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pyqg is a python solver for quasigeostrophic systems. Quasigeostrophic equations are an approximation to the full fluid equations of motion in the limit of strong rotation and stratification and are most applicable to geophysical fluid dynamics problems.

Students and researchers in ocean and atmospheric dynamics are the intended audience of pyqg. The model is simple enough to be used by students new to the field yet powerful enough for research. We strive for clear documentation and thorough testing.

pyqg supports a variety of different configurations using the same computational kernel. The different configurations are evolving and are described in detail in the documentation. The kernel, implement in cython, uses a pseudo-spectral method which is heavily dependent of the fast Fourier transform. For this reason, pyqg tries to use pyfftw and the FFTW Fourier Transform library. (If pyfftw is not available, it falls back on numpy.fft) With pyfftw, the kernel is multi-threaded but does not support mpi. Optimal performance will be achieved on a single system with many cores.
1.1 Installation

1.1.1 Requirements

The only requirements are

- Python (3.6 or later)
- numpy (1.6 or later)
- Cython (0.2 or later)

Because pyqg is a pseudo-spectral code, it relies heavily on fast-Fourier transforms (FFTs), which are the main performance bottleneck. For this reason, we try to use fftw (a fast, multithreaded, open source C library) and pyfftw (a python wrapper around fftw). These packages are optional, but they are strongly recommended for anyone doing high-resolution, numerically demanding simulations.

- fftw (3.3 or later)
- pyfftw (0.9.2 or later)

If pyqg can’t import pyfftw at compile time, it will fall back on numpy’s fft routines.

PyQG can also conveniently store model output data as an xarray dataset. The feature (which is used in some of the examples in this documentation) requires xarray.

1.1.2 Instructions

The easiest and quickest way: installing pyqg with conda

We suggest that you install pyqg using conda. This will automatically install pyfftw as well, so then you will be done and can ignore the remaining instructions on this page. To install pyqg with conda,
$ conda install -c conda-forge pyqg

**Alternatives**

In our opinion, the best way to get python and numpy is to use a distribution such as Anaconda (recommended) or Canopy. These provide robust package management and come with many other useful packages for scientific computing. The pyqg developers are mostly using anaconda.

**Note:** If you don’t want to use pyfftw and are content with numpy’s slower performance, you can skip ahead to *Installing pyqg*.

Installing fftw and pyfftw can be slightly painful. Hopefully the instructions below are sufficient. If not, please send feedback.

**Installing fftw and pyfftw**

Once you have installed pyfftw via one of these paths, you can proceed to *Installing pyqg*.

**The easy way: installing with conda**

If you are using Anaconda, we have discovered that you can easily install pyffw using the conda command. Although pyfftw is not part of the main Anaconda distribution, it is distributed as a conda package through several user channels. There is a useful blog post describing how the pyfftw conda package was created. There are currently 13 pyfftw user packages hosted on anaconda.org. Each has different dependencies and platform support (e.g. linux, windows, mac.) The nanshe channel version is the most popular and appears to have the broadest cross-platform support. We don’t know who nanshe is, but we are grateful to him/her.

To install pyfftw from the conda-forge channel, open a terminal and run the command

$ conda install -c conda-forge pyfftw

**The hard way: installing from source**

This is the most difficult step for new users. You will probably have to build FFTW3 from source. However, if you are using Ubuntu linux, you can save yourself some trouble by installing fftw using the apt package manager

$ sudo apt-get install libfftw3-dev libfftw3-doc

Otherwise you have to build FFTW3 from source. Your main resource for the FFTW homepage. Below we summarize the steps

First download the source code.

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

Then run the configure command
Note: If you don’t have root privileges on your computer (e.g. on a shared cluster) the best approach is to ask your system administrator to install FFTW3 for you. If that doesn’t work, you will have to install the FFTW3 libraries into a location in your home directory (e.g. $HOME/fftw) and add the flag `--prefix=$HOME/fftw` to the configure command above.

Then build the software

```bash
$ make
```

Then install the software

```bash
$ sudo make install
```

This will install the FFTW3 libraries into you system’s library directory. If you don’t have root privileges (see note above), remove the `sudo`. This will install the libraries into the `prefix` location you specified.

You are not done installing FFTW yet. pyfftw requires special versions of the FFTW library specialized to different data types (32-bit floats and double-long floats). You need to re-configure and re-build FFTW two more times with extra flags.

```bash
$ ./configure --enable-threads --enable-shared --enable-float
$ make
$ sudo make install

$ ./configure --enable-threads --enable-shared --enable-long-double
$ make
$ sudo make install
```

At this point, you FFTW installation is complete. We now move on to pyfftw. pyfftw is a python wrapper around the FFTW libraries. The easiest way to install it is using `pip`:

```bash
$ pip install pyfftw
```

or if you don’t have root privileges

```bash
$ pip install pyfftw --user
```

If this fails for some reason, you can manually download and install it according to the instructions on github. First clone the repository:

```bash
$ git clone https://github.com/hgomersall/pyFFTW.git
```

Then install it

```bash
$ cd pyFFTW
$ python setup.py install
```

or

```bash
$ python setup.py install --user
```

if you don’t have root privileges. If you installed FFTW in a non-standard location (e.g. $HOME/fftw), you might have to do something tricky at this point to make sure pyfftw can find FFTW. (I figured this out once, but I can’t remember how.)
Installing pyqg

**Note:** The pyqg kernel is written in Cython and uses OpenMP to parallelise some operations for a performance boost. If you are using Mac OSX Yosemite or later OpenMP support is not available out of the box. While pyqg will still run without OpenMP, it will not be as fast as it can be. See *Installing with OpenMP support on OSX* below for more information on installing on OSX with OpenMP support.

With pyfftw installed, you can now install pyqg. The easiest way is with pip:

```
$ pip install pyqg
```

You can also clone the pyqg git repository to use the latest development version.

```
$ git clone https://github.com/pyqg/pyqg.git
```

Then install pyqg on your system:

```
$ python setup.py install [--user]
```

(The `--user` flag is optional—use it if you don’t have root privileges.)

If you want to make changes in the code, set up the development mode:

```
$ python setup.py develop
```

pyqg is a work in progress, and we really encourage users to contribute to its *Development*

**Installing with OpenMP support on OSX**

There are two options for installing on OSX with OpenMP support. Both methods require using the Anaconda distribution of Python.

1. Using Homebrew

   Install the GCC-5 compiler in `/usr/local` using Homebrew:

   ```
   $ brew install gcc --without-multilib --with-fortran
   ```

   Install Cython from the conda repository

   ```
   $ conda install cython
   ```

   Install pyqg using the homebrew gcc compiler

   ```
   $ CC=/usr/local/bin/gcc-5 pip install pyqg
   ```

2. Using the HPC precompiled gcc binaries.

   The [HPC for Mac OSX](sourceforge.net) project has copies of the latest gcc precompiled for Mac OSX. Download the latest version of gcc from the HPC site and follow the installation instructions.

   Install Cython from the conda repository

   ```
   $ conda install cython
   ```

   Install pyqg using the HPC gcc compiler
1.2 Equations Solved

A detailed description of the equations solved by the various pyqg models

1.2.1 Equations For Two-Layer QG Model

The two-layer quasigeostrophic evolution equations are (1)
\[
\partial_t q_1 + \nabla (\psi_1, q_1) + \beta \psi_{1x} = \text{ssd},
\]
and (2)
\[
\partial_t q_2 + \nabla (\psi_2, q_2) + \beta \psi_{2x} = -r e k \nabla^2 \psi_2 + \text{ssd},
\]
where the horizontal Jacobian is
\[
J(A, B) = A_x B_y - A_y B_x.
\]
Also in (1) and (2) ssd denotes small-scale dissipation (in turbulence regimes, ssd absorbs enstrophy that cascades towards small scales). The linear bottom drag in (2) dissipates large-scale energy.

The potential vorticities are (3)
\[
q_1 = \nabla^2 \psi_1 + F_1 (\psi_2 - \psi_1),
\]
and (4)
\[
q_2 = \nabla^2 \psi_2 + F_2 (\psi_1 - \psi_2),
\]
where
\[
F_1 = \frac{k_d^2}{1 + \delta^2}, \quad \text{and} \quad F_2 = \delta F_1,
\]
with the deformation wavenumber
\[
k_d^2 = \frac{f^2}{g} \frac{H_1 + H_2}{H_1 H_2},
\]
where \( H = H_1 + H_2 \) is the total depth at rest.

**Forced-dissipative equations**

We are interested in flows driven by baroclinic instability of a base-state shear \( U_1 - U_2 \). In this case the evolution equations (1) and (2) become (5)
\[
\partial_t q_1 + \nabla (\psi_1, q_1) + \beta_1 \psi_{1x} = \text{ssd},
\]
and (6)
\[
\partial_t q_2 + \nabla (\psi_2, q_2) + \beta_2 \psi_{2x} = -r e k \nabla^2 \psi_2 + \text{ssd},
\]
where the mean potential vorticity gradients are (9,10)
\[
\beta_1 = \beta + F_1 (U_1 - U_2), \quad \text{and} \quad \beta_2 = \beta - F_2 (U_1 - U_2).
\]
**Equations in Fourier space**

We solve the two-layer QG system using a pseudo-spectral doubly-peridioc model. Fourier transforming the evolution equations (5) and (6) gives (7)

\[ \partial_t \hat{q}_1 = -\hat{J}(\psi_1, q_1) - i k \beta_1 \hat{\psi}_1 + \text{ssd}, \]

and

\[ \partial_t \hat{q}_2 = -\hat{J}(\psi_2, q_2) - i k \beta_2 \hat{\psi}_2 + r e_k \kappa^2 \hat{\psi}_2 + \text{ssd}, \]

where, in the pseudo-spectral spirit, \( \hat{J} \) means the Fourier transform of the Jacobian i.e., we compute the products in physical space, and then transform to Fourier space.

In Fourier space the “inversion relation” (3)-(4) is

\[
\begin{bmatrix}
-\left(\kappa^2 + F_1\right) \\
F_2 \\
\left(\kappa^2 + F_2\right)
\end{bmatrix}
\begin{bmatrix}
\hat{\psi}_1 \\
\hat{\psi}_2
\end{bmatrix}
= 
\begin{bmatrix}
\hat{q}_1 \\
\hat{q}_2
\end{bmatrix},
\]

or equivalently

\[
\begin{bmatrix}
\hat{\psi}_1 \\
\hat{\psi}_2
\end{bmatrix}
= 
\frac{1}{\det M_2}
\begin{bmatrix}
-\left(\kappa^2 + F_2\right) \\
-F_2 \\
\left(\kappa^2 + F_1\right)
\end{bmatrix}
\begin{bmatrix}
\hat{q}_1 \\
\hat{q}_2
\end{bmatrix},
\]

where

\[
\det M_2 = \kappa^2 \left(\kappa^2 + F_1 + F_2\right).
\]

**Marching forward**

We use a third-order Adams-Bashford scheme

\[ \hat{q}_i^{n+1} = E_f \times \left[ \hat{q}_i^n + \frac{\Delta t}{12} \left(23 \hat{Q}_i^n - 16 \hat{Q}_i^{n-1} + 5 \hat{Q}_i^{n-2}\right)\right], \]

where

\[ \hat{Q}_i^n = -\hat{J}(\psi_i^n, q_i^n) - i k \beta_i \hat{\psi}_i^n, \quad i = 1, 2. \]

The AB3 is initialized with a first-order AB (or forward Euler)

\[ \hat{q}_i^1 = E_f \times \left[ \hat{q}_i^0 + \frac{\Delta t}{2} \hat{Q}_i^0 \right], \]

The second step uses a second-order AB scheme

\[ \hat{q}_i^2 = E_f \times \left[ \hat{q}_i^1 + \frac{\Delta t}{2} \left(3 \hat{Q}_i^1 - \hat{Q}_i^0\right)\right]. \]

The small-scale dissipation is achieve by a highly-selective exponential filter

\[ E_f = \begin{cases} 
\exp(-23.6 (\kappa^* - \kappa_c)^4) : & \kappa \geq \kappa_c \\
1 : & \text{otherwise}.
\end{cases} \]
where the non-dimensional wavenumber is 
\[ n^* \equiv \sqrt{(k \Delta x)^2 + (l \Delta y)^2}, \]
and \( n_\text{c} \) is a (non-dimensional) wavenumber cutoff here taken as 65\% of the Nyquist scale \( n_{\text{ny}} = \pi \). The parameter \(-23.6\) is obtained from the requirement that the energy at the largest wavenumber \( (n^* = \pi) \) be zero within machine double precision:
\[ \log_{10}(0.35 \pi)^4 \approx -23.5. \]

For experiments with \(|\hat{g}_i| \ll O(1)\) one can use a smaller constant.

**Diagnostics**

The kinetic energy is
\[ E = \frac{1}{H S} \int \frac{1}{2} H_1 |\nabla \psi_1|^2 + \frac{1}{2} H_2 |\nabla \psi_2|^2 \, dS. \]

The potential enstrophy is
\[ Z = \frac{1}{H S} \int \frac{1}{2} H_1 q_1^2 + \frac{1}{2} H_2 q_2^2 \, dS. \]

We can use the enstrophy to estimate the eddy turn-over timescale
\[ T_e = \frac{2 \pi}{\sqrt{Z}}. \]

**1.2.2 Layered quasigeostrophic model**

The \( N \)-layer quasigeostrophic (QG) potential vorticity is
\[ q_1 = \nabla^2 \psi_1 + \frac{f_0^2}{H_1} \left( \frac{\psi_2 - \psi_1}{g_1^0} \right), \quad n = 1, \]
\[ q_n = \nabla^2 \psi_n + \frac{f_0^2}{H_n} \left( \frac{\psi_{n-1} - \psi_n}{g_n^{n-1}} - \frac{\psi_n - \psi_{n+1}}{g_n^0} \right), \quad n = 2, \ldots, N - 1, \]
\[ q_N = \nabla^2 \psi_N + \frac{f_0^2}{H_N} \left( \frac{\psi_{N-1} - \psi_N}{g_{N-1}^{N-1}} \right), \quad n = N, \]

where \( q_n \) is the \( n \)-th layer QG potential vorticity, and \( \psi_n \) is the streamfunction, \( f_0 \) is the inertial frequency, \( H_n \) is the layer depth. Also the \( n \)-th buoyancy jump (reduced gravity) is
\[ g_n' \equiv g \frac{\rho_n - \rho_{n+1}}{\rho_n}, \]

where \( g \) is the acceleration due to gravity and \( \rho_n \) is the layer density.

The dynamics of the system is given by the evolution of PV. In particular, assuming a background flow with background velocity \( \mathbf{V} = (U, V) \) such that
\[ \psi_n^{\text{tot}} = U_n - \psi_{ny}, \]
\[ \psi_n^{\text{tot}} = V_n + \psi_{nx}, \]
and

\[ q_n^{\text{tot}} = Q_n + \delta_n \frac{f_0}{H_N} h_b + q_n , \]

where \( Q_n + \delta_n \frac{f_0}{H_N} h_b \) is \( n \)-th layer background PV and \( h_b \) is the bottom topography, we obtain the evolution equations

\[
q_{nt} + J(\psi_n, q_n + \delta_n \frac{f_0}{H_N} h_b) + U_n(q_{nx} + \delta_n \frac{f_0}{H_N} h_{bx}) + V_n(q_{ny} + \delta_n \frac{f_0}{H_N} h_{by}) \\
+ Q_{ny} \psi_{nx} - Q_{nx} \psi_{ny} = \text{ssd} - r_{ek}\delta_n \nabla^2 \psi_n , \quad n = 1, \ldots, N ,
\]

where \( \text{ssd} \) stands for small-scale dissipation, which is achieved by a spectral exponential filter or hyperviscosity, and \( r_{ek} \) is the linear bottom drag coefficient. The Dirac delta, \( \delta_n \), indicates that the drag is only applied in the bottom layer. (Note that in QG \( h_b/H_N \ll 1 \).)

**Equations in spectral space**

The evolution equation in spectral space is

\[
\hat{q}_{nt} + (i k U + i V)(\hat{q}_n + \delta_n \frac{f_0}{H_N} \hat{h}_b) + (i k Q_y - i l Q_x)\hat{\psi}_n + \hat{J}(\psi_n, q_n + \delta_n \frac{f_0}{H_N} h_b) \\
= \text{ssd} + \delta_n r_{ek} \kappa^2 \hat{\psi}_n , \quad i = 1, \ldots, N ,
\]

where \( \kappa^2 = k^2 + l^2 \). Also, in the pseudo-spectral spirit we write the transform of the nonlinear terms and the non-constant coefficient linear term as the transform of the products, calculated in physical space, as opposed to double convolution sums. That is \( \hat{J} \) is the Fourier transform of Jacobian computed in physical space.

The inversion relationship is

\[
\hat{q}_i = (S - \kappa^2 I)\hat{\psi}_i ,
\]

where \( I \) is the \( N \times N \) identity matrix, and the stretching matrix is

\[
S = f_0^2 \begin{bmatrix}
-\frac{1}{g_i H_i} & 0 & \ldots & 0 \\
0 & -\frac{1}{g_{i-1} H_i} & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots \\
0 & \ldots & \frac{1}{g_{N-1} H_N} & -\frac{1}{g_N H_N} \\
\frac{1}{g_{N-1} H_N} & \ldots & \frac{1}{g_{N-1} H_N} & -\frac{1}{g_N H_N}
\end{bmatrix} .
\]

**Energy spectrum**

The equation for the energy spectrum,

\[
E(k, l) \equiv \frac{1}{2H} \sum_{i=1}^{N} H_i \kappa^2 |\hat{\psi}_i|^2 + \frac{1}{2H} \sum_{i=1}^{N-1} f_0^2 |\hat{\psi}_i - \hat{\psi}_{i+1}|^2 ,
\]

is

\[
\frac{d}{dt} E(k, l) = \frac{1}{H} \sum_{i=1}^{N} H_i \text{Re}[\hat{\psi}_i^* \hat{J}(\psi_i, \nabla^2 \psi_i)] + \frac{1}{H} \sum_{i=1}^{N} H_i \text{Re}[\hat{\psi}_i^* \hat{J}(\psi_i, (S\psi)_i)] \\
+ \frac{1}{H} \sum_{i=1}^{N} H_i (k U_i + l V_i) \text{Re}[i \hat{\psi}_i^*(S\hat{\psi}_i)] - r_{ek} \frac{H_N}{H} \kappa^2 |\hat{\psi}_N|^2 + E_{\text{ssd}} ,
\]
where $\ast$ stands for complex conjugation, and the terms above on the right represent, from left to right,

I: The spectral divergence of the kinetic energy flux;

II: The spectral divergence of the potential energy flux;

III: The spectrum of the potential energy generation;

IV: The spectrum of the energy dissipation by linear bottom drag;

V: The spectrum of energy loss due to small scale dissipation.

We assume that $V$ is relatively small, and that, in statistical steady state, the budget above is dominated by I through IV.

**Enstrophy spectrum**

Similarly the evolution of the barotropic enstrophy spectrum,

$$Z(k, l) = \frac{1}{2H} \sum_{i=1}^{N} H_i |\tilde{q}_i|^2,$$

is governed by

$$\frac{d}{dt} Z(k, l) = \text{Re}[\tilde{q}_i^* \tilde{J}(\psi_1, q_1)] - (kQ_y - lQ_x) \text{Re}[S \tilde{\psi}_i^* \tilde{\psi}_i] + \overline{Z_{sd}},$$

where the terms above on the right represent, from left to right,

I: The spectral divergence of barotropic potential enstrophy flux;

II: The spectrum of barotropic potential enstrophy generation;

III: The spectrum of barotropic potential enstrophy loss due to small scale dissipation.

The enstrophy dissipation is concentrated at the smallest scales resolved in the model and, in statistical steady state, we expect the budget above to be dominated by the balance between I and II.

**1.2.3 Special case: two-layer model**

With $N = 2$, an alternative notation for the perturbation of potential vorticities can be written as

$$q_1 = \nabla^2 \psi_1 + F_1 (\psi_2 - \psi_1)$$

$$q_2 = \nabla^2 \psi_2 + F_2 (\psi_1 - \psi_2),$$

where we use the following definitions where

$$F_1 = \frac{k_d^2}{1 + \delta^2}, \quad \text{and} \quad F_2 = \delta F_1,$$

with the deformation wavenumber

$$k_d^2 = \frac{f_0^2 H_1 + H_2}{H_1 H_2}.$$

With this notation, the stretching matrix is simply

$$S = \begin{pmatrix} -F_1 & F_1 \\ F_2 & -F_2 \end{pmatrix}. $$
The inversion relationship in Fourier space is
\[
\begin{bmatrix}
\hat{\psi}_1 \\
\hat{\psi}_2
\end{bmatrix} = \frac{1}{\det B} \begin{bmatrix}
-(\kappa^2 + F_2) & -F_1 \\
-F_2 & -(\kappa^2 + F_1)
\end{bmatrix}
\begin{bmatrix}
\hat{q}_1 \\
\hat{q}_2
\end{bmatrix},
\]
where
\[
\det B = \kappa^2 (\kappa^2 + F_1 + F_2).
\]

### 1.2.4 Vertical modes

Standard vertical modes, \(p_n(z)\), are the eigenvectors of the “stretching matrix”
\[
Sp_n = -R_n^{-2} p_n,
\]
where the \(R_n\) is by definition the \(n\)’th deformation radius (e.g., Flierl 1978). These orthogonal modes \(p_n\) are normalized to have unitary \(L^2\)-norm
\[
\frac{1}{H} \int_{-H}^{H} p_n p_m \, dz = \delta_{nm},
\]
where \(\delta_{nm}\).

### 1.2.5 Linear stability analysis

With \(h_b = 0\), the linear eigenproblem is
\[
A \Phi = \omega B \Phi,
\]
where
\[
A \equiv B(U k + V l) + l(k Q_y - l Q_x) + l \delta_{NN} i r_k \kappa^2,
\]
where \(\delta_{NN} = [0, 0, \ldots, 0, 1]\), and
\[
B \equiv S - l \kappa^2.
\]
The growth rate is \(\text{Im}\{\omega}\).

### 1.2.6 Equations For Equivalent Barotropic QG Model

The equivalent barotropic quasigeostrophy evolution equations is
\[
\partial_t q + J(\psi, q) + \beta \psi_x = \text{ssd}.
\]
The potential vorticity anomaly is
\[
q = \nabla^2 \psi - \kappa_d^2 \psi,
\]
where \(\kappa_d^2\) is the deformation wavenumber. With \(\kappa_d = \beta = 0\) we recover the 2D vorticity equation.

The inversion relationship in Fourier space is
\[
\hat{q} = - (\kappa^2 + \kappa_d^2) \hat{\psi}.
\]
The system is marched forward in time similarly to the two-layer model.
1.2.7 Surface Quasi-geostrophic Model

Surface quasi-geostrophy (SQG) is a relatively simple model that describes surface intensified flows due to buoyancy. One of it’s advantages is that it only has two spatial dimensions but describes a three-dimensional solution.

The evolution equation is

\[ \partial_t b + J(\psi, b) = 0, \quad \text{at} \quad z = 0, \]

where \( b = \psi_z \) is the buoyancy.

The interior potential vorticity is zero. Hence

\[ \frac{\partial}{\partial z} \left( \frac{f_0^2}{N^2} \frac{\partial \psi}{\partial z} \right) + \nabla^2 \psi = 0, \]

where \( N \) is the buoyancy frequency and \( f_0 \) is the Coriolis parameter. In the SQG model both \( N \) and \( f_0 \) are constants.

The boundary conditions for this elliptic problem in a semi-infinite vertical domain are

\[ b = \psi_z, \quad \text{and} \quad z = 0, \]

and

\[ \psi = 0, \quad \text{at} \quad z \rightarrow -\infty. \]

The solutions to the elliptic problem above, in horizontal Fourier space, gives the inversion relationship between surface buoyancy and surface streamfunction

\[ \tilde{\psi} = \frac{f_0}{N} \frac{1}{\kappa} \tilde{b}, \quad \text{at} \quad z = 0. \]

The SQG evolution equation is marched forward similarly to the two-layer model.

1.3 Examples

1.3.1 Two Layer QG Model Example

Here is a quick overview of how to use the two-layer model. See the :py:class:`pyqg.QGModel` api documentation for further details.

First import numpy, matplotlib, and pyqg:

```python
[2]: import numpy as np
from matplotlib import pyplot as plt
import pyqg
```

Initialize and Run the Model

Here we set up a model which will run for 10 years and start averaging after 5 years. There are lots of parameters that can be specified as keyword arguments but we are just using the defaults.

```python
[3]: year = 24*60*60*360.
m = pyqg.QGModel(tmax=10*year, twrite=10000, tavestart=5*year)
m.run()
```
Convert Model Output to an xarray Dataset

Model variables, coordinates, attributes, and metadata can be stored conveniently as an xarray Dataset. (Notice that this feature requires xarray to be installed on your machine. See here for installation instructions: http://xarray.pydata.org/en/stable/getting-started-guide/installing.html#instructions)

```python
m_ds = m.to_dataset()
```

```
<xarray.Dataset>

Dimensions:       (k: 33, l: 64, lev: 2, time: 1, x: 64, y: 64)

Coordinates:
* time (time) float64 3.11e+08
* lev (lev) int64 1 2
* x (x) float64 7.812e+03 2.344e+04 ... 9.766e+05 9.922e+05
* y (y) float64 7.812e+03 2.344e+04 ... 9.766e+05 9.922e+05
* l (l) float64 0.0 6.283e-06 1.257e-05 ... -1.257e-05 -6.283e-06
* k (k) float64 0.0 6.283e-06 1.257e-05 ... 0.0001948 0.0002011

Data variables: (12/20)
q (time, lev, y, x) float64 1.097e-05 7.43e-06 ... -6.064e-07
u (time, lev, y, x) float64 0.01271 -0.02153 ... 0.004449
v (time, lev, y, x) float64 0.005955 0.02975 ... -0.007719
ufull (time, lev, y, x) float64 0.03771 0.003467 ... 0.004449
vfull (time, lev, y, x) float64 0.005955 0.02975 ... -0.007719
qh (time, lev, l, k) complex128 (0.0021402319088019263+0j) ... (... ...
EKE (lev) float64 0.00222 6.157e-05
entspec (l, k) float64 1.832e-07 2.611e-12 ... 2.697e-34 9.974e-44
APEflux (l, k) float64 -0.0 3.585e-08 1.48e-07 ... 2.204e-21 4.615e-26
KEflux (l, k) float64 0.0 1.116e-08 2.814e-07 ... 1.014e-19 1.737e-24
APEgenspec (l, k) float64 0.0 -2.966e-08 1.59e-07 ... 3.403e-36 8.128e-46
APEgen (time) float64 6.914e-11

Attributes: (12/20)
pyqg:L: 1000000.0
pyqg:W: 1000000.0
pyqg:dt: 7200.0
pyqg:filterfac: 23.6
pyqg:nk: 33
pyqg:nl: 64
... ...
pyqg:tmax: 311040000.0
pyqg:twrite: 10000
pyqg:del2: 0.8
pyqg:M: 4096
```
Visualize Output

Let’s assign a new data variable, $q_{\text{upper}}$, as the upper layer PV anomaly. We access the PV values in the Dataset as $m\_ds.q$, which has two levels and a corresponding background PV gradient, $m\_ds.Qy$.

$$m\_ds['q_{\text{upper}}'] = m\_ds.q.isel(\text{lev}=0, \text{time}=0) + m\_ds.Qy.isel(\text{lev}=0)*m\_ds.y$$

$$m\_ds['q_{\text{upper}}'].attrs = \{\text{'long_name': 'upper layer PV anomaly'}\}$$

$$m\_ds.q_{\text{upper}}.\text{plot}.\text{contourf}(\text{levels}=18, \text{cmap}='\text{RdBu\_r}')$$

Plot Diagnostics

The model automatically accumulates averages of certain diagnostics. We can find out what diagnostics are available by calling

$$m.\text{describe_diagnostics}()$$

<table>
<thead>
<tr>
<th>NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>APEflux</td>
<td>spectral flux of available potential energy</td>
</tr>
<tr>
<td>APEgen</td>
<td>total available potential energy generation</td>
</tr>
<tr>
<td>APEgenspec</td>
<td>spectrum of available potential energy generation</td>
</tr>
<tr>
<td>EKE</td>
<td>mean eddy kinetic energy</td>
</tr>
<tr>
<td>EKEdiss</td>
<td>total energy dissipation by bottom drag</td>
</tr>
<tr>
<td>Ensspec</td>
<td>enstrophy spectrum</td>
</tr>
<tr>
<td>KEflux</td>
<td>spectral flux of kinetic energy</td>
</tr>
<tr>
<td>KEspec</td>
<td>kinetic energy spectrum</td>
</tr>
<tr>
<td>entspec</td>
<td>barotropic enstrophy spectrum</td>
</tr>
</tbody>
</table>

To look at the wavenumber energy spectrum, we plot the KEspec diagnostic. (Note that summing along the l-axis, as in this example, does not give us a true isotropic wavenumber spectrum.)

$$\text{kespec}_{\text{upper}} = m\_ds.\text{KEspec}.isel(\text{lev}=0).\text{sum}(\text{\text{'}l\text{'}})$$

$$\text{kespec}_{\text{lower}} = m\_ds.\text{KEspec}.isel(\text{lev}=1).\text{sum}(\text{\text{'}l\text{'}})$$

$$\text{kespec}_{\text{upper}}.\text{plot}.\text{line}(\text{\text{'}b\text{\text{-}}\text{'}}, \text{x='k', xscale='log', yscale='log', label='upper layer'})$$

$$\text{kespec}_{\text{lower}}.\text{plot}.\text{line}(\text{\text{'}g\text{\text{-}}\text{'}}, \text{x='k', xscale='log', yscale='log', label='lower layer'})$$

plt.legend(loc='lower left')

(continues on next page)
plt.ylim([1e-9, 1e-3]);
plt.xlabel(r'k (m$^{-1}$)'); plt.grid()
plt.title('Kinetic Energy Spectrum');

We can also plot the spectral fluxes of energy.

[9]:
```
    ebud = [ m_ds.APEgenspec.sum('l'),
            m_ds.APEflux.sum('l'),
            m_ds.KEflux.sum('l'),
            -m_ds.attrs['pyqg:rek']*m.del2*m_ds.KEspec.isel(lev=1).sum('l')*m.M**2 ]
    ebud.append(-np.vstack(ebud).sum(axis=0))
    ebud_labels = ['APE gen', 'APE flux', 'KE flux', 'Diss.', 'Resid.']
    [plt.semilogx(m_ds.k, term) for term in ebud]
    plt.legend(ebud_labels, loc='upper right')
    plt.xlim([m_ds.k.min(), m_ds.k.max()])
    plt.xlabel(r'k (m$^{-1}$)'); plt.grid()
    plt.title('Spectral Energy Transfers');
```
1.3.2 Fully developed baroclinic instability of a 3-layer flow

[1]: import numpy as np
    from numpy import pi
    from matplotlib import pyplot as plt

    import pyqg
    from pyqg import diagnostic_tools as tools

Set up

[2]:
L = 1000.e3  # length scale of box  [m]
Ld = 15.e3   # deformation scale  [m]
k_d = 1./Ld  # deformation wavenumber [m^-1]
Nx = 64      # number of grid points

H1 = 500.   # layer 1 thickness  [m]
H2 = 1750.  # layer 2
H3 = 1750.  # layer 3

U1 = 0.05   # layer 1 zonal velocity [m/s]
U2 = 0.025  # layer 2
U3 = 0.0    # layer 3

rho1 = 1025.
rho2 = 1025.275
rho3 = 1025.640

rek = 1.e-7  # linear bottom drag coeff.  [s^-1]
f0 = 0.0001236812857687059 # coriolis param [s^-1]
beta = 1.2130692965249345e-11 # planetary vorticity gradient [m^-1 s^-1]

Ti = Ld/abs(U1)  # estimate of most unstable e-folding time scale [s]
\[ dt = \frac{Ti}{200}. \quad \text{# time-step [s]} \]
\[ tmax = 300 \times Ti \quad \text{# simulation time [s]} \]

\[ m = \text{pyqg.LayeredModel}(nx=Nx, \ nz=3, \ U = [U1,U2,U3], \ V = \{0.,0.,0.\}, \ L=L, \ f=f0, \ beta=beta, \ H = [H1,H2,H3], \ rho=[\rho_1,\rho_2,\rho_3], \ rek=rek, \ dt=dt, \ tmax=tmax, \ twrite=5000, \ tavestart=Ti \times 10) \]

INFO: Logger initialized

**Initial condition**

\[ \text{sig} = 1.e^{-7} \]
\[ qi = \text{sig} \times \text{np.vstack}([\text{np.random.randn}(m.nx,m.ny)[\text{np.newaxis},], \]
\[ \text{np.random.randn}(m.nx,m.ny)[\text{np.newaxis},], \]
\[ \text{np.random.randn}(m.nx,m.ny)[\text{np.newaxis},]) \]
\[ m.\text{set}_q(qi) \]

**Run the model**

\[ m.\text{run}() \]

INFO: Step: 5000, Time: 7.50e+06, KE: 2.56e-06, CFL: 0.006
INFO: Step: 10000, Time: 1.50e+07, KE: 1.78e-04, CFL: 0.009
INFO: Step: 15000, Time: 2.25e+07, KE: 6.31e-03, CFL: 0.059
INFO: Step: 20000, Time: 3.00e+07, KE: 3.25e-02, CFL: 0.100
INFO: Step: 25000, Time: 3.75e+07, KE: 8.46e-02, CFL: 0.153
INFO: Step: 30000, Time: 4.50e+07, KE: 2.16e-01, CFL: 0.232
INFO: Step: 35000, Time: 5.25e+07, KE: 3.49e-01, CFL: 0.233
INFO: Step: 40000, Time: 6.00e+07, KE: 3.01e-01, CFL: 0.192
INFO: Step: 45000, Time: 6.75e+07, KE: 2.31e-01, CFL: 0.180
INFO: Step: 50000, Time: 7.50e+07, KE: 2.05e-01, CFL: 0.229
INFO: Step: 55000, Time: 8.25e+07, KE: 3.01e-01, CFL: 0.221
INFO: Step: 60000, Time: 9.00e+07, KE: 2.24e-01, CFL: 0.183

**Xarray Dataset**


\[ ds = m.\text{to}_\text{dataset}() \]
\[ ds \]

\[ <\text{xarray.Dataset}> \]
Dimensions: \[(k: 33, \ l: 64, \ lev: 3, \ lev\_mid: 2, \ time: 1, \ x: 64, \ y: 64)\]
Coordinates:
* time (time) float64 9e+07
  lev (lev) int64 1 2 3
  lev\_mid (lev\_mid) float64 1.5 2.5
  x (x) float64 7.812e+03 2.344e+04 ... 9.766e+05 9.922e+05
  y (y) float64 7.812e+03 2.344e+04 ... 9.766e+05 9.922e+05
  l (l) float64 0.0 6.283e-06 1.257e-05 ... -1.257e-05 -6.283e-06
  k (k) float64 0.0 6.283e-06 1.257e-05 ... 0.0001948 0.0002011 \]  (continues on next page)
Data variables: (12/24)

- `q` (time, lev, y, x) float64 -7.827e-05 -0.0001178 ... -3.031e-06
- `u` (time, lev, y, x) float64 0.5062 0.4731 ... 0.1182 0.1011
- `v` (time, lev, y, x) float64 0.2718 0.2065 ... 0.2098 0.1877
- `ufull` (time, lev, y, x) float64 0.5562 0.5231 ... 0.1182 0.1011
- `vfull` (time, lev, y, x) float64 0.2718 0.2065 ... 0.2098 0.1877
- `qh` (time, lev, l, k) complex128 (4.194438926138098e-06+0j) ...
  ...
- `APEspec` (l, k) float64 0.0 1.663e+05 2.119e+04 ... 2.2e-25 9.251e-35
- `KEflux_div` (l, k) float64 0.0 0.02921 0.001374 ... 1.336e-17 2.765e-22
- `APEflux_div` (l, k) float64 0.0 -0.1028 -0.007152 ... 3.757e-18 9.383e-23
- `APEgenspec` (l, k) float64 0.0 0.1023 0.007533 ... 1.664e-33 -3.719e-44
- `ENSflux` (l, k) float64 0.0 -7.638e-10 ... 8.308e-25 1.893e-29
- `ENSgenspec` (l, k) float64 -0.0 7.62e-10 5.593e-11 ... 2.334e-41 -2.27e-52

Attributes: (12/24)

- `pyqg:beta`: 1.2130692965249345e-11
- `pyqg:delta`: None
- `pyqg:dt`: 1500.0
- `pyqg:filterfac`: 23.6
- `pyqg:L`: 1000000.0
- `pyqg:M`: 4096
  ...
- `pyqg:tc`: 60000
- `pyqg:tmax`: 90000000.0
- `pyqg:twrite`: 5000
- `pyqg:W`: 1000000.0
- `title`: pyqg: Python Quasigeostrophic Model

Snapshots

[7]: PV = ds.q + ds.Qy * ds.y
PV['x'] = ds.x/ds.attrs['pyqg:rd']; PV.x.attrs = {'long_name': r'\$x/L_d\$'}
PV['y'] = ds.y/ds.attrs['pyqg:rd']; PV.y.attrs = {'long_name': r'\$y/L_d\$'}

[8]: plt.figure(figsize=(18,4))
plt.subplot(131)
PV.sel(lev=1).plot(cmap='Spectral_r')
plt.subplot(132)
PV.sel(lev=2).plot(cmap='Spectral_r')
plt.subplot(133)
PV.sel(lev=3).plot(cmap='Spectral_r')

[8]: <matplotlib.collections.QuadMesh at 0x7fe53b3f7fd0>
pyqg has a built-in method that computes the vertical modes. It is stored as an attribute in the Dataset.

```
[9]: print(f"The first baroclinic deformation radius is \( \frac{\text{ds.attrs['pyqg:radii'][1]}}{1.e3} \) km")
print(f"The second baroclinic deformation radius is \( \frac{\text{ds.attrs['pyqg:radii'][2]}}{1.e3} \) km")
```

The first baroclinic deformation radius is 15.375382785987185 km
The second baroclinic deformation radius is 7.975516271996243 km

We can project the solution onto the modes

```
[10]: pn = m.modal_projection(m.p)
```

```
[11]: plt.figure(figsize=(18,4))
    plt.pcolormesh(m.x/m.rd, m.y/m.rd, pn[0]/(U1*Ld), cmap='Spectral_r', shading='auto')
    plt.xlabel(r'$x/L_d$')
    plt.ylabel(r'$y/L_d$')
    plt.colorbar()
    plt.title('Barotropic streamfunction')
    plt.subplot(132)
    plt.pcolormesh(m.x/m.rd, m.y/m.rd, pn[1]/(U1*Ld), cmap='Spectral_r', shading='auto')
    plt.xlabel(r'$x/L_d$')
    plt.ylabel(r'$y/L_d$')
    plt.colorbar()
    plt.title('1st baroclinic streamfunction')
    plt.subplot(133)
    plt.pcolormesh(m.x/m.rd, m.y/m.rd, pn[2]/(U1*Ld), cmap='Spectral_r', shading='auto')
    plt.xlabel(r'$x/L_d$')
    plt.ylabel(r'$y/L_d$')
    plt.colorbar()
    plt.title('2nd baroclinic streamfunction');
```
Diagnostics

[12]: kr, kespec_1 = tools.calc_ispec(m, ds.KEspec.sel(lev=1).data)
    _, kespec_2 = tools.calc_ispec(m, ds.KEspec.sel(lev=2).data)
    _, kespec_3 = tools.calc_ispec(m, ds.KEspec.sel(lev=3).data)

    plt.loglog( kr, kespec_1, '.-' )
    plt.loglog( kr, kespec_2, '.-' )
    plt.loglog( kr, kespec_3, '.-' )

    plt.legend(['layer 1', 'layer 2', 'layer 3'], loc='lower left')
    plt.ylim([1e-14,1e-6]);
    plt.xlabel(r'k (m$^{-1}$)'); plt.grid()
    plt.title('Kinetic Energy Spectrum');

By default the modal KE and PE spectra are also calculated

[13]: kr, modal_kespec_1 = tools.calc_ispec(m, ds.KEspec_modal.sel(lev=1).data)
    _, modal_kespec_2 = tools.calc_ispec(m, ds.KEspec_modal.sel(lev=2).data)
    _, modal_kespec_3 = tools.calc_ispec(m, ds.KEspec_modal.sel(lev=3).data)

    _, modal_pespec_2 = tools.calc_ispec(m, ds.PEspec_modal.sel(lev_mid=1.5).data)
    _, modal_pespec_3 = tools.calc_ispec(m, ds.PEspec_modal.sel(lev_mid=2.5).data)
plt.figure(figsize=(15,5))
plt.subplot(121)
plt.loglog(kr, modal_kespec_1, '.-')
plt.loglog(kr, modal_kespec_2, '.-')
plt.loglog(kr, modal_kespec_3, '.-')
plt.legend(['barotropic', '1st baroclinic', '2nd baroclinic'], loc='lower left')
plt.ylim([1e-14,1e-6]);
plt.xlabel(r'$k$ (m$^{-1}$)'); plt.grid()
plt.title('Kinetic Energy Spectra');
plt.subplot(122)
plt.loglog(kr, modal_pespec_2, '.-')
plt.loglog(kr, modal_pespec_3, '.-')
plt.legend(['1st baroclinic', '2nd baroclinic'], loc='lower left')
plt.ylim([1e-14,1e-6]);
plt.xlabel(r'$k$ (m$^{-1}$)'); plt.grid()
plt.title('Potential Energy Spectra');

_, APEgenspec = tools.calc_ispec(m, ds.APEgenspec.data)
_, APEflux = tools.calc_ispec(m, ds.APEflux_div.data)
_, KEflux = tools.calc_ispec(m, ds.KEflux_div.data)
_, KEspec = tools.calc_ispec(m, (ds.KEspec.sel(lev=1) * ds.attrs['pyqg:M']**2).data)

ebud = [ APEgenspec,
         APEflux,
         KEflux,
         -ds.attrs['pyqg:rek']*(m.Hi[-1]/m.H)*KEspec ]
ebud.append(-np.vstack(ebud).sum(axis=0))
ebud_labels = ['APE gen','APE flux div. ','KE flux div. ','Diss. ','Resid. ']
plt.semilogx(kr, term for term in ebud)
plt.legend(ebud_labels, loc='upper right')
plt.xlabel(r'$k$ (m$^{-1}$)'); plt.grid()
plt.title('Spectral Energy Transfers');
The dynamics here is similar to the reference experiment of Larichev & Held (1995). The APE generated through baroclinic instability is fluxed towards deformation length scales, where it is converted into KE. The KE the experiments and inverse transfer, cascading up to the scale of the domain. The mechanical bottom drag essentially removes the large scale KE.

### 1.3.3 Barotropic Model

Here will will use pyqg to reproduce the results of the paper: J. C. Mcwilliams (1984). The emergence of isolated coherent vortices in turbulent flow. Journal of Fluid Mechanics, 146, pp 21-43 doi:10.1017/S0022112084001750

```python
import numpy as np
import matplotlib.pyplot as plt

import pyqg

McWilliams performed freely-evolving 2D turbulence ($R_d = \infty, \beta = 0$) experiments on a $2\pi \times 2\pi$ periodic box.

```python
# create the model object
m = pyqg.BTModel(L=2.*np.pi, nx=256,
                  beta=0., H=1., rek=0., rd=None,
                  tmax=40, dt=0.001, taveint=1,
                  ntd=4)

# in this example we used ntd=4, four threads
# if your machine has more (or fewer) cores available, you could try changing it
```

**Initial condition**

The initial condition is random, with a prescribed spectrum

$$|\psi|^2 = A \kappa^{-1} \left[1 + \left(\frac{\kappa}{6}\right)^4\right]^{-1},$$

where $\kappa$ is the wavenumber magnitude. The constant $A$ is determined so that the initial energy is $KE = 0.5$.  

1.3. Examples
# generate McWilliams 84 IC condition

\[
\begin{align*}
    & \text{fk} = \text{m.wv} \neq 0 \\
    & \text{ckappa} = \text{np.zeros_like(m.wv2)} \\
    & \text{ckappa}[\text{fk}] = \text{np.sqrt( m.wv2[\text{fk}]*(1. + (m.wv2[\text{fk}]/36.)**2) )**-1} \\
    & \text{nhx, nhy} = \text{m.wv2.shape} \\
    & \text{Pi_hat} = \text{np.random.randn(nhx,nhy)} \times \text{ckappa} + \text{1j*np.random.randn(nhx,nhy)} \times \text{ckappa} \\
    & \text{Pi} = \text{m.ifft( Pi_hat[np.newaxis,:,:] )} \\
    & \text{Pi} = \text{Pi} - \text{Pi}.\text{mean}() \\
    & \text{Pi_hat} = \text{m.fft( Pi )} \\
    & \text{KEaux} = \text{m.spec_var( m.wv*Pi_hat )} \\
    & \text{pih} = (\text{Pi_hat/np.sqrt(KEaux)}) \\
    & \text{qih} = -\text{m.wv2*pih} \\
    & \text{qi} = \text{m.ifft(qih)} \\
\end{align*}
\]

# initialize the model with that initial condition

\[
\begin{align*}
    & \text{m.set_q(qi)} \\
\end{align*}
\]

# define a quick function for plotting and visualize the initial condition

\[
\begin{align*}
    & \text{def plot_q(m, qmax=40):} \\
    & \quad \text{fig, ax} = \text{plt.subplots()} \\
    & \quad \text{pc} = \text{ax.pcolormesh(m.x,m.y,m.q.squeeze(), cmap='RdBu_r')} \\
    & \quad \text{pc.set_clim([-qmax, qmax])} \\
    & \quad \text{ax.set_xlim([0, 2*np.pi])} \\
    & \quad \text{ax.set_ylim([0, 2*np.pi])} \\
    & \quad \text{ax.set_aspect(1)} \\
    & \quad \text{plt.colorbar(pc)} \\
    & \quad \text{plt.title('Time = $g$' % m.t)} \\
    & \quad \text{plt.show()} \\
    & \text{plot_q(m)} \\
\end{align*}
\]
Runing the model

Here we demonstrate how to use the `run_with_snapshots` feature to periodically stop the model and perform some action (in this case, visualization).

```python
for _ in m.run_with_snapshots(tsnapstart=0, tsnapint=10):
    plot_q(m)
```

<table>
<thead>
<tr>
<th>t</th>
<th>tc</th>
<th>cfl</th>
<th>ke</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1000</td>
<td>0.1044</td>
<td>0.4964</td>
</tr>
<tr>
<td>2</td>
<td>2000</td>
<td>0.1106</td>
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</tr>
<tr>
<td>3</td>
<td>3000</td>
<td>0.1013</td>
<td>0.4943</td>
</tr>
<tr>
<td>4</td>
<td>4000</td>
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<td>0.4938</td>
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<tr>
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<td>6000</td>
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<td>0.4932</td>
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<tr>
<td>7</td>
<td>7000</td>
<td>0.0925</td>
<td>0.4931</td>
</tr>
<tr>
<td>8</td>
<td>8000</td>
<td>0.0962</td>
<td>0.4929</td>
</tr>
<tr>
<td>9</td>
<td>9000</td>
<td>0.0979</td>
<td>0.4929</td>
</tr>
<tr>
<td>10</td>
<td>10000</td>
<td>0.1033</td>
<td>0.4928</td>
</tr>
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<td>11</td>
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<td>0.1027</td>
<td>0.4927</td>
</tr>
<tr>
<td>12</td>
<td>12000</td>
<td>0.0998</td>
<td>0.4927</td>
</tr>
<tr>
<td>13</td>
<td>13000</td>
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<td>0.4926</td>
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<tr>
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<td>14000</td>
<td>0.1029</td>
<td>0.4926</td>
</tr>
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<td>0.4925</td>
</tr>
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<td>17</td>
<td>17000</td>
<td>0.1225</td>
<td>0.4925</td>
</tr>
<tr>
<td>18</td>
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<td>0.1206</td>
<td>0.4925</td>
</tr>
<tr>
<td>19</td>
<td>19000</td>
<td>0.1037</td>
<td>0.4924</td>
</tr>
</tbody>
</table>

1.3. Examples
Time = 20

<table>
<thead>
<tr>
<th>t</th>
<th>tc</th>
<th>cfl</th>
<th>ke</th>
</tr>
</thead>
<tbody>
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<td>0.113210</td>
<td>0.492452605</td>
</tr>
<tr>
<td>21</td>
<td>21000</td>
<td>0.095246</td>
<td>0.492439588</td>
</tr>
<tr>
<td>22</td>
<td>22000</td>
<td>0.092449</td>
<td>0.492429553</td>
</tr>
<tr>
<td>23</td>
<td>23000</td>
<td>0.115412</td>
<td>0.492419773</td>
</tr>
<tr>
<td>24</td>
<td>24000</td>
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<td>0.492407434</td>
</tr>
<tr>
<td>25</td>
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<td>0.098588</td>
<td>0.492396021</td>
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<tr>
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<td>0.492361675</td>
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Time = 30

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<th>cfl</th>
<th>ke</th>
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<td>0.492352666</td>
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<td>0.492331664</td>
</tr>
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<td>0.492317502</td>
</tr>
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<td>0.101901</td>
<td>0.492302225</td>
</tr>
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<td>37000</td>
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<td>38000</td>
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<td>39</td>
<td>39000</td>
<td>0.110105</td>
<td>0.492278000</td>
</tr>
</tbody>
</table>

Chapter 1. Contents
The genius of McWilliams (1984) was that he showed that the initial random vorticity field organizes itself into strong coherent vortices. This is true in significant part of the parameter space. This was previously suspected but unproven, mainly because people did not have computer resources to run the simulation long enough. Thirty years later we can perform such simulations in a couple of minutes on a laptop!

Also, note that the energy is nearly conserved, as it should be, and this is a nice test of the model.

### Plotting spectra

```python
[7]:
   energy = m.get_diagnostic('KEspec')
   enstrophy = m.get_diagnostic('Ensspec')

[11]:
   # this makes it easy to calculate an isotropic spectrum
   from pyqg import diagnostic_tools as tools
   kr, energy_iso = tools.calc_ispec(m,energy.squeeze())
   _, enstrophy_iso = tools.calc_ispec(m,enstrophy.squeeze())

[17]:
   ks = np.array([3.,80])
   es = 5*ks**-4
   plt.loglog(kr,energy_iso)
   plt.loglog(ks,es,'k--')
   plt.text(2.5,.0001,r'$k^{-4}$',fontsize=20)
   plt.ylim(1.e-10,1.e0)
   plt.xlabel('wavenumber')
   plt.title('Energy Spectrum')

[17]: <matplotlib.text.Text at 0x10c1b1a90>
```
ks = np.array([3., 80])
es = 5 * ks ** (-5./3)
plt.loglog(kr, enstrophy_iso)
plt.loglog(ks, es, 'k--')
plt.text(5.5, .01, r'$k^{-5/3}$', fontsize=20)
plt.ylim(1.e-3, 1.e0)
plt.xlabel('wavenumber')
plt.title('Enstrophy Spectrum')
1.3.4 Surface Quasi-Geostrophic (SQG) Model


```python
import matplotlib.pyplot as plt
import numpy as np
from numpy import pi
%matplotlib inline
from pyqg import sqg_model
```

Surface quasi-geostrophy (SQG) is a relatively simple model that describes surface intensified flows due to buoyancy. One of it’s advantages is that it only has two spatial dimensions but describes a three-dimensional solution.

If we define $b$ to be the buoyancy, then the evolution equation for buoyancy at each the top and bottom surface is

$$\partial_t b + J(\psi, b) = 0.$$ 

The invertibility relation between the streamfunction, $\psi$, and the buoyancy, $b$, is hydrostatic balance

$$b = \partial_z \psi.$$ 

Using the fact that the Potential Vorticity is exactly zero in the interior of the domain and that the domain is semi-infinite, yields that the inversion in Fourier space is,

$$\hat{b} = K \hat{\psi}.$$ 

Held et al. studied several different cases, the first of which was the nonlinear evolution of an elliptical vortex. There are several other cases that they studied and people are welcome to adapt the code to study those as well. But here we focus on this first example for pedagogical reasons.

```python
# create the model object
year = 1.
m = sqg_model.SQGModel(L=2.*pi,nx=512, tmax = 26.005,
    beta = 0., Nb = 1., H = 1., rek = 0., rd = None, dt = 0.005,
    taveint=1, twrite=400, ntd=4)
# in this example we used ntd=4, four threads
# if your machine has more (or fewer) cores available, you could try changing it
```

Initial condition

The initial condition is an elliptical vortex,

$$b = 0.01 \exp(- (x^2 + (4y)^2)/(L/y)^2)$$
where $L$ is the length scale of the vortex in the $x$ direction. The amplitude is 0.01, which sets the strength and speed of the vortex. The aspect ratio in this example is 4 and gives rise to an instability. If you reduce this ratio sufficiently you will find that it is stable. Why don’t you try it and see for yourself?

```python
# Choose ICs from Held et al. (1995)
# case i) Elliptical vortex
x = np.linspace(m.dx/2,2*np.pi,m.nx) - np.pi
y = np.linspace(m.dy/2,2*np.pi,m.ny) - np.pi
x,y = np.meshgrid(x,y)
qi = -np.exp(-(x**2 + (4.0*y)**2)/(m.L/6.0)**2)

# initialize the model with that initial condition
m.set_q(qi[np.newaxis,:,::])

# Plot the ICs
plt.rcParams['image.cmap'] = 'RdBu'
p1 = plt.imshow(m.q.squeeze() + m.beta * m.y)
plt.title('b(x,y,t=0)')
plt.colorbar()
plt.clim([-1, 0])
plt.xticks([])
plt.yticks([])
plt.show()
```

Running the model

Here we demonstrate how to use the `run_with_snapshots` feature to periodically stop the model and perform some action (in this case, visualization).
for snapshot in m.run_with_snapshots(tsnapstart=0., tsnapint=400*m.dt):
    plt.clf()
    pl = plt.imshow(m.q.squeeze() + m.beta * m.y)
    #plt.clim([-30., 30.])
    plt.title('t='+str(m.t))
    plt.colorbar()
    plt.clim([-1, 0])
    plt.xticks([])
    plt.yticks([])
    plt.show()
INFO: Step: 1600, Time: 8.00e+00, KE: 5.21e-03, CFL: 0.273

INFO: Step: 2000, Time: 1.00e+01, KE: 5.21e-03, CFL: 0.267
1.3. Examples
INFO: Step: 4800, Time: 2.40e+01, KE: 5.18e-03, CFL: 0.242

INFO: Step: 5200, Time: 2.60e+01, KE: 5.17e-03, CFL: 0.263
Compare these results with Figure 2 of the paper. In this simulation you see that as the cyclone rotates it develops thin arms that spread outwards and become unstable because of their strong shear. This is an excellent example of how smaller scale vortices can be generated from a mesoscale vortex.

You can modify this to run it for longer time to generate the analogue of their Figure 3.

### 1.3.5 Built-in linear stability analysis

```python
[11]: import numpy as np
    from numpy import pi
    import matplotlib.pyplot as plt
    %matplotlib inline

    import pyqg

[12]: m = pyqg.LayeredModel(nx=256, nz = 2, U = [.01, -.01], V = [0., 0.], H = [1., 1.],
            L=2*pi,beta=1.5, rd=1./20., rek=0.05, f=1.,delta=1.)

INFO: Logger initialized
INFO: Kernel initialized

To perform linear stability analysis, we simply call pyqg’s built-in method `stability_analysis`:

```python
[3]: evals,evecs = m.stability_analysis()
```

The eigenvalues are stored in `omg`, and the eigenvectors in `evec`. For plotting purposes, we use `fftshift` to reorder the entries.

```python
[4]: evals = np.fft.fftshift(evals.imag,axes=(0,))

k,l = m.k*m.radii[1], np.fft.fftshift(m.l,axes=(0,))*m.radii[1]
```

It is also useful to analyze the fastest-growing mode:

```python
[5]: argmax = evals[m.Ny/2,:].argmax()
    evec = np.fft.fftshift(evecs,axes=(1))[:,m.Ny/2,argmax]
    kmax = k[m.Ny/2,argmax]
```

(continues on next page)
x = np.linspace(0, 4.*pi/kmax, 100)
mag, phase = np.abs(evec), np.arctan2(evec.imag, evec.real)

By default, the stability analysis above is performed without bottom friction, but the stability method also supports bottom friction:

```python
[6]: evals_fric, evecs_fric = m.stability_analysis(bottom_friction=True)
evals_fric = np.fft.fftshift(evals_fric.imag, axes=(0,))
argmax = evals_fric[m.Ny/2, :].argmax()
evec_fric = np.fft.fftshift(evecs_fric, axes=(1))[::-1, m.Ny/2, argmax]
kmax_fric = k[m.Ny/2, argmax]
mag_fric, phase_fric = np.abs(evec_fric), np.arctan2(evec_fric.imag, evec_fric.real)
```

Plotting growth rates

```python
[10]: plt.figure(figsize=(14, 4))
plt.subplot(121)
plt.contour(k, l, evals, colors='k')
plt.pcolormesh(k, l, evals, cmap='Blues')
plt.colorbar()
plt.xlim(0, 2.); plt.ylim(-2., 2.)
plt.clim([0., 0.1])
plt.xlabel(r'$k \ L_d$'); plt.ylabel(r'$l \ L_d$')
plt.title('without bottom friction')
plt.subplot(122)
plt.contour(k, l, evals_fric, colors='k')
plt.pcolormesh(k, l, evals_fric, cmap='Blues')
plt.colorbar()
plt.xlim(0, 2.); plt.ylim(-2., 2.)
plt.clim([0., 0.1])
plt.xlabel(r'$k \ L_d$'); plt.ylabel(r'$l \ L_d$')
plt.title('with bottom friction')
```

![Plotting growth rates](image-url)
Plotting the wavestructure of the most unstable modes

```python
[9]: plt.figure(figsize=(12,5))
plt.plot(x,mag[0]*np.cos(kmax*x + phase[0]),'b',label='Layer 1')
plt.plot(x,mag[1]*np.cos(kmax*x + phase[1]),'g',label='Layer 2')
plt.plot(x,mag_fric[0]*np.cos(kmax_fric*x + phase_fric[0]),'b--')
plt.plot(x,mag_fric[1]*np.cos(kmax_fric*x + phase_fric[1]),'g--')
plt.legend(loc=8)
plt.xlabel(r'\$x/L_d\$'); plt.ylabel(r'\$y/L_d\$')
```

[9]: <matplotlib.text.Text at 0x114c6d410>
This calculation shows the classic phase-tilting of baroclinic unstable waves (e.g. Vallis 2006).

1.3.6 Parameterizations

In this example, we’ll implement the physical parameterization learned by symbolic regression in Zanna and Bolton 2020:

```
[2]:
def zb2020_parameterization(m, factor=-46761284):
    """Implements the parameterization from Equation 6 of https://doi.org/10.1029/2020GL088376""
    ik = 1j * m.k
    il = 1j * m.l

    # Compute relative velocity derivatives in spectral space
    uh = m.fft(m.u)
    vh = m.fft(m.v)
    vx = m.ifft(vh * ik)
    vy = m.ifft(vh * il)
    uy = m.ifft(uh * il)
    ux = m.ifft(uh * ik)

    # Compute ZB2020 basis functions
    rel_vort = vx - uy
```
shearing = vx + uy
stretching = ux - vy

# Combine them in real space and take their FFT
rv_stretch = m.fft(rel_vort * stretching)
rv_shear = m.fft(rel_vort * shearing)
sum_sqs = m.fft(rel_vort**2 + shearing**2 + stretching**2) / 2.0

# Take spectral-space derivatives and multiply by the scaling factor
Su = factor * m.ifft(ik*(sum_sqs - rv_shear) + il*rv_stretch)
Sv = factor * m.ifft(il*(sum_sqs + rv_shear) + ik*rv_stretch)

return Su, Sv

This function parameterizes subgrid forcing in terms of changes that should be applied to the real-space velocity tendencies. To use it in a pyqg.Model, we can pass it during initialization as `uv_parameterization`, and then its outputs will be added to the spectral-space potential vorticity tendency $\partial_t q$ (after suitable transformations, and at each timestep). Note that we can also define parameterizations in terms of PV directly by initializing the model with a `q_parameterization` function (which should return a single array rather than a tuple of two).

Run models

To illustrate the effect of the parameterization, we’ll run three variants of models:

- one without parameterization at $nx=64$ resolution (where $\Delta x$ is larger than the deformation radius $r_d$, preventing the model from fully resolving eddies),
- one with parameterization at $nx=64$ resolution,
- one at a higher $nx=256$ resolution (where $\Delta x$ is ~4x finer than the deformation radius, so eddies can be almost fully resolved).

[3]:
```python
%%time
m_unparam = pyqg.QGModel(nx=64, dt=3600., tmax=10*year, tavestart=5*year,
--> twrite=10000)
m_unparam.run()
```

INFO: Logger initialized
INFO: Step: 10000, Time: 3.60e+07, KE: 1.92e-05, CFL: 0.007
INFO: Step: 20000, Time: 7.20e+07, KE: 4.28e-04, CFL: 0.051
INFO: Step: 30000, Time: 1.08e+08, KE: 4.88e-04, CFL: 0.045
INFO: Step: 40000, Time: 1.44e+08, KE: 4.98e-04, CFL: 0.042
INFO: Step: 50000, Time: 1.80e+08, KE: 4.54e-04, CFL: 0.052
INFO: Step: 60000, Time: 2.16e+08, KE: 5.30e-04, CFL: 0.052
INFO: Step: 70000, Time: 2.52e+08, KE: 4.62e-04, CFL: 0.040
INFO: Step: 80000, Time: 2.88e+08, KE: 4.90e-04, CFL: 0.044

CPU times: user 20.4 s, sys: 70.4 ms, total: 20.5 s
Wall time: 20.7 s

[4]:
```python
%%time
m_param = pyqg.QGModel(nx=64, dt=3600., tmax=10*year, tavestart=5*year, twrite=10000,
--> uv_parameterization=zb2020_parameterization)
m_param.run()
```

INFO: Logger initialized
INFO: Step: 10000, Time: 3.60e+07, KE: 1.69e-05, CFL: 0.006

(continues on next page)
INFO: Step: 20000, Time: 7.20e+07, KE: 3.78e-04, CFL: 0.047
INFO: Step: 30000, Time: 1.08e+08, KE: 4.27e-04, CFL: 0.043
INFO: Step: 40000, Time: 1.44e+08, KE: 3.65e-04, CFL: 0.039
INFO: Step: 50000, Time: 1.80e+08, KE: 4.37e-04, CFL: 0.048
INFO: Step: 60000, Time: 2.16e+08, KE: 4.26e-04, CFL: 0.045
INFO: Step: 70000, Time: 2.52e+08, KE: 3.90e-04, CFL: 0.040
INFO: Step: 80000, Time: 2.88e+08, KE: 3.94e-04, CFL: 0.047

CPU times: user 57.8 s, sys: 202 ms, total: 58 s
Wall time: 59 s

Note that parameterization does slow down the simulation, but it’s still significantly faster than running a high-resolution simulation.

Plot spectra

Now let’s examine how adding the parameterization to our simulation changed its energetic properties:

```python
from pyqg import diagnostic_tools as tools
from scipy.stats import linregress
plt.figure(figsize=(10,6))
plt.title("Comparison of kinetic energy spectra", fontsize=16)
for m, label in zip([m_unparam, m_param, m_hires], ['Lo-res', 'Lo-res + parameterization', 'Hi-res']):
    # Calculate the spectrum
    k, spectrum = tools.calc_ispec(m, m.get_diagnostic('KEspec').sum(axis=0))
    # Do a power law fit on data in the intertial range
    kmin = 5e-5
    kmax = 1e-4
    i = np.argmin(np.abs(np.log(k) - np.log(kmin)))
    j = np.argmin(np.abs(np.log(k) - np.log(kmax)))
    lr = linregress(np.log(k[i:j]), np.log(spectrum[i:j]))
    # Plot the spectrum with the linear fit
    loglog_plot = plt.loglog(k, spectrum, lw=5, alpha=0.9,
```

(continues on next page)
Although the overall energy is lower, the parameterization ends up with an inverse cascade whose decay rate (log-log slope over inertial length scales) is much closer to that of the high-resolution model.

1.4 API

1.4.1 Base Model Class

This is the base class from which all other models inherit. All of these initialization arguments are available to all of the other model types. This class is not called directly.

```python
class pyqg.Model(nz=1, nx=64, ny=None, L=1000000.0, W=None, dt=7200.0, twrite=1000.0, tmax=1576800000.0, tavestart=315360000.0, taveint=86400.0, useAB2=False, rek=5.787e-07, filterfac=23.6, f=None, g=9.81, q_parameterization=None, uv_parameterization=None, diagnostics_list='all', ntd=1, log_level=1, log_file=None)
```

A generic pseudo-spectral inversion model.
Attributes

nx, ny [int] Number of real space grid points in the x, y directions (cython)

nk, nl [int] Number of spectral space grid points in the k, l directions (cython)

nz [int] Number of vertical levels (cython)

kk, ll [real array] Zonal and meridional wavenumbers (nk) (cython)

a [real array] inversion matrix (nk, nk, nl, nk) (cython)

q [real array] Potential vorticity in real space (nz, ny, nx) (cython)

qh [complex array] Potential vorticity in spectral space (nk, nl, nk) (cython)

ph [complex array] Streamfunction in spectral space (nk, nl, nk) (cython)

u, v [real array] Zonal and meridional velocity anomalies in real space (nz, ny, nx) (cython)

Ubg [real array] Background zonal velocity (nk) (cython)

Qy [real array] Background potential vorticity gradient (nk) (cython)

ufull, vfull [real arrays] Zonal and meridional full velocities in real space (nz, ny, nx) (cython)

uh, vh [complex arrays] Velocity anomaly components in spectral space (nk, nl, nk) (cython)

rek [float] Linear drag in lower layer (cython)

t [float] Model time (cython)

tc [int] Model timestep (cython)

dt [float] Numerical timestep (cython)

L, W [float] Domain length in x and y directions

filterfac [float] Amplitude of the spectral spherical filter

twrite [int] Interval for cfl writeout (units: number of timesteps)

tmax [float] Total time of integration (units: model time)

tavestart [float] Start time for averaging (units: model time)

tsnapstart [float] Start time for snapshot writeout (units: model time)

taveint [float] Time interval for accumulation of diagnostic averages. (units: model time)

tsnapint [float] Time interval for snapshots (units: model time)

ntd [int] Number of threads to use. Should not exceed the number of cores on your machine.

pmodes [real array] Vertical pressure modes (unitless)

radii [real array] Deformation radii (units: model length)

q_parameterization [function] Optional function which takes the model as input and returns a numpy array of shape (nz, ny, nx) to be added to dq/dt before stepping forward. This can be used to implement subgrid forcing parameterizations.

uv_parameterization [function] Optional function which takes the model as input and returns a tuple of two numpy arrays, each of shape (nz, ny, nx), to be added to the zonal and meridional velocity derivatives (respectively) at each timestep. This can also be used to implemented subgrid forcing parameterizations, but expressed in terms of velocity rather than potential vorticity.
Note: All of the test cases use \(nx==ny\). Expect bugs if you choose these parameters to be different.

Note: All time intervals will be rounded to nearest \(dt\) interval.

Parameters

\(nx\) [int] Number of grid points in the x direction.
\(ny\) [int] Number of grid points in the y direction (default: \(nx\)).
\(L\) [number] Domain length in x direction. Units: meters.
\(W\) : Domain width in y direction. Units: meters (default: \(L\)).
\(rek\) [number] linear drag in lower layer. Units: seconds \(^{-1}\).
\(filterfac\) [number] amplitude of the spectral spherical filter (originally 18.4, later changed to 23.6).
\(dt\) [number] Numerical timstep. Units: seconds.
\(twrite\) [int] Interval for cfl writeout. Units: number of timesteps.
\(tmax\) [number] Total time of integration. Units: seconds.
\(tavestart\) [number] Start time for averaging. Units: seconds.
\(tsnapstart\) [number] Start time for snapshot writeout. Units: seconds.
\(taveint\) [number] Time interval for accumulation of diagnostic averages. Units: seconds. (For performance purposes, averaging does not have to occur every timestep)
\(tsnapint\) [number] Time interval for snapshots. Units: seconds.
\(ntd\) [int] Number of threads to use. Should not exceed the number of cores on your machine.
\(q\_parameterization\) [function] Optional function which takes the model as input and returns a \textit{numpy} array of shape \((nz, ny, nx)\) to be added to \(dq/dt\) before stepping forward. This can be used to implement subgrid forcing parameterizations.
\(uv\_parameterization\) [function] Optional function which takes the model as input and returns a tuple of two \textit{numpy} arrays, each of shape \((nz, ny, nx)\), to be added to the zonal and meridional velocity derivatives (respectively) at each timestep. This can also be used to implemented subgrid forcing parameterizations, but expressed in terms of velocity rather than potential vorticity.

\texttt{describe_diagnostics()}\n
Print a human-readable summary of the available diagnostics.

\texttt{modal_projection}(p, forward=True)\n
Performs a field \(p\) into modal amplitudes \(pn\) using the basis \([pmodes]\). The inverse transform calculates \(p\) from \(pn\)

\texttt{run()}\n
Run the model forward without stopping until the end.

\texttt{run_with_snapshots}(tsnapstart=0.0, tsnapint=432000.0)\n
Run the model forward, yielding to user code at specified intervals.

Parameters
tsnapstart  [int] The timestep at which to begin yielding.

tstapint  [int] The interval at which to yield.

**spec_var** *(ph)*
compute variance of p from Fourier coefficients ph

**stability_analysis** *(bottom_friction=False)*

**Performs the baroclinic linear instability analysis given**
given the base state velocity :math: (U, V) and
the stretching matrix :math: S:

\[
A \Phi = \omega B \Phi,
\]

where

\[
A = B(U_k + V_l) + I(kQ_y - lQ_x) + 1j\delta_{NN} r_{ek} \kappa^2
\]

where \(\delta_{NN} = [0, 0, \ldots, 0, 1]\),

and

\[
B = S - I\kappa^2.
\]

The eigenstructure is

\[
\Phi
\]

and the eigenvalue is

\[
'\omega'.
\]

The growth rate is \(\text{Im}\{\omega}\).

**Parameters**

*bottom_friction*: *optional inclusion linear bottom drag* in the linear stability calculation
(default is False, as if :math: r_{ek} = 0)

**Returns**

*omega*: *complex array* The eigenvalues with largest complex part (units: inverse model time)

*phi*: *complex array* The eigenvectors associated with omega (unitless)

**to_dataset** ()
Convert outputs from model to an xarray dataset

**vertical_modes** ()
Calculate standard vertical modes. Simply the eigenvectors of the stretching matrix S

### 1.4.2 Specific Model Types

These are the actual models which are run.
class `pyqg.QGModel` *(beta=1.5e-11, rd=15000.0, delta=0.25, H1=500, U1=0.025, U2=0.0, **kwargs)*

Two layer quasigeostrophic model.

This model is meant to represent flows driven by baroclinic instability of a base-state shear $U_1 - U_2$. The upper and lower layer potential vorticity anomalies $q_1$ and $q_2$ are

$$q_1 = \nabla^2 \psi_1 + F_1 (\psi_2 - \psi_1)$$

$$q_2 = \nabla^2 \psi_2 + F_2 (\psi_1 - \psi_2)$$

with

$$F_1 = \frac{k_2^2}{1 + \delta^2}$$

$$F_2 = \delta F_1 .$$

The layer depth ratio is given by $\delta = H_1/H_2$. The total depth is $H = H_1 + H_2$.

The background potential vorticity gradients are

$$\beta_1 = \beta + F_1 (U_1 - U_2)$$

$$\beta_2 = \beta - F_2 (U_1 - U_2) .$$

The evolution equations for $q_1$ and $q_2$ are

$$\partial_t q_1 + J(\psi_1, q_1) + \beta_1 \psi_{1x} = \text{ssd}$$

$$\partial_t q_2 + J(\psi_2, q_2) + \beta_2 \psi_{2x} = -r_{ek} \nabla^2 \psi_2 + \text{ssd} .$$

where $\text{ssd}$ represents small-scale dissipation and $r_{ek}$ is the Ekman friction parameter.

**Parameters**

- `beta` [number] Gradient of coriolis parameter. Units: meters $^{-1}$ seconds $^{-1}$
- `bek` [number] Linear drag in lower layer. Units: seconds $^{-1}$
- `delta` [number] Layer thickness ratio (H1/H2)
- `U1` [number] Upper layer flow. Units: m/s
- `U2` [number] Lower layer flow. Units: m/s

**set_U1U2** *(U1, U2)*

Set background zonal flow.

**Parameters**

- `U1` [number] Upper layer flow. Units: meters seconds $^{-1}$
- `U2` [number] Lower layer flow. Units: meters seconds $^{-1}$

**set_q1q2** *(q1, q2, check=False)*

Set upper and lower layer PV anomalies.

**Parameters**

- `q1` [array-like] Upper layer PV anomaly in spatial coordinates.
- `q1` [array-like] Lower layer PV anomaly in spatial coordinates.
class pyqg.LayeredModel (g=9.81, beta=1.5e-11, nz=4, rd=15000.0, H=None, U=None, V=None, rho=None, delta=None, **kwargs)

Layered quasigeostrophic model.

This model is meant to represent flows driven by baroclinic instability of a base-state shear. The potential vorticity anomalies $q_i$ are related to the streamfunction $\psi_i$ through

$$q_i = \nabla^2 \psi_i + \frac{f^2_0}{H_i} \left( \psi_{i-1} - \psi_i - \psi_{i+1} \right), \quad i = 2, N - 1,$$

$$q_1 = \nabla^2 \psi_1 + \frac{f^2_0}{H_1} \left( \psi_2 - \psi_1 \right), \quad i = 1,$$

$$q_N = \nabla^2 \psi_N + \frac{f^2_0}{H_N} \left( \psi_{N-1} - \psi_N \right) + \frac{f_0}{H_N} h_b, \quad i = N,$$

where the reduced gravity, or buoyancy jump, is

$$g'_i = g \frac{\rho_{i+1} - \rho_i}{\rho_i}.$$

The evolution equations are

$$q_{i,t} + J(\psi_i, q_i) + Q_y \psi_{i,x} - Q_x \psi_{i,y} = ssd - r_{ek} \delta_{iN} \nabla^2 \psi_i, \quad i = 1, N,$$

where the mean potential vorticity gradients are

$$Q_x = SV,$$

and

$$Q_y = \beta I - SU,$$

where $S$ is the stretching matrix, $I$ is the identity matrix, and the background velocity is $\vec{V}(z) = (U, V)$.

**Parameters**

- **nz** [integer number] Number of layers (> 1)
- **beta** [number] Gradient of coriolis parameter. Units: meters$^{-1}$ seconds$^{-1}$
- **rd** [number] Deformation radius. Units: meters. Only necessary for the two-layer (nz=2) case.
- **delta** [number] Layer thickness ratio (H1/H2). Only necessary for the two-layer (nz=2) case. Unitless.
- **U** [list of size nz] Base state zonal velocity. Units: meters s$^{-1}$
- **V** [array of size nz] Base state meridional velocity. Units: meters s$^{-1}$
- **H** [array of size nz] Layer thickness. Units: meters
- **rho**: array of size nz. Layer density. Units: kilograms meters$^{-3}$

class pyqg.BTModel (beta=0.0, rd=0.0, H=1.0, U=0.0, **kwargs)

Single-layer (barotropic) quasigeostrophic model. This class can represent both pure two-dimensional flow and also single reduced-gravity layers with deformation radius $rd$.

The equivalent-barotropic quasigeostrophic evolution equations is

$$\partial_t q + J(\psi, q) + \beta \psi_x = ssd$$

The potential vorticity anomaly is

$$q = \nabla^2 \psi - \kappa_d^2 \psi$$
Parameters

- **beta** [number, optional] Gradient of coriolis parameter. Units: meters $^{-1}$ seconds $^{-1}$
- **rd** [number, optional] Deformation radius. Units: meters.
- **U** [number, optional] Upper layer flow. Units: meters seconds $^{-1}$.

**set_U(U)**
Set background zonal flow.

**class** `pyqg.SQGModel` *(beta=0.0, Nb=1.0, rd=0.0, H=1.0, U=0.0, **kwargs)*
Surface quasigeostrophic model.

Parameters

- **beta** [number] Gradient of coriolis parameter. Units: meters $^{-1}$ seconds $^{-1}$
- **Nb** [number] Buoyancy frequency. Units: seconds $^{-1}$.
- **U** [number] Background zonal flow. Units: meters.

**set_U(U)**
Set background zonal flow

### 1.4.3 Lagrangian Particles

**class** `pyqg.LagrangianParticleArray2D` *(x0, y0, periodic_in_x=False, periodic_in_y=False, xmin=-inf, xmax=inf, ymin=-inf, ymax=inf, particle_dtype='f8')*
A class for keeping track of a set of lagrangian particles in two-dimensional space. Tries to be fast.

Parameters

- **x0**, **y0** [array-like] Two arrays (same size) representing the particle initial positions.
- **periodic_in_x** [bool] Whether the domain wraps in the x direction.
- **periodic_in_y** [bool] Whether the domain ‘wraps’ in the y direction.
- **xmin**, **xmax** [numbers] Maximum and minimum values of x coordinate
- **ymin**, **ymax** [numbers] Maximum and minimum values of y coordinate
- **particle_dtype** [dtype] Data type to use for particles

**step_forward_with_function** *(uv0fun, uv1fun, dt)*
Advance particles using a function to determine u and v.

Parameters

- **uv0fun** [function] Called like `uv0fun(x, y)`. Should return the velocity field u, v at time t.
- **uv1fun(x,y)** [function] Called like `uv1fun(x, y)`. Should return the velocity field u, v at time t + dt.
- **dt** [number] Timestep.

**class** `pyqg.GriddedLagrangianParticleArray2D` *(x0, y0, Nx, Ny, grid_type='A', **kwargs)*
Lagrangian particles with velocities given on a regular cartesian grid.
Parameters

\( x_0, y_0 \) [array-like] Two arrays (same size) representing the particle initial positions.

Nx, Ny: int Number of grid points in the x and y directions

grid_type: {'A'} Arakawa grid type specifying velocity positions.

interpolate_gridded_scalar \((x, y, c, order=1, pad=1, offset=0)\)
Interpolate gridded scalar \(C\) to points \(x,y\).

Parameters

\( x, y \) [array-like] Points at which to interpolate

\( c \) [array-like] The scalar, assumed to be defined on the grid.

order [int] Order of interpolation

pad [int] Number of pad cells added

offset [int] ???

Returns

\( ci \) [array-like] The interpolated scalar

step_forward_with_gridded_uv \((U0, V0, U1, V1, dt, order=1)\)
Advance particles using a gridded velocity field. Because of the Runge-Kutta timestepping, we need two velocity fields at different times.

Parameters

\( U0, V0 \) [array-like] Gridded velocity fields at time \(t - dt\).

\( U1, V1 \) [array-like] Gridded velocity fields at time \(t\).

\( dt \) [number] Timestep.

order [int] Order of interpolation.

1.4.4 Diagnostic Tools

Utility functions for pyqg model data.

pyqg.diagnostic_tools.calc_ispec \((model, ph)\)
Compute isotropic spectrum \(phr\) of \(ph\) from 2D spectrum.

Parameters

\( model \) [pyqg.Model instance] The model object from which \(ph\) originates

\( ph \) [complex array] The field on which to compute the variance

Returns

\( kr \) [array] isotropic wavenumber

\( phr \) [array] isotropic spectrum

pyqg.diagnostic_tools.spec_sum \((ph2)\)
Compute total spectral sum of the real spectral quantity\(^2\).

Parameters

\( model \) [pyqg.Model instance] The model object from which \(ph\) originates

\( ph2 \) [real array] The field on which to compute the sum
Returns

`var_dens` [float] The sum of `ph2`

```python
pyqg.diagnostic_tools.spec_var(model, ph)
```

Compute variance of `p` from Fourier coefficients `ph`.

Parameters

- `model` [pyqg.Model instance] The model object from which `ph` originates
- `ph` [complex array] The field on which to compute the variance

Returns

`var_dens` [float] The variance of `ph`

### 1.5 Development

#### 1.5.1 Team

- Malte Jansen, University of Chicago
- Ryan Abernathey, Columbia University / LDEO
- Cesar Rocha, Woods Hole Oceanographic Institution
- Francis Poulin, University of Waterloo

#### 1.5.2 History

The numerical approach of pyqg was originally inspired by a MATLAB code by Glenn Flierl of MIT, who was a teacher and mentor to Ryan and Malte. It would be hard to find anyone in the world who knows more about this sort of model than Glenn. Malte implemented a python version of the two-layer model while at GFDL. In the summer of 2014, while both were at the WHOI GFD Summer School, Ryan worked with Malte refactor the code into a proper python package. Cesar got involved and brought pyfftw into the project. Ryan implemented a cython kernel. Cesar and Francis implemented the barotropic and sqg models.

#### 1.5.3 Future

By adopting open-source best practices, we hope pyqg will grow into a widely used, community-based project. We know that many other research groups have their own “in house” QG models. You can get involved by trying out the model, filing issues if you find problems, and making pull requests if you make improvements.

#### 1.5.4 Development Workflow

Anyone interested in helping to develop pyqg needs to create their own fork of our git repository. (Follow the github forking instructions. You will need a github account.)

Clone your fork on your local machine.

```
$ git clone git@github.com:USERNAME/pyqg
```

(In the above, replace USERNAME with your github user name.)

Then set your fork to track the upstream pyqg repo.)
```
$ cd pyqg
$ git remote add upstream git://github.com/pyqg/pyqg.git
```

You will want to periodically sync your master branch with the upstream master.

```
$ git fetch upstream
$ git rebase upstream/master
```

Never make any commits on your local master branch. Instead open a feature branch for every new development task.

```
$ git checkout -b cool_new_feature
```

(Replace `cool_new_feature` with an appropriate description of your feature.) At this point you work on your new feature, using `git add` to add your changes. When your feature is complete and well tested, commit your changes

```
$ git commit -m 'did a bunch of great work'
```

and push your branch to github.

```
$ git push origin cool_new_feature
```

At this point, you go find your fork on github.com and create a pull request. Clearly describe what you have done in the comments. If your pull request fixes an issue or adds a useful new feature, the team will gladly merge it.

After your pull request is merged, you can switch back to the master branch, rebase, and delete your feature branch. You will find your new feature incorporated into `pyqg`.

```
$ git checkout master
$ git fetch upstream
$ git rebase upstream/master
$ git branch -d cool_new_feature
```

### 1.5.5 Virtual Environment

This is how to create a virtual environment into which to test-install `pyqg`, install it, check the version, and tear down the virtual environment.

```
$ conda create --yes -n test_env python=3.9 pip nose numpy cython scipy nose
$ conda install --yes -n test_env -c nanshe pyfftw
$ source activate test_env
$ pip install pyqg
$ python -c 'import pyqg; print(pyqg.__version__);'
$ source deactivate
$ conda env remove --yes -n test_env
```

### 1.5.6 Release Procedure

Once we are ready for a new release, someone needs to make a pull request which updates the version number in `setup.py`. Also make sure that `whats-new.rst` in the docs is up to date.

After the new version number PR has been merged, create a new release in github.

The step of publishing to pypi has to be done manually from the command line. (Note: I figured out how this works from these instructions). After the new release has been created, do the following.
Note that pypi will not let you publish the same release twice, so make sure you get it right!

# 1.6 What’s New

## 1.6.1 v0.3.1 (unreleased)

## 1.6.2 v0.3.0 (23 Nov. 2019)

- Revived development after long hiatus
- Reverted some experimental changes
- Several small bug fixes and documentation corrections
- Updated CI and doc build environments
- Adopted to versioneer for package versioning

## 1.6.3 v0.2.0 (27 April 2016)

Added compatibility with python 3.
Implemented linear baroclinic stability analysis method.
Implemented vertical mode methods and modal KE and PE spectra diagnostics.
Implemented multi-layer subclass.
Added new logger that leverages on built-in python logging.
Changed license to MIT.

## 1.6.4 v0.1.4 (22 Oct 2015)

Fixed bug related to the sign of advection terms (GH86).
Fixed bug in _calc_diagnostics (GH75). Now diagnostics start being averaged at tavestart.

## 1.6.5 v0.1.3 (4 Sept 2015)

Fixed bug in setup.py that caused openmp check to not work.
1.6.6 v0.1.2 (2 Sept 2015)

Package was not building properly through pip/pypi. Made some tiny changes to setup script. pypi forces you to increment the version number.

1.6.7 v0.1.1 (2 Sept 2015)

A bug-fix release with no api or feature changes. The kernel has been modified to support numpy fft routines.

- Removed pyfftw dependency (GH53)
- Cleaning of examples

1.6.8 v0.1 (1 Sept 2015)

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