The MiniWeather Mini App

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1 Introduction

The miniWeather code mimics the basic dynamics seen in atmospheric weather and climate. The dynamics themselves are dry compressible, stratified, non-hydrostatic flows dominated by buoyant forces that are relatively small perturbations on a hydrostatic background state. The equations in this code themselves form the backbone of pretty much all fluid dynamics codes, and this particular flavor forms the base of all weather and climate modeling.

With about 500 total lines of code (and only about 200 lines that you care about), it serves as an approachable place to learn parallelization and porting using MPI + X, where X is OpenMP, OpenACC, CUDA, or potentially other approaches to CPU and accelerated parallelization. The code uses periodic boundary conditions in the x-direction and solid wall boundary conditions in the z-direction.

1.1 Brief Description of the Code

1.1.1 Domain Parameters

A fuller description of the science, math, and dynamics are play are in Section 5, but this section is reserved to describing some of the main variables and flow in the code. The code is decomposed in two spatial dimensions, x and z, with `nx_glob` and `nz_glob` cells in the global domain and `nx` and `nz` cells in the local domain, using straightforward domain decomposition for MPI-level parallelization. The global domain is of size `xlen` and `zlen` meters, and `hs` "halo" cells are appended to both sides of each dimension for convenience in forming stencils of cells for reconstruction.

1.1.2 Fluid State Variables

There are four main arrays used in this code: `state`, `state_tmp`, `flux`, and `tend`, and the dimensions for each are given in the code upon declaration in the comments. Each of these arrays is described briefly below:

- `state`: This is the fluid state at the current time step, and it is the only array that persists from one time step to the next. The other four are only used within the calculations to advance the model to the next time step. The fluid state describes the *average* state over each cell area in the spatial domain. This variable contains four fluid states, which are the traditional mass, momenta, and thermodynamic quantities of most fluid models:

1. Density (`ID_DENS`): The 2-D density of the fluid in $\mathrm{kg\,m^{-2}}$ (note this is normally $\mathrm{kg\,m^{-3}}$, but this is a 2-D model, not 3-D)
2. U-momentum (`ID_UMOM`): The momentum per unit area of the fluid in the x-direction calculated as ρu, where u is the x-direction wind velocity. The units are $\mathrm{kg\,m^{-1}\,s^{-1}}$. Note that to get true momentum, you must integrate over the cell.
3. W-momentum (`ID_WMOM`): The momentum per unit area of the fluid in the z-direction calculated as ρw, where w is the w-direction wind velocity. The units are $\mathrm{kg\,m^{-1}\,s^{-1}}$. Note that to get true momentum, you must integrate over the cell.
4. Potential Temperature (`ID_RHOT`): The product of density and potential temperature, $\rho\theta$, where $\theta = T\left(P_0/P\right)^{R_d/c_p}$, $P_0 = 10^5\,\mathrm{Pa}$, T is the true temperature, and R_d and c_p are the dry air constant and specific heat at constant pressure for dry air, respectively. The units of this quantity are $\mathrm{K\,kg\,m^{-2}}$.

- `state_tmp`: This is a temporary copy of the fluid state used in the Runge-Kutta integration to keep from overwriting the state at the beginning of the time step, and it has the same units and meaning.

- `flux`: This is fluid state at cell boundaries in the x- and z-directions, and the units and meanings are the same as for `state` and `state_tmp`. In the x-direction update, the values of `flux` at indices `i` and `i+1` represents the fluid state at the left- and right-hand boundaries of cell `i`. The indexing is analagous in the z-direction. The fluxes are used to exchange fluid properties with neighboring cells.

- `tend`: This is the time tendency of the fluid state $\partial\mathbf{q}/\partial t$, where $\mathbf{q}$ is the the `state` vector, and as the name suggests, it has the same meaning and units as `state`, except per unit time (appending $\mathrm{s^{-1}}$ to the units). In the Finite-Volume method, the time tendency of a cell is equivalent to the divergence of the flux across a cell.

1.1.3 Overal Model Flow

This code follows a traditional Finite-Volume control flow.

To compute the time tendency, given an initial state at the beginning of a time step that contains cell-averages of the fluid state, the value of the state at cell boundaries is reconstructed using a stencil. Then, a viscous term is added to the fluid state at the cell boundaries to improve stability. Next, the tendencies are computed as the divergence of the flux across the cell. Finally, the tendencies are applied to the fluid state.

Once the time tendency is computed, the fluid PDEs are essentially now cast as a set of ODEs varying only in time, and this is called the "semi-discretized" form of the equations. To solve the equations in time, an ODE solver is used, in this case, a Runge-Kutta method. Finally, at the highest level, the equations are split into separate solves in each dimension, x and z.

2 Compiling and Running the Code

2.1 Required Libraries

To run everything in this code, you need MPI, parallel-netcdf, ncview, and an OpenACC compiler (preferably PGI 17+) to be installed. The serial code still uses MPI because I figured it was best to start with parallel I/O in place so that it's ready to go when the MPI implementation is done.

You can download parallel-netcdf from:
`https://trac.mcs.anl.gov/projects/parallel-netcdf`
Also, you can download a free version of PGI Community Edition (which has OpenACC implemented) from:
`https://www.pgroup.com/products/community.htm`
You'll probably also want to have "ncview" installed so you can easily view the NetCDF files. Ncview also makes it easy to see a movie of the solution as it evolves in time:
`http://meteora.ucsd.edu/~pierce/ncview_home_page.html`

2.2 Directories and Compiling

There are three main directories in the mini app: (1) a Fortran source directory; (2) a C source directory; and (3) a documentation directory, which you presumably know about because it contains this text you're reading now. The C code is technically C++ code but only because I wanted to use the ampersand pass by reference notation.

To compile the code, first edit the Makefile and change the flags to point to your parallel-netcdf installation as well as change the flags based on which compiler you are using. There are four versions of the code: serial, mpi, mpi+openmp, and mpi+openacc. The filenames make it clear which file is associated with which programming paradigm. To make all of these at once, simply type "make". To make them individually, you can type "make serial", "make mpi", "make openmp", and "make openacc".

2.3 Altering the Code's Configurations

There are four aspects of the configuration you can edit easily, and they are clearly labeled in the code as "USER-CONFIGURABLE PARAMETERS". These include: (1) the number of cells to use ["nx_glob" and "nz_glob"]; (2) the amount of time to simulate ["sim_time"]; (3) the frequency to output data to file ["output_freq"]; and (4) the initial data to use ["data_spec_int"].

2.4 Running the Code

To run the code, simply call "mpirun -n [# ranks] ./mini_weather_[version]". Since parameters are set in the code itself, you don't need to pass any parameters. Some machines use different tools instead of mpirun (e.g., OLCF's Titan uses "aprun").

2.5 Viewing the Output

The file I/O is done in the netCDF format: (`https://www.unidata.ucar.edu/software/netcdf/`). To me, the easiest way to view the data is to use a tool called "ncview" (`http://meteora.ucsd.edu/~pierce/ncview_home_page.html`). To use it, you can simply type "ncview output.nc", making sure you have X-forwarding enabled in your ssh session. Further, you can call "ncview -frames output.nc", and it will dump out all of your frames in the native resolution you're viewing the data in, and you you can render a movie with tools like ffmpeg.

3 Parallelization

This code was designed to parallelize with MPI first and then OpenMP or OpenACC next, but you can always parallelize with OpenMP or OpenACC without MPI if you want. But it is rewarding to be able to run it on multiple nodes at higher resolution for more and sharper eddies in the dynamics.

As you port the code, you'll want to change relatively little code at a time, re-compile, re-run, and look at the output to see that you're still getting the right answer. There are advantages to using a visual tool to check the answer, as it can sometimes give you clues as to why you're not getting the right answer.

Note that you only need to make changes code within the first 450 source lines. Everything below that is initialization and I/O code that doesn't need to be parallelized (unless you want to). There's a note in the serial code that tells you at what point the rest of the code will remain the same, even after parallelization.

3.1 Indexing

The code makes room for so-called "halo" cells in the fluid state. This is a common practice in any algorithm that uses stencil-based reconstruction to estimate variation within a domain. In this code, there are "hs" halo cells on either side of each dimension, and I pretty much hard-code hs=2.

3.1.1 Fortran

In the Fortran code's fluid state ("state"), the x- and z-dimensions are dimensioned as multi-dimensional arrays that range from 1-hs:nx+hs. In the x-direction, 1-hs:0 belong to the MPI task to the left, cells 1:nx belong to the current MPI task, and nx+1:nx+hs belong to the MPI task to the right. In the z-dimension, 1-hs:0 are artificially set to mimic a solid wall boundary condition at the bottom, and nz+1:nz+hs are the same for the top boundary. The cell-interface fluxes ("flux") are dimensioned as 1:nx+1 and 1:nz+1 in the x- and z-directions, and the cell average tendencies ("tend") are dimensioned 1:nx and 1:nz in the x- and z-directions. The cell of index i will have left- and right-hand interface fluxes of index i and i+1, respectively, and it will be evolved by the tendency at index i. The analog of this is also true in the z-direction.

3.1.2 C

In the C code, the fluid state array is dimensioned to size (nz+2*hs) and (nx+2*hs) in the x- and z-directions. In the x-direction, cells 0 to hs-1 belong to the left MPI task, cells hs to nx+hs-1 belong to the current MPI taks, and cells nx+hs to nx+2*hs-1 belong to the right MPI task. The z-direction's halo cells are used to mimic solid wall boundaries. The cell-interface fluxes ("flux") are dimensioned as nx+1 and nz+1 in the x- and z-directions, and the cell average tendencies ("tend") are dimensioned nx and nz in the x- and z-directions. The cell of index i+hs will have left- and right-hand interface fluxes of index i and i+1, respectively, and it will be evolved by the tendency at index i.The analog of this is also true in the z-direction.

3.2 MPI

This code was designed to use domain decomposition, where each MPI rank "owns" a certain set of cells in the x-direction and contains two "halo" cells from the left- and right-hand MPI tasks in the x-direction as well. The domain is only decomposed in the x-direction and not the z-direction.

IMPORTANT: Please be sure to set "nranks", "myrank", "nx", "i_beg", "left_rank", and "right_rank". These are clearly marked in the serial source code. You can set more variables, but these are used elsewhere in the code (particularly in the parallel file I/O), so they must be set.

To parallelize with MPI, there are only two places in the code that need to be altered. The first is the initialization, a subroutine / function named "init", where you must determine the number of ranks, you process's rank, the beginning index of your rank's first cell in the x-direction, the number of x-direction cells your rank will own, and the MPI rank IDs that are to your left and your right. Because the code is periodic in the x-direction, your left and right neighboring ranks will wrap around. For instance, if your are rank zero, your left-most rank will be nranks-1.

The second place is in the routine that sets the halo values in the x-direction. In this routine, you need to:

1. Create MPI data buffers (at the same place the other arrays are declared) to hold the data that needs to be sent and received, allocate them in the init() routine, and deallocate them in the finalize() routine.
2. Pack the data you need to send to your left and right MPI neighbors
3. Send the data to your left and right MPI neighbors
4. Receive the data from your left and right MPI neighbors
5. Unpack the data from your left and right neighbors and place the data into your MPI rank's halo cells.

Once you complete this, the code will be fully parallelized in MPI. Both of the places you need to add code for MPI are marked in the serial code, and there are some extra hints in the "set_halo_values_x()" routine as well.

3.3 OpenMP

For the OpenMP code, you basically need to decorate the loops with “omp parallel do” or “omp parallel for” and pay attention to any variables you need to make “private” so that each thread has its own copy. Keep in mind that OpenMP works best on “outer” loops rather than “inner” loops. Also, for sake of performance, there are a couple of instances where it is wise to use the “collapse” clause because the outermost loop is not large enough to support the number of threads most CPUs have.

3.4 OpenACC

The OpenACC approach will differ depending on whether you’re in Fortran or C. Just a forewarning, OpenACC is much more convenient in Fortran when it comes to data movement because in Fortran, the compiler knows how big your arrays are, and therefore the compiler can (and does) create all of the data movement for you. All you have to do is optimize the data movement after the fact.

3.4.1 Fortran Code

The OpenACC parallelization is a bit more involved when it comes to performance. But, it’s a good idea to just start with the kernels themselves, since the compiler will generate all of your data statements for you on a per-kernel basis. You need to pay attention to private variables here as well.

Once you’re getting the right answer with the kernels on the GPU, you can look at optimizing data movement by putting in data statements. I recommend putting data statements for the state, tend, flux, hy_*, and the MPI buffers around the main time stepping loop. Then, you need to move the data to the host before sending MPI data, back to the device once you receive MPI data, and to the host before file I/O.

3.4.2 C Code

In the C code, you’ll need to put in manual copy, copyin, and copyout statements on a per-kernel basis, and you’ll need to explicitly declare the size of each array as well. Other than this, the approach is the same as with the Fortran case. Once you have your kernels ported, you can optimize the data movement by wrapping the main time stepping loop in data statements, making sure the host has the data for I/O and sending MPI buffers and the device has the data after receiving MPI buffers.

3.5 C++ Performance Portability

The C++ code is in the “`cpp`” directory, and it uses a custom multi-dimensional array class from “`Array.h`”. For adding MPI to the serial code, please follow the instructions in the above MPI section. The real purpose of the C++ code is to get used to what performance portability looks like in C++, and this is moving from the `miniWeather_mpi.cpp` code to the `miniWeather_mpi_parallelfor.cpp` code, where you change all of the loops into `parallel_for` kernel launches, similar to the Kokkos syntax. For a description of how to move loops to `parallel_for`, please see the following webpage:

`https://github.com/mrnorman/YAKL/wiki/CPlusPlus-Performance-Portability-For-OpenACC-and-OpenMP-Folks`

I strongly recommend moving to parallel_for while compiling for the CPU so you don't have to worry about separate memory address spaces at the same time. Be sure to use array bounds checking during this process to ensure you don't mess up the indexing in the parallel_for launch. You can do this by adding `-DARRAY_DEBUG` to the `CXX_FLAGS`. After you've transformed all of the for loops to `parallel_for`, you can deal with the complications of separate memory spaces.

You'll have to pay attention to asynchronicity. `parallel_for` is asynchronous, and therefore, you'll need to add `yakl::fence()` in a few places (MPI and File I/O). If a `parallel_for`'s kernel uses variables with global scope, you will get a compile time error when running on the GPU. C++ Lambdas do not capture variables with global scope, and therefore, you'll be using CPU copies of that data, which nvcc does not allow. The most convenient way to handle this is to create local references as follows: `auto &varName = ::varName`

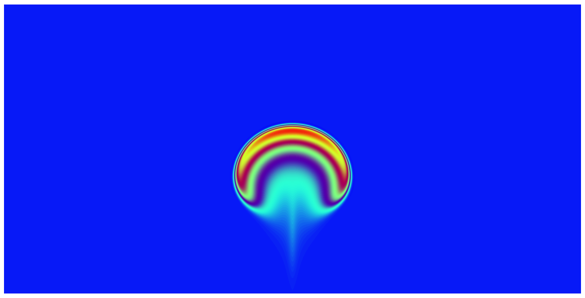
You will run into similar issues if you attempt to use data from your own class because the `"this"` pointer is typically into CPU memory because class objects are often allocated on the CPU. This can also be circumvented via local references. You have to put `YAKL_INLINE` in front of the following functions because they are called from kernels: `injection, density_current, turbulence, mountain_waves, thermal, collision, hydro_const_` `hydro_const_theta, and sample_ellipse_cosine`. Finally, you'll need to create new send and receive buffers in the x-direction halo exchange that are valid on the CPU using the `realArrHost typdef` in `const.h`. Then you'll need to copy the data to the CPU with the `deep_copy_to` function in `Array` class. See more information here:
`https://github.com/mrnorman/YAKL`

4 Numerical Experiments

A number of numerical experiments are in the code for you to play around with. You can set these by changing the "data_spec_int" variable.

4.1 Rising Thermal

data_spec_int = DATA_SPEC_THERMAL
sim_time = 1000
This simulates a rising thermal in a neutral atmosphere, which will look something like a "mushroom" cloud (without all of the violence).


(a) 500s

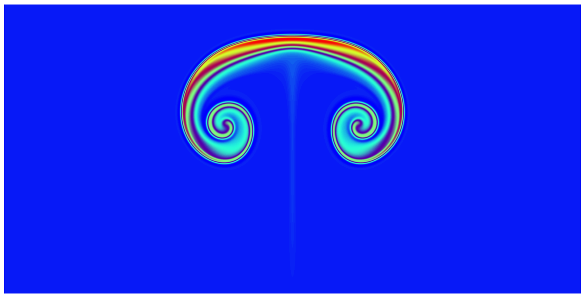
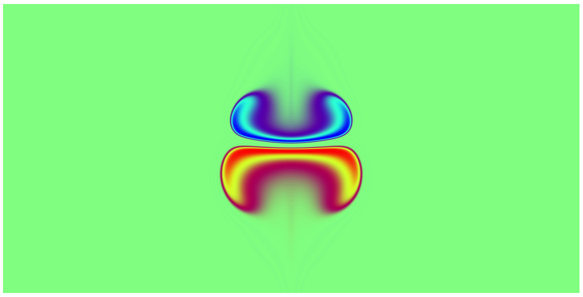
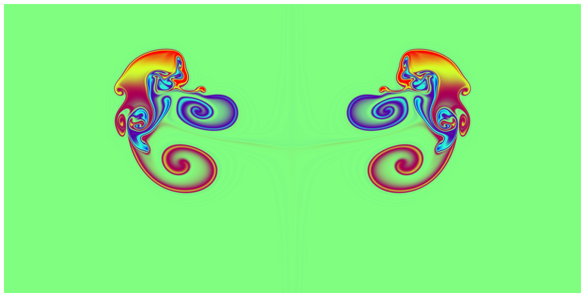

(b) 1,000s

Figure 1: Rising Thermal test case: Potential Temperature perturbation with 1600x800 cells.

4.2 Colliding Thermals

data_spec_int = DATA_SPEC_COLLISION
sim_time = 600
This is similar to the rising thermal test case except with a cold bubble at the model top colliding with a warm bubble at the model bottom to produce some cool looking eddies. This test case is mainly for looks, not physics.


(a) 200s


(b) 400s

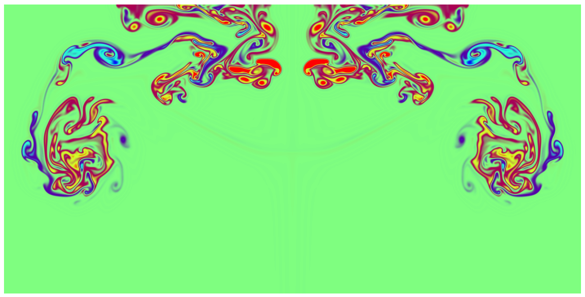

(c) 700s

Figure 2: Colliding Thermals test case: Potential Temperature perturbation with 1600x800 cells.

4.3 Mountain Gravity Waves

data_spec_int = DATA_SPEC_MOUNTAIN
sim_time = 1500
This test cases passes a horizontal wind over a faked mountain at the model bottom in a stable atmosphere to generate a train of stationary gravity waves across the model domain.

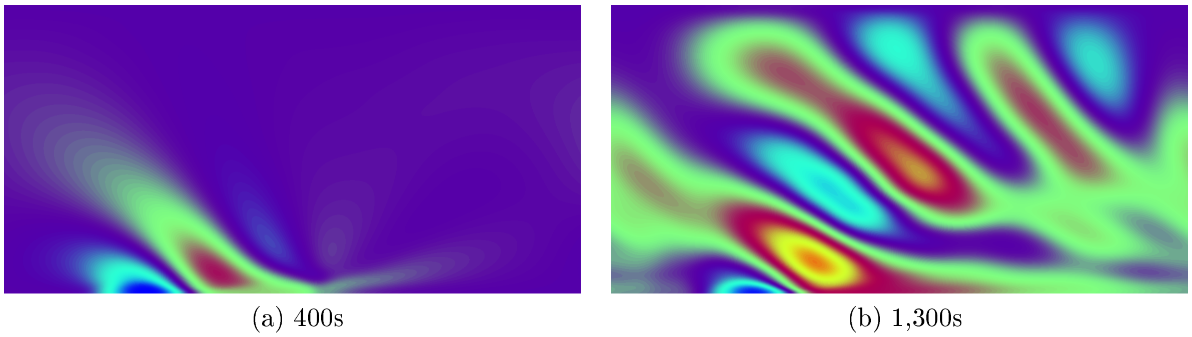

(a) 400s (b) 1,300s

Figure 3: Mountain Gravity Waves test case: Potential Temperature perturbation with 400x200 cells.

4.4 Density Current

data_spec_int = DATA_SPEC_DENSITY_CURRENT
sim_time = 600
This test case creates a neutrally stratified atmosphere with a strong cold bubble in the middle of the domain that crashes into the ground to give the feel of a weather front (more of a downburst, really).

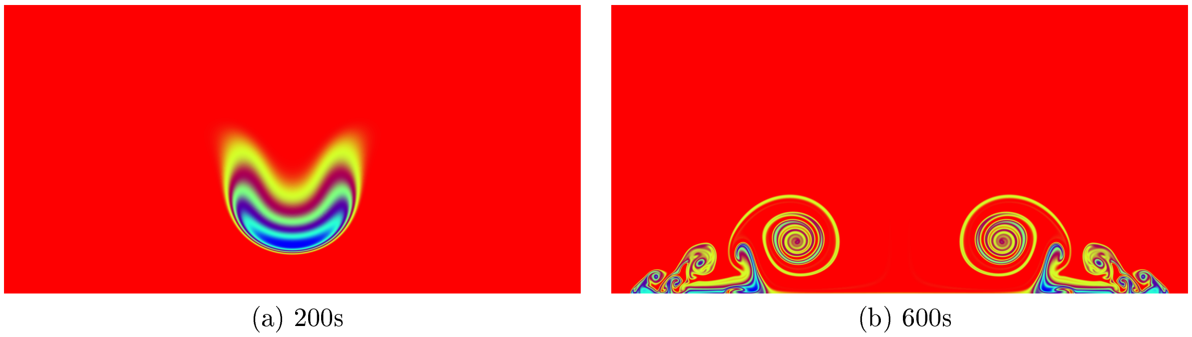

(a) 200s (b) 600s

Figure 4: Density Current test case: Potential Temperature perturbation with 1600x800 cells.

4.5 Injection

data_spec_int = DATA_SPEC_INJECTION
sim_time = 1200

A narrow jet of fast and slightly cold wind is injected into a balanced, neutral atmosphere at rest from the left domain near the model top. This has nothing to do with atmospheric flows. It's just here for looks.

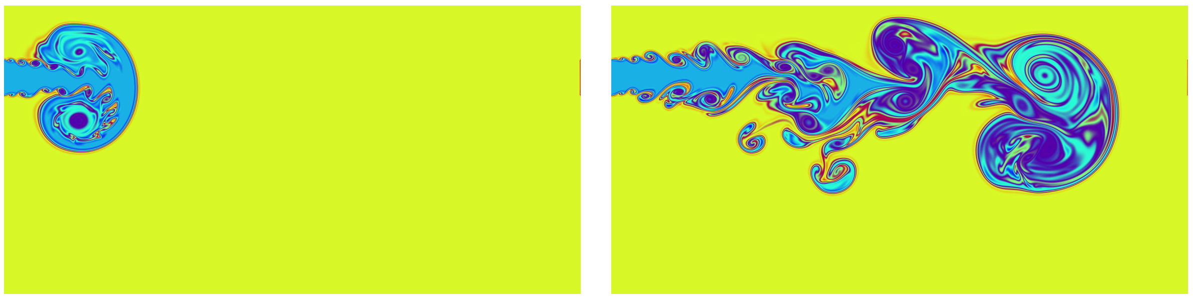

(a) 300s (b) 1,000s

Figure 5: Injection test case: Potential Temperature perturbation with 1600x800 cells.

5 Physics, PDEs, and Numerical Approximations

I put this section last just for the sake of completion in case you're curious what's actually going on in the code. While the numerical approximations in this code are certainly cheap and dirty, they are a fast and easy way to get the job done in a relatively small amount of code. For instance, on 16 K20x GPUs, you can perform a "colliding thermals" simulation with 5 million grid cells (3200×1600) in just a few minutes.

5.1 The 2-D Euler Equations

This app simulates the 2-D inviscid Euler equations for stratified fluid dynamics, which are defined as follows:

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho w\\ \rho\theta\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uw\\ \rho u\theta\end{bmatrix}+\frac{\partial}{\partial z}\begin{bmatrix}\rho w\\ \rho wu\\ \rho w^2+p\\ \rho w\theta\end{bmatrix}=\begin{bmatrix}0\\ 0\\ -\rho g\\ 0\end{bmatrix} \tag{1}$$

$$\rho_H = -\frac{1}{g}\frac{\partial p}{\partial z}$$

where ρ is density, u, and w are winds in the x-, and z-directions, respectively, θ is potential temperature related to temperature, T, by $\theta = T\left(P_0/P\right)^{R_d/c_p}$, $P_0 = 10^5\,\mathrm{Pa}$ is the surface pressure, $g = 9.8\ \mathrm{m\,s^{-2}}$ is acceleration due to gravity, $p = C_0\left(\rho\theta\right)^{\gamma}$ is the pressure as determined by an alternative form of the ideal gas equation of state, $C_0 = R_d^{\gamma} p_0^{-R_d/c_v}$, $R_d = 287\,\mathrm{J\,kg^{-1}\,K^{-1}}$ is the dry gas constant, $\gamma = c_p/c_v$, $c_p = 1004\,\mathrm{J\,kg^{-1}\,K^{-1}}$ is specific heat at constant pressure, and $c_v = 717\,\mathrm{J\,kg^{-1}\,K^{-1}}$ is specific heat at constant volume. This can be cast in a more convenient form as:

$$\frac{\partial \mathbf{q}}{\partial t}+\frac{\partial \mathbf{f}}{\partial x}+\frac{\partial \mathbf{h}}{\partial z}=\mathbf{s} \tag{2}$$

where a bold font represents a vector quantity.

5.2 Maintaining Hydrostatic Balance

The flows this code simulates are relatively small perturbations off of a "hydrostatic" balance, which balances gravity with a difference in pressure:

$$\frac{dp}{dz} = -\rho g$$

Because small violations of this balance lead to significant noise in the vertical momentum, it's best not to try to directly reconstruct this balance but rather to only reconstruct the perturbations. Therefore, hydrostasis is subtracted from (1) to give:

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho' \\ \rho u \\ \rho w \\ (\rho\theta)'\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ \rho u w \\ \rho u\theta\end{bmatrix} + \frac{\partial}{\partial z}\begin{bmatrix}\rho w \\ \rho w u \\ \rho w^2 + p' \\ \rho w\theta\end{bmatrix} = \begin{bmatrix}0 \\ 0 \\ -\rho' g \\ 0\end{bmatrix} \tag{3}$$

where a "prime" quantity represents that variable with the hydrostatic background state subtracted off.

5.3 Dimensional Splitting

This equation is solved using dimensional splitting for simplicity and speed. The equations are split into x- and z-direction solves that are, respectively:

$$x: \qquad \frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = \mathbf{0}$$

$$z: \qquad \frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{h}}{\partial x} = \mathbf{s}$$

Each time step, the order in which the dimensions are solved is reversed, giving second-order accuracy overall.

5.4 Finite-Volume Spatial Discretization

A Finite-Volume discretization is used in which the PDE in a given dimension is integrated over a cell domain, $\Omega_i \in \left[x_{i-1/2}, x_{i+1/2}\right]$, where $x_{i\pm1/2} = x_i \pm \Delta x$, x_i is the cell center, and Δx is the width of the cell. The integration is the same in the z-direction. Using the Gauss divergence theorem, this turns the equation into (using the z-direction as an example):

$$\frac{\partial \overline{\mathbf{q}}_{i,k}}{\partial t} = -\frac{\mathbf{h}_{i,k+1/2} - \mathbf{h}_{i,k-1/2}}{\Delta z} + \overline{\mathbf{s}}_{i,k} \tag{4}$$

where $\overline{\mathbf{q}}_{i,k}$ and $\overline{\mathbf{s}}_{i,k}$ are the cell-average of the fluid state and source term over the cell of index i, k.

To compute the update one needs the flux vector at the cell interfaces and the cell-averaged source term. To compute the flux vector at interfaces, fourth-order-accurate polynomial interpolation is used using the four cell averages surrounding the cell interface in question.

5.5 Runge-Kutta Time Integration

The equation (4) still has a time derivative that needs integrating, and a simple low-storage Runge-Kutta ODE solver is used to integrate the time derivative, and it is solved as follows:

$$\mathbf{q}^{\star} = \mathbf{q}^{n} + \frac{\Delta t}{3} RHS\left(\mathbf{q}^{n}\right)$$

$$\mathbf{q}^{\star\star} = \mathbf{q}^{n} + \frac{\Delta t}{2} RHS\left(\mathbf{q}^{\star}\right)$$

$$\mathbf{q}^{n+1} = \mathbf{q}^{n} + \Delta t RHS\left(\mathbf{q}^{\star\star}\right)$$

When it comes to time step stability, I simply assume the maximum speed of propagation is $450\,\mathrm{m\,s^{-1}}$, which basically means that the maximum wind speed is assumed to be $100\,\mathrm{m\,s^{-1}}$, which is a safe assumption. I set the CFL value to 1.5 for this code.

5.6 "Hyper-viscosity"

The centered fourth-order discretization in Section 5.4 is unstable as is and requires extra dissipation to damp out small-wavelength energy that would otherwise blow up the simulation. This damping is accomplished with a scale-selective fourth-order so-called "hyper"-viscosity that is defined as:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial}{\partial x}\left(-\kappa \frac{\partial^3 \mathbf{q}}{\partial x^3}\right) = \mathbf{0}$$

and this is also solved with the Finite-Volume method just like above. The hyperviscosity constant is defined as:

$$\kappa = -\beta \left(\Delta x\right)^4 2^{-4} \left(\Delta t\right)^{-1}$$

where $\beta \in [0,1]$ is a user-defined parameter to control the strength of the diffusion, where a higher value gives more diffusion. The parameter β is not sensitive to the grid spacing, and it seems that $\beta = 0.25$ is generally enough to get rid of $2\Delta x$ noise contamination.