inf)
- **min_change** (*float, optional*) – Minimum fractional change between timesteps (default: 0.)
- **threshold** (*float, optional*) – Fractional change threshold for changing timestep (default: 0.)

Notes

The new timestep is computed by summing across the provided frequencies for each grid point, and then reciprocating the maximum "total" frequency from the entire grid.

compute_dt(*self*)
Compute CFL-limited timestep.

add_frequency(*self*, *freq*)
Add an on-grid frequency.

add_velocity(*self*, *velocity*, *axis*)
Add grid-crossing frequency from a velocity along one axis.

add_velocities(*self*, *components*)
Add grid-crossing frequencies from a tuple of velocity components.

dedalus.extras.plot_tools

Module Contents

class FieldWrapper(*field*)
Class to mimic h5py dataset interface for Dedalus fields.

shape

class DimWrapper(*field*, *axis*)
Wrapper class to mimic h5py dimension scales.

label

plot_bot(*dset*, *image_axes*, *data_slices*, *image_scales=(0, 0)*, *clim=None*, *even_scale=False*, *cmap='RdBu_r'*, *axes=None*, *figkw={}*, *title=None*, *func=None*)
Plot a 2d slice of the grid data of a dset/field.

Parameters

- **dset** (*h5py dset or Dedalus Field object*) – Dataset to plot
- **image_axes** (*tuple of ints (xi, yi)*) – Data axes to use for image x and y axes
- **data_slices** (*tuple of slices, ints*) – Slices selecting image data from global data
- **image_scales** (*tuple of ints or strs (xs, ys)*) – Axis scales (default: (0,0))
- **clim** (*tuple of floats, optional*) – Colorbar limits (default: (data min, data max))
- **even_scale** (*bool, optional*) – Expand colorbar limits to be symmetric around 0 (default: False)
- **cmap** (*str, optional*) – Colormap name (default: 'RdBu_r')
- **axes** (*matplotlib.Axes object, optional*) – Axes to overplot. If None (default), a new figure and axes will be created.
- **figkw** (*dict, optional*) – Keyword arguments to pass to plt.figure (default: {})
- **title** (*str, optional*) – Title for plot (default: dataset name)
- **func** (*function(xmesh, ymesh, data), optional*) – Function to apply to selected meshes and data before plotting (default: None)

plot_bot_2d(*dset*, *transpose=False*, ***kw*)
Plot the grid data of a 2d field.

Parameters

- **field** (*field object*) – Field to plot
- **transpose** (*bool, optional*) – Flag for transposing plot (default: False)
- **Other keyword arguments are passed on to plot_bot.**

plot_bot_3d(*dset*, *normal_axis*, *normal_index*, *transpose=False*, ***kw*)
Plot a 2d slice of the grid data of a 3d field.

Parameters

- **field** (*field object*) – Field to plot
- **normal_axis** (*int or str*) – Index or name of normal axis
- **normal_index** (*int*) – Index along normal direction to plot

- **transpose** (*bool, optional*) – Flag for transposing plot (default: False)
- **Other keyword arguments are passed on to plot_bot.**

class MultiFigure(*nrows*, *ncols*, *image*, *pad*, *margin*, *scale=1.0*, ***kw*)
An array of generic images within a matplotlib figure.

Parameters

- **nrows, ncols** (*int*) – Number of image rows/columns.
- **image** (*Box instance*) – Box describing the image shape.
- **pad** (*Frame instance*) – Frame describing the padding around each image.
- **margin** (*Frame instance*) – Frame describing the margin around the array of images.
- **scale** (*float, optional*) – Scaling factor to convert from provided box/frame units to figsize. Margin will be automatically expanded so that fig dimensions are integers.
- **Other keywords passed to plt.figure.**

add_axes(*self*, *i*, *j*, *rect*, ***kw*)
Add axes to a subfigure.

Parameters

- **i, j** (*int*) – Image row/column
- **rect** (*tuple of floats*) – (left, bottom, width, height) in fractions of image width and height
- **Other keywords passed to Figure.add_axes.**

class Box(*x*, *y*)
2d-vector-like object for representing image sizes and offsets.

Parameters **x, y** (*float*) – Box width/height.

xbox

ybox

class Frame(*top*, *bottom*, *left*, *right*)
Object for representing a non-uniform frame around an image.

Parameters **top, bottom, left, right** (*float*) – Frame widths.

bottom_left

top_right

quad_mesh(*x*, *y*, *cut_x_edges=False*, *cut_y_edges=False*)
Construct quadrilateral mesh arrays from two grids. Intended for use with e.g. plt.pcolor.

Parameters

- **x** (*1d array*) – Grid for last axis of the mesh.
- **y** (*1d array*) – Grid for first axis of the mesh.
- **cut_x_edges, cut_y_edges** (*bool, optional*) – True to truncate edge quadrilaterals at x/y grid edges. False (default) to center edge quadrilaterals at x/y grid edges.

get_1d_vertices(*grid*, *cut_edges=False*)
Get vertices dividing a 1d grid.

Parameters

- **grid** (*1d array*) – Grid.

- **cut_edges** (*bool, optional*) – True to set edge vertices at grid edges. False (default) to center edge segments at grid edges.

pad_limits(*xgrid*, *ygrid*, *xpad=0.0*, *ypad=0.0*, *square=None*)
Compute padded image limits for x and y grids.

Parameters

- **xgrid** (*array*) – Grid for x axis of image.
- **ygrid** (*array*) – Grid for y axis of image.
- **xpad** (*float, optional*) – Padding fraction for x axis (default: 0.).
- **ypad** (*float, optional*) – Padding fraction for y axis (default: 0.).
- **square** (*axis object, optional*) – Extend limits to have a square aspect ratio within an axis.

get_plane(*dset*, *xaxis*, *yaxis*, *slices*, *xscale=0*, *yscale=0*, ***kw*)
Select plane from dataset. Intended for use with e.g. plt.pcolor.

Parameters

- **dset** (*h5py dataset*) – Dataset
- **xaxis, yaxis** (*int*) – Axes for plotting
- **xscale, yscale** (*int or str*) – Corresponding axis scales
- **slices** (*tuple of ints, slice objects*) – Selection object for dataset
- **Other keywords passed to quad_mesh**

dedalus.libraries

Subpackages

dedalus.tests

Subpackages

dedalus.tests.special_functions

Submodules

dedalus.tests.special_functions.airy

Compute Airy functions by solving the Airy equation:

f_xx - (A + Bx) f = 0 f(-1) = C f(+1) = D

Module Contents

default_params

dedalus_domain(*N*)
Construct Dedalus domain for solving the Airy equation.

dedalus_solution(*A*, *B*, *C*, *D*, *N*)
Use Dedalus to solve the Airy equation.

exact_solution(*A*, *B*, *C*, *D*, *N*)
Use scipy to construct exact solution to the Airy equation.

test_airy(*params=default_params*)
Compare Dedalus and exact results.

dedalus.tests.special_functions.bessel

Compute Bessel function by solving the Bessel equation:

x**2 f_xx + x f_x + (x**2 - A**2) f = 0 f(0) = 0 f(30) = B

Module Contents

default_params

dedalus_domain(*N*)
Construct Dedalus domain for solving the Airy equation.

dedalus_solution(*A*, *B*, *N*)
Use Dedalus to solve the Airy equation.

exact_solution(*A*, *B*, *N*)
Use scipy to construct exact solution to the Airy equation.

test_bessel(*params=default_params*)
Compare Dedalus and exact results.

dedalus.tools

Submodules

dedalus.tools.array

Tools for array manipulations.

Module Contents

interleaved_view(*data*)
View n-dim complex array as (n+1)-dim real array, where the last axis separates real and imaginary parts.

reshape_vector(*data*, *dim=2*, *axis=-1*)
Reshape 1-dim array as a multidimensional vector.

axslice(*axis*, *start*, *stop*, *step=None*)
Slice array along a specified axis.

zeros_with_pattern(**args*)
Create sparse matrix with the combined pattern of other sparse matrices.

expand_pattern(*input*, *pattern*)
Return copy of sparse matrix with extended pattern.

apply_matrix(*matrix*, *array*, *axis*, ***kw*)
Contract any direction of a multidimensional array with a matrix.

add_sparse(*A*, *B*)
Add sparse matrices, promoting scalars to multiples of the identity.

dedalus.tools.cache

Tools for caching computations.

Module Contents

class CachedAttribute(*method*)
Descriptor for building attributes during first access.

class CachedFunction(*function*, *max_size=None*)
Decorator for caching function outputs.

class CachedMethod
Bases:*dedalus.tools.cache.CachedFunction*

Descriptor for caching method outputs.

class CachedClass(*cls*, **args*, ***kw*)
Bases:`type`

Metaclass for caching instantiation.

serialize_call(*args*, *kw*, *argnames*, *defaults*)
Serialize args/kw into cache key.

dedalus.tools.config

Configuration handling.

Module Contents

config

dedalus.tools.dispatch

Tools for emulating multiple dispatch.

Module Contents

class MultiClass
Bases:`type`

Metaclass for dispatching instantiation to subclasses.

class CachedMultiClass
Bases:*dedalus.tools.dispatch.MultiClass*, *dedalus.tools.cache.CachedClass*

Metaclass for dispatching and caching instantiantation to subclasses.

dedalus.tools.exceptions

Custom exception classes.

Module Contents

exception NonlinearOperatorError
Bases:Exception

Exceptions for nonlinear LHS terms.

exception SymbolicParsingError
Bases:Exception

Exceptions for syntactic and mathematical problems in equations.

exception UnsupportedEquationError
Bases:Exception

Exceptions for valid but unsupported equations.

exception UndefinedParityError
Bases:Exception

Exceptions for data/operations with undefined parity.

dedalus.tools.general

Extended built-ins, etc.

Module Contents

class OrderedSet
Bases:collections.OrderedDict

Ordered set based on uniqueness of dictionary keys.

update(*self*, **args*)

add(*self*, *item*)

rev_enumerate(*sequence*)
Simple reversed enumerate.

natural_sort(*iterable*, *reverse=False*)
Sort alphanumeric strings naturally, i.e. with "1" before "10". Based on http://stackoverflow.com/a/4836734.

oscillate(*iterable*)
Oscillate forward and backward through an iterable.

unify(*objects*)
Check if all objects in a collection are equal. If so, return one of them. If not, raise.

dedalus.tools.logging

Logging setup.

Module Contents

MPI_RANK

MPI_SIZE

stdout_level

file_level

nonroot_level

filename

rootlogger

formatter

stdout_handler

file_path

dedalus.tools.parallel

Tools for running in parallel.

Module Contents

class Sync(*comm=MPI.COMM_WORLD*, *enter=True*, *exit=True*)
Context manager for synchronizing MPI processes.

Parameters

- **enter** (*boolean, optional*) – Apply MPI barrier on entering context. Default: True
- **exit** (*boolean, optional*) – Apply MPI barrier on exiting context. Default: True

sync_glob(*path*, *glob*, *comm=MPI.COMM_WORLD*)
Syncronized pathlib globbing for consistent results across processes.

Parameters

- **path** (*str or pathlib.Path*) – Base path for globbing.
- **pattern** (*str*) – Glob pattern.
- **comm** (*mpi4py communicator, optional*) – MPI communicator. Default: MPI.COMM_WORLD

dedalus.tools.parsing

Tools for equation parsing.

Module Contents

split_equation(*equation*)
Split equation string into LHS and RHS strings.

Examples

```
>>> split_equation('f(x, y=5) = x**2')
('f(x, y=5)', 'x**2')
```

split_call(*call*)
Convert math-style function definitions into head and arguments.

Examples

```
>>> split_call('f(x, y)')
('f', ('x', 'y'))
>>> split_call('f')
('f', ())
```

lambdify_functions(*call*, *result*)
Convert math-style function definitions into lambda expressions. Pass other statements without modification.

Examples

```
>>> lambdify_functions('f(x, y)', 'x*y')
('f', 'lambda x,y: x*y')
>>> lambdify_functions('f', 'a*b')
('f', 'a*b')
```

dedalus.tools.plot_op

Module Contents

class Node(*label*, *level*)

class Leaf(**args*)
Bases: *dedalus.tools.plot_op.Node*

count = 0.0

class Tree(*operator*)

build(*self*, *arg*, *level*)

set_position(*self*, *node*)

plot_operator(*operator*, *fontsize=8*, *figsize=8*, *saveas=None*)

pad(*xmin*, *xmax*, *ymin*, *ymax*, *pad=0.0*, *square=False*)

dedalus.tools.post

Post-processing helpers.

Module Contents

logger

visit_writes(*set_paths*, *function*, *comm=MPI.COMM_WORLD*, ***kw*)
Apply function to writes from a list of analysis sets.

Parameters

- **set_paths** (*list of str or pathlib.Path*) – List of set paths
- **function** (*function(set_path, start, count, **kw)*) – A function on an HDF5 file, start index, and count.
- **comm** (*mpi4py.MPI.Intracomm, optional*) – MPI communicator (default: COMM_WORLD)
- **Other keyword arguments are passed on to 'function'**

Notes

This function is parallelized over writes, and so can be effectively parallelized up to the number of writes from all specified sets.

get_assigned_writes(*set_paths*, *comm=MPI.COMM_WORLD*)
Divide writes from a list of analysis sets between MPI processes.

Parameters

- **set_paths** (*list of str or pathlib.Path*) – List of set paths
- **comm** (*mpi4py.MPI.Intracomm, optional*) – MPI communicator (default: COMM_WORLD)

get_all_writes(*set_paths*)
Get write numbers from a list of analysis sets.

Parameters **set_paths** (*list of str or pathlib.Path*) – List of set paths

get_assigned_sets(*base_path*, *distributed=False*, *comm=MPI.COMM_WORLD*)
Divide analysis sets from a FileHandler between MPI processes.

Parameters

- **base_path** (*str or pathlib.Path*) – Base path of FileHandler output
- **distributed** (*bool, optional*) – Divide distributed sets instead of merged sets (default: False)
- **comm** (*mpi4py.MPI.Intracomm, optional*) – MPI communicator (default: COMM_WORLD)

merge_process_files(*base_path*, *cleanup=False*, *comm=MPI.COMM_WORLD*)
Merge process files from all distributed analysis sets in a folder.

Parameters

- **base_path** (*str or pathlib.Path*) – Base path of FileHandler output

- **cleanup** (*bool, optional*) – Delete distributed files after merging (default: False)
- **comm** (*mpi4py.MPI.Intracomm, optional*) – MPI communicator (default: COMM_WORLD)

Notes

This function is parallelized over sets, and so can be effectively parallelized up to the number of distributed sets.

merge_process_files_single_set(*set_path*, *cleanup=False*)
Merge process files from a single distributed analysis set.

Parameters

- **set_path** (*str of pathlib.Path*) – Path to distributed analysis set folder
- **cleanup** (*bool, optional*) – Delete distributed files after merging (default: False)

merge_setup(*joint_file*, *proc_path*)
Merge HDF5 setup from part of a distributed analysis set into a joint file.

Parameters

- **joint_file** (*HDF5 file*) – Joint file
- **proc_path** (*str or pathlib.Path*) – Path to part of a distributed analysis set

merge_data(*joint_file*, *proc_path*)
Merge data from part of a distributed analysis set into a joint file.

Parameters

- **joint_file** (*HDF5 file*) – Joint file
- **proc_path** (*str or pathlib.Path*) – Path to part of a distributed analysis set

merge_sets(*joint_path*, *set_paths*, *cleanup=False*, *comm=MPI.COMM_WORLD*)
Merge analysis sets.

Parameters

- **joint_path** (*string or pathlib.Path*) – Path for merged file.
- **set_paths** (*list of strings or pathlib.Path objects*) – Paths of all sets to be merged
- **cleanup** (*bool, optional*) – Delete set files after merging (default: False)
- **comm** (*mpi4py.MPI.Intracomm, optional*) – MPI communicator (default: COMM_WORLD)

merge_analysis

dedalus.tools.progress

Tools for tracking iteration progress.

Module Contents

log_progress(*iterable*, *logger*, *level*, ***kw*)
Log iteration progress.

print_progress(*iterable*, *stream=sys.stdout*, ***kw*)
Print iteration progress to a stream.

track(*iterable*, *write*, *desc='Iteration'*, *iter=1*, *frac=1.0*, *dt=np.inf*)
Track an iterator attaching messages at set cadences.

format_time(*total_sec*)
Format time strings.

dedalus.tools.sparse

Tools for working with sparse matrices.

Module Contents

STORE_LU

PERMC_SPEC

USE_UMFPACK

scipy_sparse_eigs(*A*, *B*, *N*, *target*, ***kw*)
Perform targeted eigenmode search using the scipy/ARPACK sparse solver for the reformulated generalized eigenvalue problem

$$A.x = \lambda\ B.x \Longrightarrow (A - \sigma B)B.x = (1/(\lambda-\sigma))\ x$$

for eigenvalues λ near the target σ.

Parameters

- **A, B** (*scipy sparse matrices*) – Sparse matrices for generalized eigenvalue problem
- **N** (*int*) – Number of eigenmodes to return
- **target** (*complex*) – Target σ for eigenvalue search
- **Other keyword options passed to scipy.sparse.linalg.eigs.**

2.3.2 Submodules

dedalus.dev

Interface for accessing all submodules.

dedalus.public

Interface for tools typically accessed for solving a problem.

CHAPTER 3

Other Links

- Project homepage: http://dedalus-project.org
- Code repository: http://bitbucket.org/dedalus-project/dedalus
- Documentation: http://dedalus-project.readthedocs.org
- User mailing list: https://groups.google.com/forum/#!forum/dedalus-users
- Development mailing list: https://groups.google.com/forum/#!forum/dedalus-dev

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