

# Welcome to the MPAS tutorial practice guide

This web page is intended to serve as a guide through the practice exercises of this tutorial. Exercises are split into seven main sections, each of which focuses on a particular aspect of using the MPAS-Atmosphere model.

While going through this practice guide, you may find it helpful to have a copy of the MPAS-Atmosphere Users' Guide available in another window. Click <a href="https://example.com/here">here</a> to open the Users' Guide in a new window.

In case you would like to refer to any of the lecture slides from previous days, you can open the <u>Tutorial</u> Agenda in another window.

You can proceed through the sections of this practical guide at your own pace. It is highly recommended to go through the exercises in order, since later exercises may require the output of earlier ones. Clicking the grey headers will expand each section or subsection.

# 0. Prerequisites and environment setup

The practical exercises in this tutorial have been tailored to work on the <u>Derecho</u> system. Derecho is an HPC cluster that provides most of the libraries needed by MPAS and its pre- and post-processing tools through *modules*. In general, before compiling and running MPAS-Atmosphere on your own system, you will need an MPI-2 implementation as well as the NetCDF-4, PnetCDF, and PIO libraries.

Beginning with MPAS v8.0, a built-in alternative to the PIO library is available: the Simple MPAS I/O Layer (SMIOL). SMIOL requires just the PnetCDF library, and there is no need for the NetCDF-4 and PIO libraries when compiling MPAS itself. In this tutorial, we will be using MPAS with the SMIOL library.

Before going through any of the exercises in subsequent sections, we will need to run several commands to prepare our environment. Firstly, we will purge all loaded modules to begin from a known starting point (with no modules loaded); then, we will load several modules to give access to the GNU compilers as well as an MPI implementation:

```
$ module --force purge
$ module load ncarenv/23.09
$ module load craype/2.7.23
$ module load gcc/13.2.0
$ module load ncarcompilers/1.0.0
$ module load cray-mpich/8.1.27
```

Next, we will load modules for additional libraries needed by the MPAS-Atmosphere model. Besides the Parallel-NetCDF module (parallel-netcdf/1.12.3) needed by MPAS itself, the netcdf/4.9.2 module is being loaded to support compilation of pre- and post-processing tools and so that we have access to the standard ncdump program for showing the contents of NetCDF files.

```
$ module load parallel-netcdf/1.12.3
$ module load netcdf/4.9.2
```

At this point, running module list should print the following:

```
$ module list
```

```
Currently Loaded Modules:
```

```
1) ncarenv/23.09 (S) 3) gcc/13.2.0 5) cray-mpich/8.1.27 7) hdf5/1.14.3 2) craype/2.7.23 4) ncarcompilers/1.0.0 6) parallel-netcdf/1.12.3 8) netcdf/4.9.2
```

#### Where

```
S: Module is Sticky, requires --force to unload or purge
```

Post-processing exercises will need Python along with the NumPy, PyNGL, NetCDF4, and miscellaneous other Python packages. On Derecho, these are available in a Conda environment named 'npl'. The npl environment also provides the NCAR Command Language (NCL). We can load the conda module and activate the npl environment with the following commands:

```
$ module load conda
$ conda activate npl
```

Some Python plotting scripts that will be used in this tutorial rely on additional Python code that is located in a non-standard location. In order for these plotting scripts to work, we'll need to set our PYTHONPATH environment variable using the following command:

```
$ export PYTHONPATH=/glade/campaign/mmm/wmr/mpas tutorial/python scripts
```

Additionally, we can load a module to provide access to the 'ncview' tool:

```
$ module load noview
```

When running limited-area simulations, we will need to use Metis to create our own graph partition files. We can add the <code>gpmetis</code> command to our PATH with the following:

\$ export PATH=/glade/campaign/mmm/wmr/mpas tutorial/metis/bin:\${PATH}

IMPORTANT NOTE: The 'npl' Conda environment on Derecho modifies our PATH such that the wrong MPI compiler wrappers appear first. To remedy this, we can simply reload the 'gcc' module as a final step:

```
$ module reload gcc/13.2.0
```

If you've logged out of Derecho and would like a quick list of commands to set up your environment again after logging back in, you can copy and paste the following commands into your terminal:

```
module --force purge
module load ncarenv/23.09
module load craype/2.7.23
module load gcc/13.2.0
module load ncarcompilers/1.0.0
module load cray-mpich/8.1.27
module load parallel-netcdf/1.12.3
module load netcdf/4.9.2
module load conda
conda activate npl
export PYTHONPATH=/glade/campaign/mmm/wmr/mpas_tutorial/python_scripts
module load ncview
export PATH=/glade/campaign/mmm/wmr/mpas_tutorial/metis/bin:${PATH}
module reload gcc/13.2.0
```

We will run all of the practical exercises in this tutorial in our *scratch* directories, i.e., /glade/derecho/scratch/\${USER}/mpas\_tutorial. To keep the MPAS tutorial exercises separate from other work, we'll create a sub-directory named "mpas\_tutorial":

```
$ mkdir /glade/derecho/scratch/${USER}/mpas tutorial
```

Running jobs on Derecho requires the submission of a job script to a batch queueing system, which will allocate requested computing resources to your job when they become available. In general, it's best to avoid running any compute-intensive jobs on the login nodes, and the practical instructions to follow will guide you in the process of submitting jobs when necessary.

As a first introduction to running jobs on Derecho, there are several key commands worth noting:

- qcmd -A UMMM0006 This command runs the specified command on a batch node under the UMMM0006 project for this tutorial
- qsub This command submits a job script, which describes a job to be run on one or more batch nodes; it
  offers increased control over running a simple command with qcmd
- qstat -u \$user This command tells you the status of your pending and running jobs. Note that you
  may need to wait about 30 seconds for a recently submitted job to show up.
- qdel This command deletes a queued or running job

At various points in the practical exercises, we'll need to submit jobs to Derecho's queueing system using the qsub command, and after doing so, we may often check on the status of the job with the qstat command, monitoring the log files produced by the job once we see that the job has begun to run.

With your shell environment set up as described in this section, you're ready to begin with the practical exercises of this tutorial!

# 1. Compiling MPAS, and creating static files and idealized ICs

In this section, our goal is to obtain a copy of the MPAS source code directly from the MPAS GitHub repository. We'll then compile both the <code>init\_atmosphere\_model</code> and <code>atmosphere\_model</code> programs before using the former to begin the processing of time-invariant, terrestrial fields for use in a real-data simulation. While this processing is taking place, in another terminal window (<code>don't forget to set up your environment!</code>) we can practice preparing idealized initial conditions.

### 1.1 Obtaining the MPAS-Model source code

Since our default login shell is bash, all shell commands throughout this tutorial will be written for bash. However, if you prefer a different shell and don't mind mentally translating, e.g., export commands to

setenv commands, then feel free to switch shells.

As described in the lectures, the MPAS code is distributed directly from the GitHub repository where it is developed. While it's possible to navigate to <a href="https://github.com/MPAS-Dev/MPAS-Model">https://github.com/MPAS-Dev/MPAS-Model</a> and obtain the code by clicking on the "Releases" tab, it's much faster to *clone* the repository directly on the command-line. After changing to our /glade/derecho/scratch/\${USER}/mpas\_tutorial directory, we can make a clone of the MPAS-Model repository:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ git clone https://github.com/MPAS-Dev/MPAS-Model.git
```

Cloning the MPAS-Model repository may take a few seconds, and at the end of the process, the output to the terminal should look something like the following:

```
Cloning into 'MPAS-Model'...
remote: Enumerating objects: 64819, done.
remote: Counting objects: 100% (29/29), done.
remote: Compressing objects: 100% (13/13), done.
remote: Total 64819 (delta 16), reused 25 (delta 16), pack-reused 64790
Receiving objects: 100% (64819/64819), 35.63 MiB | 20.78 MiB/s, done.
Resolving deltas: 100% (48230/48230), done.
Updating files: 100% (1540/1540), done.
```

We should now have an MPAS-Model directory:

That's it! We now have a copy of the latest release of the MPAS source code.

# 1.2 Compiling the MPAS init\_atmosphere and atmosphere cores

As mentioned in the lectures, there are two "cores" that need to be compiled from the same MPAS source code: the <code>init\_atmosphere</code> core and the <code>atmosphere</code> core.

Before beginning the compilation process, it's worth verifying that we have MPI compiler wrappers in our path, and that environment variable pointing to the Parallel-NetCDF library is set:

```
$ which mpif90
/glade/u/apps/derecho/23.09/spack/opt/spack/ncarcompilers/1.0.0/gcc/13.2.0/g5ig/bin/mpi/mpif90

$ which mpicc
/glade/u/apps/derecho/23.09/spack/opt/spack/ncarcompilers/1.0.0/gcc/13.2.0/g5ig/bin/mpi/mpicc

$ echo $PNETCDF
/glade/u/apps/derecho/23.09/spack/opt/spack/parallel-netcdf/1.12.3/cray-mpich/8.1.27/gcc/13.2.0/xqnd
```

If all of the above commands were successful, our shell environment should be sufficient to allow the MPAS cores to be compiled.

We'll begin by compiling the *init\_atmosphere* core, producing an executable named <code>init\_atmosphere\_model</code>.

IMPORTANT NOTE: Before compiling on Derecho specifically, there's an important point that needs explanation! In order to avoid saturating the Derecho login nodes with compilation processes and negatively impacting other users, we will run our compilation command on a batch node with the special qcmd command. The qcmd command launches the specified command on a batch node and returns when the command has finished. So, although you would normally not use "qcmd" when compiling MPAS on other systems, for this tutorial we will prefix the usual compilation command with qcmd -A UMMM0006 -- (where UMMM0006 is the computing project we're working under).

After changing to the MPAS-Model directory

```
$ cd MPAS-Model
```

we can issue the following command to build the *init atmosphere* core with the GNU compilers:

```
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=init atmosphere
```

In the build command, we have also added the -j8 flag to tell *make* to use eight tasks to build the code; this should reduce the time to compile the init atmosphere model executable significantly!

After issuing the make command, above, compilation should take just a couple of minutes, and if the compilation was successful, the end of the build process should have produced messages like the following:

If compilation of the <code>init\_atmosphere</code> core was successful, we should also have an executable file named <code>init\_atmosphere</code> model:

Note, also, that default namelist and streams files for the <code>init\_atmosphere</code> core have also been generated as part of the compilation process: these are the files named <code>namelist.init\_atmosphere</code> and <code>streams.init atmosphere</code>.

Now, we're ready to compile the *atmosphere* core. If we try this without cleaning any of the common infrastructure code, first, e.g.,

\$ make gnu CORE=atmosphere

we would get an error like the following:

To remove the init\_atmosphere\_model\_model executable and clean the MPAS infrastructure, run: make clean CORE=init\_atmosphere\_model

To preserve all executables except atmosphere model and clean the MPAS infrastructure, run:
make clean CORE=atmosphere

Alternatively, AUTOCLEAN=true can be appended to the make command to force a clean, build a new atmosphere model executable, and preserve all other executables.

\*

After compiling one MPAS core, we need to clean up the shared infrastructure before compiling a different core. We can clean all parts of the infrastructure that are needed by the *atmosphere* core by running the following command:

\$ make clean CORE=atmosphere

Having cleaned up, we can proceed to compile the atmosphere core with:

```
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=atmosphere
```

The compilation of the atmosphere\_model executable can take several minutes or longer to complete (depending on which compiler is used). Similar to the compilation of the *init\_atmosphere* core, a successful compilation of the *atmosphere* core should give the following message:

Now, our MPAS-Model directory should contain an executable file named atmosphere\_model, as well as default namelist.atmosphere and streams.atmosphere files:

```
$ 1s -1L
total 33018
-rwxr-xr-x 1 duda ncar 5644864 Apr 26 20:37 atmosphere_model
-rwxr-xr-x 1 duda ncar 209256 Apr 26 20:36 build tables
-rw-r--r- 1 duda ncar 20580056 Apr 26 20:34 CAM ABS DATA.DBL
TWALF-XF-X 2 duda ncar 4096 Apr 26 20:37 default_inputs
-rw-r--r- 1 duda ncar 18208 Apr 26 20:34 CAM AEROPT DATA.DBL
-rwxr-xr-x 1 duda ncar 2014592 Apr 26 20:32 init atmosphere model
-rw-r--r 1 duda ncar 3131 Apr 26 20:26 INSTALL
-rw-r--r 1 duda ncar 29820 Apr 26 20:34 LANDUSE.TBL
-rw-r--r-- 1 duda ncar
                                2311 Apr 26 20:26 LICENSE
-rw-r--r- 1 duda ncar 27864 Apr 26 20:26 Makefile

-rw-r--r- 1 duda ncar 1774 Apr 26 20:37 namelist.atmosphere

-rw-r--r- 1 duda ncar 1379 Apr 26 20:32 namelist.init_atmosphere
-rw-r--r- 1 duda ncar 543744 Apr 26 20:34 OZONE_DAT.TBL
-rw-r--r 1 duda ncar 536 Apr 26 20:34 OZONE LAT.TBL
-rw-r--r 1 duda ncar 708 Apr 26 20:34 OZONE PLEV.TB:
                                   708 Apr 26 20:34 OZONE PLEV.TBL
-rw-r--r-- 1 duda ncar
                                 2555 Apr 26 20:26 README.md
-rw-r--r- 1 duda ncar 847552 Apr 26 20:34 RRTMG_LW_DATA
-rw-r--r- 1 duda ncar 1694976 Apr 26 20:34 RRTMG_LW_DATA.DBL
-rw-r--r-- 1 duda ncar 680368 Apr 26 20:34 RRTMG SW DATA
-rw-r--r- 1 duda ncar 1360572 Apr 26 20:34 RRTMG_SW_DATA.DBL
-rw-r--r- 1 duda ncar 4399 Apr 26 20:34 SOILPARM.TBL
drwxr-xr-x 14 duda ncar 4096 Apr 26 20:37 src
-rw-r--r-- 1 duda ncar
                                  1203 Apr 26 20:37 stream list.atmosphere.diagnostics
-rw-r--r-- 1 duda ncar
-rw-r--r-- 1 duda ncar
                                  927 Apr 26 20:37 stream_list.atmosphere.output
                                     9 Apr 26 20:37 stream list.atmosphere.surface
-rw-r--r-- 1 duda ncar
                                1571 Apr 26 20:37 streams.atmosphere
-rw-r--r-- 1 duda ncar
                                  920 Apr 26 20:32 streams.init_atmosphere
drwxr-xr-x 4 duda ncar
                                  4096 Apr 26 20:26 testing and setup
-rw-r--r-- 1 duda ncar 22986 Apr 26 20:34 VEGPARM.TBL
```

Note, also, the presence of files named stream\_list.atmosphere.\*. These are lists of output fields that are referenced by the streams.atmosphere file.

The new files like CAM\_ABS\_DATA.DBL, LANDUSE.TBL, RRTMG\_LW\_DATA, etc. are look-up tables and other data files used by physics schemes in MPAS-Atmosphere. These files should all be symbolic links to files in the src/core atmosphere/physics/physics wrf/files/ directory.

If we have <code>init\_atmosphere\_model</code> and <code>atmosphere\_model</code> executables, then compilation of both MPAS-Atmosphere cores was successful, and we're ready to proceed to the next sub-section.

#### 1.3 Static, terrestrial field processing

For our first MPAS simulation in this tutorial, we'll use a quasi-uniform 240-km mesh. Since we'll later be working with a variable-resolution mesh, it will be helpful to maintain separate sub-directories for these two simulations.

To begin processing of the static, terrestrial fields for the 240-km quasi-uniform mesh, let's change to our /glade/derecho/scratch/\${USER}/mpas\_tutorial directory and make a new sub-directory named 240km\_uniform:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ mkdir 240km_uniform
$ cd 240km_uniform
```

We can find a copy of the 240-km quasi-uniform mesh at /glade/campaign/mmm/wmr/mpas\_tutorial/meshes/x1.10242.grid.nc. To save disk space, we'll symbolically link this file into our directory:

```
$ ln -s /glade/campaign/mmm/wmr/mpas tutorial/meshes/x1.10242.grid.nc .
```

We will also need the init\_atmosphere\_model executable, as well as copies of the namelist.init\_atmosphere and streams.init\_atmosphere files. We'll make a symbolic link to the executable, and copies of the other files (since we will be changing them):

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/init_atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.init_atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.init_atmosphere .
```

Finally, so that we can make use of multiple MPI tasks for the static field processing, we will symbolically link a graph partition file with 16 partitions into our working directory:

```
$ ln -s /glade/campaign/mmm/wmr/mpas_tutorial/meshes/x1.10242.graph.info.part.16 .
```

Before running the init\_atmosphere\_model program, we'll need to set up the namelist.init\_atmosphere file as described in the lectures. With your preferred editor, edit the highlighted options in the default namelist.init atmosphere file so that they match the following:

```
&nhyd model
    config init case = 7
&data sources
    config_geog_data_path = '/glade/campaign/mmm/wmr/mpas tutorial/mpas static/'
    config landuse data = 'MODIFIED IGBP MODIS NOAH'
    config topo data = 'GMTED2010'
    config_vegfrac_data = 'MODIS'
    config albedo data = 'MODIS'
    config maxsnowalbedo data = 'MODIS'
    config supersample factor = 3
&preproc_stages
    config static interp = true
    config native gwd static = true
    config_vertical_grid = false
    config met interp = false
   config_input_sst = false
    config frac seaice = false
&decomposition
    config block decomp file prefix = 'x1.10242.graph.info.part.'
```

Note, in particular, the setting of the path to the geographical datasets, and the settings to enable only the processing of static data and the gravity wave drag ("gwd") static fields. Note, too, that we only specify the *prefix* of the graph partition file; the number of MPI tasks will be appended to the filename automatically by MPAS.

After editing the namelist.init\_atmosphere file, it will also be necessary to tell the init\_atmosphere\_model program the name of our input grid file, as well as the name of the "static" output file that we would like to create. We do this by editing the streams.init\_atmosphere file, where we first set the name of the grid file for the "input" stream:

and then set the name of the static file to be created for the "output" stream:

When interpolating geographical fields to a mesh, the "surface" and "lbc" streams can be ignored (but, you should not delete the "surface" or "lbc" streams, or the init\_atmosphere\_model program will complain).

After editing the streams.init\_atmosphere file, we can begin the processing of the static, time-invariant fields for the 240-km quasi-uniform mesh. Rather than running the init\_atmosphere\_model program on a batch node with qcmd, we will use a job script to run the program, returning a command prompt to us where we can monitor the progress of the job. To begin, we'll copy a prepared job script to our working directory:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/init_real.pbs .
```

If you're interested in doing so, you can take a look at the init\_real.pbs job script. Once you're ready, you can submit the script to the queueing system with the qsub command:

```
$ qsub init real.pbs
```

Now, we need to wait for our job to start running; we can check on its status every minute or so with the qstat command:

```
$ qstat -u $USER
```

Once we see that our job is running — indicated by an "R" in the second-to-last column, e.g,

```
$ qstat -u $USER
```

```
| September | Sept
```

we can check on the progress of the init\_atmosphere\_model program by following the messages written to the log.init\_atmosphere.0000.out file:

```
$ tail -f log.init_atmosphere.0000.out
```

We should expect to see lines of output similar to the following being printed every few seconds:

```
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/04801-06000.16801-18|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/03601-04800.16801-18|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/02401-03600.16801-18|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/01201-02400.16801-18|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/00001-01200.16801-18|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/00001-01200.15601-16|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/00001-01200.15601-16|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/42001-43200.15601-16|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/42001-43200.15601-15|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/42001-43200.15401-15|
Processing tile: /glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/topo_gmted2010_30s/42001-43200.15401-15|
```

The processing of the static, time-invariant fields will take some time — perhaps 10 minutes or so.

If lines similar to the above are being periodically written, we can kill the tail process with CTRL-C before proceeding to the next sub-section, where we will create idealized initial conditions while the static, terrestrial fields are interpolated.

IMPORTANT NOTE: If lines of output are not being periodically written to the terminal when running the tail command as described above, look for a file named log.init\_atmosphere.0000.err and determine what went wrong before going on to the next sub-section! Exercises in the second section of this tutorial will require the successful processing of static, time-invariant fields!

# 1.4 Preparing idealized initial conditions

While the init\_atmosphere\_model program is processing static, time-invariant fields for a real-data simulation in the 240km\_uniform directory, we can try initializing and running an idealized simulation in a separate directory.

The init\_atmosphere\_model program supports the creation of idealized initial conditions for the following cases:

- 3-d baroclinic wave on the sphere
- 3-d supercell thunderstorm on a doubly-periodic Cartesian plane
- 2-d mountain wave in the xz-plane

For each of these idealized cases, prepared input files are available on the MPAS-Atmosphere download page. We'll go through the process of creating initial conditions for the idealized supercell case; the general process is similar for the other two cases.

The prepared input files for MPAS-Atmosphere idealized cases may be found by going to the MPAS Homepage and clicking on the "MPAS-Atmosphere download" link at the left. Then, clicking on the "Configurations for idealized test cases" link will take you to the download links for idealized cases.

Although the input files for these idealized cases can be downloaded through the web page, we can also download, e.g., the supercell input files with wget once we know the URL. Beginning from our /glade/derecho/scratch/\${USER}/mpas\_tutorial directory, we can download the supercell input file archive and unpack it with:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ wget http://www2.mmm.ucar.edu/projects/mpas/test_cases/v7.0/supercell.tar.gz
$ tar xzvf supercell.tar.gz
```

After changing to the resulting supercell directory, the README file will give an overview of how to initialize and run the test case. The key points are that we need to symbolically link both the init\_atmosphere\_model and atmosphere\_model executables into the supercell directory:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/init_atmosphere_model .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model .
```

Unlike as described in the README file, however, we will not run the init\_atmosphere\_model and atmosphere\_model programs directly on the command-line.

We will run the init atmosphere model program through qcmd with:

```
$ qcmd -A UMMM0006 -- ./init_atmosphere_model
```

Once the initial conditions have been created as described in the README file, it's helpful to verify that there were no errors; the end of the log.init\_atmosphere.0000.out file should look something like the following:

```
Total log messages printed:
Output messages = 304
Warning messages = 13
Error messages = 0
Critical error messages = 0
```

Assuming there were no errors, we can run the simulation with 32 processors by first copying a prepared job script to our working directory and submitting the script with qsub:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/supercell.pbs .
$ qsub supercell.pbs
```

As with the static field interpolation, we need to wait for our job to start running. We can check on its status every minute or so with the qstat command:

```
$ qstat -u $USER
```

Once we see that our job is running, we can move on to the next section. The simulation may take about 10 minutes to run with 32 MPI tasks. During one of the later practical section, if you would like to revisit the simulation to see the results, running the supercell.ncl NCL script should produce plots of the time evolution of several model fields:

```
$ ncl supercell.ncl
```

# 2. Creating real-data ICs and running a simulation

Having compiled both the <code>init\_atmosphere</code> and <code>atmosphere</code> cores, and also having interpolated time-invariant, terrestrial fields to create a "static" file for real-data simulations, we'll interpolate atmospheric and land-surface fields to create complete initial conditions for an MPAS simulation in this section. We'll also process 10 days' worth of SST and sea-ice data to update these fields periodically as the model runs. Then, we'll start a five-day simulation, which will take around an hour to complete. Once the model has started running, we can use any extra time to compile the <code>convert mpas</code> utility program.

If you've reached this point and the static field interpolation from Section 1.3 has not yet finished, you can first go through Section 2.4, before returning to Sections 2.1 - 2.3 after the static field interpolation has completed.

# 2.1 Interpolating real-data initial conditions

In an earlier section, we started the process of interpolating static geographical fields to the 240-km, quasi-uniform mesh in the 240km\_uniform directory. If this interpolation was successful, this directory should contain two new files: log.init atmosphere.0000.out and x1.10242.static.nc.

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutoria1/240km_uniform
$ ls -l log.init atmosphere.0000.out x1.10242.static.nc
```

The end of the log.init atmosphere.0000.out file should show that there were no errors:

```
Total log messages printed:

Output messages = 673

Warning messages = 6

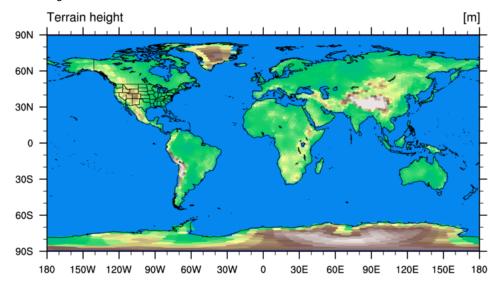
Error messages = 0

Critical error messages = 0
```

We can also make a plot of the terrain elevation field in the x1.10242.static.nc file with a Python script named plot\_terrain.py. We'll discuss the use of Python and NCL scripts for visualization in a later section, so for now we can simply execute the following commands to plot the terrain field:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/python_scripts/plot_terrain.py .
$ ./plot_terrain.py x1.10242.static.nc
$ display terrain.png
```

Running the script may take 10 or 15 seconds, but the result should be a figure that looks like the following:



Now that we have convinced ourselves that the processing of static, geographical fields was successful, we can proceed to interpolate atmosphere and land-surface initial conditions for our 240-km simulation. Generally, it is necessary to use the *ungrib* component of the WRF Pre-Processing System to prepare atmospheric datasets in the *intermediate format* used by MPAS. For the purposes of this tutorial, we will simply assume that these data have already been processed with the *ungrib* program in /glade/campaign/mmm/wmr/mpas tutorial/met data/.

To interpolate the ERA5 analysis valid at 0000 UTC on 10 September 2014 to our 240-km mesh, we will symbolically link the ERA5:2014-09-10 00 file to our working directory:

```
$ ln -s /glade/campaign/mmm/wmr/mpas_tutorial/met_data/ERA5:2014-09-10_00 .
```

Then, we will need to edit the namelist.init\_atmosphere as described in the lectures to instruct the init\_atmosphere\_model program to interpolate the ERA5 data to our mesh. The critical items to set in the namelist.init\_atmosphere file are:

```
&nhyd_model
    config init case = 7
    config_start_time = '2014-09-10_00:00:00'
&dimensions
    config_nvertlevels = 55
    config_nsoillevels = 4
    config_nfglevels = 38
    config_nfgsoillevels = 4
&data_sources
    config_met_prefix = 'ERA5'
    config_use_spechumd = false
&vertical_grid
    config ztop = 30000.0
    config_nsmterrain = 1
    config_smooth_surfaces = true
    config_dzmin = 0.3
    config_nsm = 30
    config tc vertical grid = true
    config_blend_bdy_terrain = false
&interpolation_control
    config_extrap_airtemp = 'lapse-rate'
&preproc_stages
    config_static_interp = false
    config_native_gwd_static = false
    config_vertical_grid = true
    config_met_interp = true
    config_input_sst = false
    config frac seaice = true
&decomposition
```

```
config_block_decomp_file_prefix = 'x1.10242.graph.info.part.'
/
```

You may find it easier to copy the default namelist.init\_atmosphere file from /glade/derecho/scratch/\${USER}/mpas\_tutorial/MPAS-Model/namelist.init\_atmosphere before making the edits highlighted above.

When editing the namelist.init\_atmosphere file, the key changes are to the starting time for our real-data simulation, the prefix of the *intermediate file* that contains the ERA5 atmospheric and land-surface fields, and the pre-processing stages that will be run.

After editing the namelist.init\_atmosphere file, we will also need to set the name of the input file in the streams.init\_atmosphere file to the name of the "static" file that we just produced:

and we will also need to set the name of the output file, which will be the MPAS real-data initial conditions file:

Once we've made the above changes to the namelist.init\_atmosphere and streams.init\_atmosphere files, we can run the init\_atmosphere\_model program by submitting our init\_real.pbs script again:

```
$ qsub init_real.pbs
```

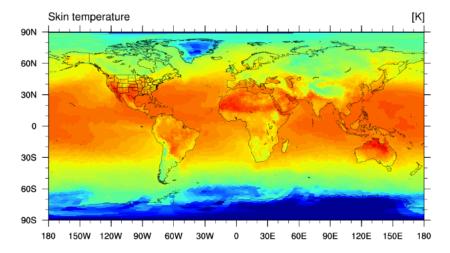
As before, we can check on the status of our job periodically by running

```
$ qstat -u $USER
```

After it begins to run, the program should take just a minute or two to finish running, and the result should be an x1.10242.init.nc file and a new log.init\_atmosphere.0000.out file. Assuming no errors were reported at the end of the log.init\_atmosphere.0000.out file, we can plot, e.g., the skin temperature field in the x1.10242.init.nc file using the plot tsk.py Python script:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/python_scripts/plot_tsk.py .
$ ./plot_tsk.py x1.10242.init.nc
$ display tsk.png
```

Again, we'll examine the use of Python and NCL scripts for visualization later, so for now we only need to verify that a plot like the following is produced:



If a plot like the above is produced, then we have completed the generation of an initial conditions file for our 240-km real-data simulation!

### 2.2 Generating SST and sea-ice update files

Because MPAS-Atmosphere — at least, when run as a stand-alone model — does not contain prognostic equations for the SST and sea-ice fraction, these fields would remain constant if not updated from an external source; this is, of course, not realistic, and it will generally impact the quality of longer model simulations. Consequently, for MPAS-Atmosphere simulations longer than roughly a week, it is typically

necessary to periodically update the sea-surface temperature (SST) field in the model. For real-time simulations, this is generally not an option, but it is feasible for *retrospective* simulations, where we have observed SST analyses available to us.

In order to create an SST update file, we will make use of a sequence of intermediate files containing SST and sea-ice analyses that are available in /glade/campaign/mmm/wmr/mpas\_tutorial/met\_data. Before proceeding, we'll link all of these SST intermediate files into our working directory:

```
$ ln -sf /glade/campaign/mmm/wmr/mpas_tutorial/met_data/SST* .
```

Following Section 8.1 of the MPAS-Atmosphere Users' Guide, we must edit the namelist.init\_atmosphere file to specify the range of dates for which we have SST data, as well as the frequency at which the SST intermediate files are available. The key namelist options that must be set are shown below; other options can be ignored.

```
&nhyd_model
    config_init_case = 8
    config_start_time = '2014-09-10 00:00:00'
    config_stop_time = '2014-09-20_00:00:00'
&data_sources
    config sfc prefix = 'SST'
    config_fg_interval = 86400
&preproc_stages
   config static interp = false
    config_native_gwd_static = false
    config vertical grid = false
    config_met_interp = false
    config_input_sst = true
    config_frac_seaice = true
&decomposition
    config_block_decomp_file_prefix = 'x1.10242.graph.info.part.'
```

Note in particular that we have set the *config\_init\_case* variable to **8**! This is the initialization case used to create surface update files, instead of real-data initial conditions files.

As before, we also need to edit the streams.init\_atmosphere file, this time setting the name of the SST update file to be created by the "surface" stream, as well as the frequency at which this update file should contain records:

Note that we have set both the *filename\_template* and *output\_interval* attributes of the "surface" stream. The output\_interval should match the interval specified in the namelist for the *config\_fg\_interval* variable. The other streams ("input", "output", and "lbc") can remain unchanged — the input file should still be set to the name of the static file.

After setting up the namelist.init\_atmosphere and streams.atmosphere files, we're ready to run the init\_atmosphere\_model program by submitting our init\_real.pbs script again:

```
$ qsub init real.pbs
```

As before, we can check on the status of our job periodically by running

```
$ qstat -u $USER
```

After the job completes, the log.init\_atmosphere.0000.out file should report that there were no errors. Additionally, the file x1.10242.sfc update.nc file should have been created.

We can confirm that the x1.10242.sfc\_update.nc contains the requested valid times for the SST and sea-ice fields by printing the "xtime" variable from the file; in MPAS, the "xtime" variable in a netCDF file is always used to store the times at which records in the file are valid.

```
$ ncdump -v xtime x1.10242.sfc_update.nc
```

This ncdump command should print the following times:

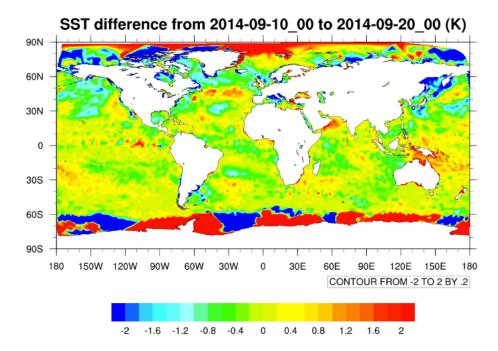
If the times shown above were printed, then we have successfully created an SST and sea-ice update file for MPAS-Atmosphere. As a final check, we can use the Python script from

/glade/campaign/mmm/wmr/mpas\_tutorial/python\_scripts/plot\_delta\_sst.py to plot the difference in the SST field between the last time in the surface update file and the first time in the file.

Because the surface update file contains no information about the latitude and longitude of grid cells, we provide two command-line arguments when running this script: one to give the name of the grid file, which contains cell latitude and longitude fields, and the second to specify the surface update file:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/python_scripts/plot_delta_sst.py .
$ ./plot_delta_sst.py x1.10242.static.nc x1.10242.sfc_update.nc
$ display delta sst.png
```

This script may take a minute or so to run.



In this plot, we have masked out the SST differences over land, since the values of the field over land are not representative of actual SST differences, but may represent differences in, e.g., skin temperature or 2-m air temperature, depending on the source of the SST analyses.

## 2.3 Model integration

Assuming that an initial condition file and a surface update file have been created, we're ready to run the MPAS-Atmosphere model itself!

Working from our 240km\_uniform directory, we'll begin by creating a symbolic link to the atmosphere\_model executable that we compiled in

/glade/derecho/scratch/\${USER}/mpas\_tutorial/MPAS-Model. We'll also make copies of the namelist.atmosphere and streams.atmosphere files as well. Recall from when we compiled the model that there are stream\_list.atmosphere.\* files that accompany the streams.atmosphere file; we'll copy these, too.

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/stream_list.atmosphere.* .
```

You'll also recall that there were many look-up tables and other data files that are needed by various physics parameterizations in the model. Before we can run MPAS-Atmosphere, we'll need to create symbolic links to these files as well in our working directory:

Before running the model, we will need to edit the namelist.atmosphere file, which is the namelist for the MPAS-Atmosphere model itself. The default namelist.atmosphere is set up for a 120-km mesh; in order to run the model on a different mesh, there is one key parameter that depends on the model resolution:

• config dt — the model integration time step (delta-t), in seconds.

As will be described in the lectures, the model integration step is generally chosen based on the finest horizontal resolution in a simulation domain.

To tell the model the date and time at which integration will begin (important, e.g., for computing solar radiation parameters), and to specify the length of the integration to be run, there are two other parameters that must be set for each simulation:

- config\_start\_time the start time of the integration.
- config\_run\_duration the length of the integration.

Lastly, when running the MPAS-Atmosphere model in parallel, we must tell the model the prefix of the filenames that contain mesh partitioning information for different MPI task counts:

 config\_block\_decomp\_file\_prefix — the file prefix (to be suffixed with processor count) of the file containing mesh partitioning information.

Accordingly, we must edit at least these parameters in the namelist.atmosphere file; other parameters are described in Appendix B of the MPAS-Atmosphere Users' Guide, and do not necessarily need to be changed:

```
&nhyd_model
    config_dt = 1200.0
    config_start_time = '2014-09-10_00:00:00'
    config_run_duration = '5_00:00:00'

&decomposition
    config_block_decomp_file_prefix = 'x1.10242.graph.info.part.'
//
```

For a relatively coarse mesh like the 240-km mesh, we can also call the radiation schemes less frequently to allow the model to run a little more quickly. Let's set the radiation calling interval to 1 hour:

```
&physics
    config_radtlw_interval = '01:00:00'
    config_radtsw_interval = '01:00:00'
/
```

After changing the parameters shown above in the namelist.atmosphere file, we must also set the name of the initial condition file, the name of the surface update file, and the interval at which we would like to read the surface update file in the streams.atmosphere file:

Having set up the namelist.atmosphere and streams.atmosphere files, we're almost ready to run the model in parallel. You'll recall from the lectures that we need to supply a *graph partition file* to tell MPAS how the horizontal domain is partitioned among MPI tasks. Accordingly, we'll create a symbolic link to the partition file for 128 MPI tasks for the 240-km mesh in our working directory:

```
$ In -s /glade/campaign/mmm/wmr/mpas_tutorial/meshes/x1.10242.graph.info.part.128 .
```

As a general rule, a mesh with N grid columns should be run on at most N/160 processors in MPAS-Atmosphere to make efficient use of the processors. So, for the mesh in this exercise, which has 10242 grid columns, we could in principle use up to about 64 MPI tasks while still making relatively efficient use of the computing resources. For this exercise, however, we will use a single, full Derecho node with 128 cores.

Now, we should be able to run MPAS using 128 MPI tasks. Before submitting a job with qsub, we can copy a prepared job script to our working directory.

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/run_model.pbs .
$ qsub run model.pbs
```

We can check on the status of our job with qstat -u \$USER. Once the model begins to run, it will write information about its progress to the log.atmosphere.0000.out file. We can use tail -f to follow the updates to the log file as the model runs:

```
$ tail -f log.atmosphere.0000.out
```

If the model has started up successfully and begun to run, we should see messages like this

```
Begin timestep 2014-09-10_06:00:00
--- time to run the LW radiation scheme L_RADLW =T
--- time to run the SW radiation scheme L_RADSW =T
--- time to run the convection scheme L_CONV =T
--- time to apply limit to accumulated rainc and rainnc L_ACRAIN =F
--- time to apply limit to accumulated radiation diags. L_ACRADT =F
--- time to calculate additional physics_diagnostics =F
split dynamics-transport integration 3

global min, max w -0.177687 0.512867
global min, max u -112.127 112.008
Timing for integration step: 5.78077 s
```

written for each timestep that the model takes. If not, a log.atmosphere.0000.err file may have been created, and if so, it may have messages to indicate what might have gone wrong.

The model simulation should take less than about a five minutes to complete. As the model runs, you may notice that several netCDF output files are being created:

- diag.2014.09.\*.nc These files contain mostly 2-d diagnostic fields that were listed in the stream\_list.atmosphere.diagnostics file.
- history.2014.09.\*.nc These files contain mostly 3-d prognostic and diagnostic fields from the model.
- restart.2014.09.\*.nc These are model restart files that are essentially checkpoints of the model state; a simulation can be re-started from any of these checkpoint/restart files.

If the model has successfully begun running, we can move to the next sub-section to obtain and compile the convert mpas utility for interpolating model output files to a lat-lon grid for quick visualization.

## 2.4 Obtaining and compiling the convert\_mpas program

We saw in earlier sections that Python scripts may be used to visualize fields in MPAS netCDF files. Although these scripts can produce publication-quality figures, many times all that is needed is a way to quickly inspect the fields in a file. The <code>convert\_mpas</code> program is designed to interpolate fields from the unstructured MPAS mesh to a regular lat-lon grid for easy checking, e.g., with neview.

As with the MPAS-Model code, the convert\_mpas code may be obtained most easily by cloning a GitHub repository. Working from our /glade/derecho/scratch/\${USER}/mpas\_tutorial directory, we'll download the code in this way:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ git clone https://github.com/mgduda/convert_mpas.git
$ cd convert mpas
```

The convert\_mpas utility is compiled via a simple Makefile. In general, one can edit the Makefile in the main convert mpas directory; for this tutorial, however, no changes are needed.

We can build the convert mpas utility by simply running make with no command-line arguments:

```
$ make
```

If compilation was successful, there should now be an executable file named <code>convert\_mpas</code>. So that we can run this program from any of our working directories, we'll add our current directory to our shell <code>\${PATH}</code> environment variable:

```
$ export PATH=/glade/derecho/scratch/${USER}/mpas_tutorial/convert_mpas:${PATH}
```

You may like to take a few minutes to read through the **README.md** file to familiarize yourself with the usage of the **convert\_mpas** program. We'll have a chance to exercise the **convert\_mpas** utility in the next section.

# 3. Running MPAS with variable resolution, and basic visualization

In the previous section, we were able to make a five-day, real-data simulation on a 240-km quasi-uniform mesh. In this section, we'll practice preparing a variable-resolution, 240km – 48km mesh with the <code>grid\_rotate</code> tool, after which we'll proceed as we did for the quasi-uniform case to process static, terrestrial fields on this variable-resolution mesh.

As we saw in the first section, processing the static fields can take some time, so while this processing is taking place, we'll practice using the <code>convert\_mpas</code> tool to interpolate output from our 240-km quasi-uniform simulation to a lat-lon grid for quick visualization.

Once the static field processing has completed for the 240km – 48km variable-resolution mesh, we'll interpolate the initial conditions fields and start a simulation on this mesh. This simulation will take about half an hour to complete, so we'll want to get this running so that it will have completed by the next section.

### 3.1 Obtaining, building, and running the grid\_rotate program

A common theme with MPAS is the need to obtain source code from *git* repositories hosted on GitHub. The <code>grid\_rotate</code> utility is no exception in this regard. One difference, however, is that the <code>grid\_rotate</code> code is contained in a repository that houses many different tools for MPAS cores, including the MPAS-Albany Land Ice core, the MPAS-Ocean core, and the MPAS-Sea Ice core.

The grid\_rotate utility is found in the MPAS-Tools repository, which we can clone into our mpas tutorial working directory with the following commands:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ git clone https://github.com/MPAS-Dev/MPAS-Tools.git
```

Within the MPAS-Tools repository, the grid\_rotate code resides in the mesh\_tools/grid\_rotate subdirectory. We can change to this directory and build the grid rotate utility with the make command.

```
$ cd MPAS-Tools/mesh_tools/grid_rotate
$ make
```

So that we can more easily run the <code>grid\_rotate</code> program from any working directory, we'll add our current working directory to our shell <code>\${PATH}</code>.

\$ export PATH=/glade/derecho/scratch/\${USER}/mpas tutorial/MPAS-Tools/mesh tools/grid rotate:\${PATH}

Now that we have a means of rotating the location of refinement in a variable-resolution MPAS mesh, we can begin the process of preparing such a mesh. For this tutorial, we'll be using a mesh that refines from 240-km grid spacing down to about 48-km grid spacing over an elliptic region.

When creating initial conditions and running the 240-km quasi-uniform simulation, we worked in a sub-directory named 240km\_uniform. For our variable-resolution simulation, we'll work in a sub-directory named 240-48km\_variable to keep our work separated. Let's create the 240-48km\_variable directory and link in the variable-resolution mesh from /glade/campaign/mmm/wmr/mpas\_tutorial/meshes into that directory:

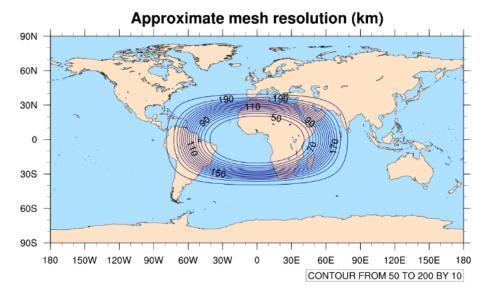
```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ mkdir 240-48km_variable
$ cd 240-48km_variable
$ ln -s /glade/campaign/mmm/wmr/mpas_tutorial/meshes/x5.30210.grid.nc .
```

The x5.30210.grid.nc mesh contains 30210 grid cells and refines by a factor of five (from 240-km grid spacing to 48-km grid spacing). The refinened region is centered over (0.0 lat, 0.0 lon), and we can get a quick idea of the size of the refinement by plotting contours of the approximate mesh resolution with the mesh\_resolution.ncl NCL script:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/ncl_scripts/mesh_resolution.ncl .
$ export FNAME=x5.30210.grid.nc
$ ncl mesh_resolution.ncl
```

When running the mesh\_resolution.ncl script, a plot like the one below should be produced in a file named 'mesh\_resolution.png', and which you can view with the display command:

```
$ display mesh_resolution.png
```



Using the <code>grid\_rotate</code> tool, we can change the location and orientation of this refinement to an area of our choosing. Before running the <code>grid\_rotate</code> program, we need a copy of the input namelist that is read by this program:

\$ cp /glade/derecho/scratch/\${USER}/mpas tutorial/MPAS-Tools/mesh tools/grid rotate/namelist.input .

As described in the lectures, we'll set the parameters in the namelist.input file to relocate the refined region in the mesh. For example, to move the refinement over South America, we might use:

```
&input
   config_original_latitude_degrees = 0
   config_original_longitude_degrees = 0

   config_new_latitude_degrees = -19.5
   config_new_longitude_degrees = -62
   config_birdseye_rotation_counter_clockwise_degrees = 90
//
```

Feel free to place the refinement wherever you would like!

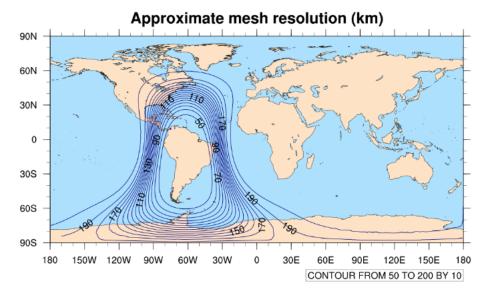
After making changes to the namelist.input file, we can rotate the x5.30210.grid.nc file to create a new "grid" file with any name we choose. For example:

\$ grid\_rotate x5.30210.grid.nc SouthAmerica.grid.nc

As with the original x5.30210.grid.nc file, we can plot the approximate resolution of our rotated grid file with commands like the following:

```
$ export FNAME=SouthAmerica.grid.nc
$ ncl mesh_resolution.ncl
```

Of course, the name <code>southAmerica.grid.nc</code> should be replaced with the name that you have chosen for your rotated grid when setting the <code>FNAME</code> environment variable. In our example, the resulting plot looks like the one below.



It may take some iteration to get the refinement just where you would like it. You can go back and edit the namelist.input file, then re-run the grid\_rotate program, and finally, re-run the ncl mesh resolution.ncl command until you are satisfied!

## 3.2 Static, terrestrial field processing

Interpolating static, geographical fields to a variable-resolution MPAS mesh works in essentially the same way as it does for a quasi-uniform mesh. So, the steps taken in this section should seem familiar — they mirror what we did in Section 1.3!

To begin the process, we'll symbolically link the init\_atmosphere\_model executable into our 240-48km\_variable directory, and we'll copy the default namelist.init\_atmosphere and streams.init\_atmosphere files as well:

```
$ In -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/init_atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.init_atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.init_atmosphere .
```

So that we can make use of multiple MPI tasks for the static field processing, we will symbolically link a graph partition file with 16 partitions for the x5.30210 mesh into our working directory:

```
$ ln -s /glade/campaign/mmm/wmr/mpas tutorial/meshes/x5.30210.graph.info.part.16 .
```

Note that graph partition files for a mesh are independent of any rotation that may be applied to the mesh. The graph partitioning depends only on the connectivity among cells in the mesh and not on the geographic locations of cells, and rotating a mesh does not alter the local connections among cells.

As before, we'll set the following variables in the namelist.init\_atmosphere file:

```
&nhyd model
    config_init_case = 7
&data sources
    config_geog_data_path = '/glade/campaign/mmm/wmr/mpas_tutorial/mpas_static/'
    config landuse data = 'MODIFIED IGBP MODIS NOAH'
    config_topo_data = 'GMTED2010'
    config vegfrac data = 'MODIS'
    config_albedo_data = 'MODIS'
    config maxsnowalbedo data = 'MODIS'
    config_supersample_factor = 3
&preproc stages
    config_static_interp = true
    config native gwd static = true
    config_vertical_grid = false
    config met interp = false
    config input sst = false
    config_frac_seaice = false
&decomposition
    config_block_decomp_file_prefix = 'x5.30210.graph.info.part.'
```

In editing the streams.init\_atmosphere file, we'll choose the filename for the "input" stream to match whatever name we chose for our rotated grid file:

and we'll set the filename for the "output" stream to follow the same naming convention, but using "static" instead of "grid":

With these changes, we're ready to run the init\_atmosphere\_model program. In order to submit the job to the queuing system, we can copy the same prepared job script as in Section 1.3 and submit it with qsub:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/init_real.pbs .
$ qsub init real.pbs
```

As before, processing of the static, geographical fields may take roughly 10 minutes to complete.

# 3.3 Using the convert\_mpas utility

While the static, geographical fields are being processed for our 240km – 48km variable-resolution mesh, we can experiment with the use of the convert\_mpas utility to interpolate output from our 240-km, quasi-uniform simulation.

If you didn't have a chance to download and compile the <code>convert\_mpas</code> program back in Section 2.4, you will need to go back to that section before proceeding with the rest of this section.

We'll change directories to the 240km\_uniform directory, and we may also need to add the directory containing the convert mpas utility to our shell \${PATH} variable again:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform
$ export PATH=/glade/derecho/scratch/${USER}/mpas_tutorial/convert_mpas:${PATH}
```

In the 240km\_uniform directory, we should see output files from MPAS that are named history\*nc and diag\*nc:

```
$ 1s -1 history*nc diag*nc
-rw-r--r- 1 duda ncar 4525528 Apr 8 23:56 diag.2014-09-10_00.00.00.nc
-rw-r--r- 1 duda ncar 4525528 Apr 8 23:56 diag.2014-09-10_03.00.00.nc
...
-rw-r--r- 1 duda ncar 4525528 Apr 8 23:59 diag.2014-09-14_21.00.00.nc
-rw-r--r- 1 duda ncar 4525528 Apr 8 23:59 diag.2014-09-15_00.00.00.nc
-rw-r--r- 1 duda ncar 94449804 Apr 8 23:56 history.2014-09-10_06.00.00.nc
...
-rw-r--r- 1 duda ncar 94449804 Apr 8 23:59 history.2014-09-14_18.00.00.nc
-rw-r--r- 1 duda ncar 94449804 Apr 8 23:59 history.2014-09-15_00.00.00.nc
```

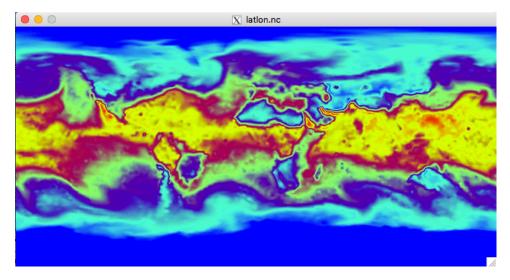
As a first try, we can interpolate the fields from the final model "history" file, history.2014-09-15\_00.00.00.nc, to a 0.5-degree lat-lon grid with the command:

```
$ convert mpas history.2014-09-15 00.00.00.nc
```

The interpolation should take less than a minute, and the result should be a file named latlon.nc. Let's take a look at this file with the noview utility:

```
$ ncview latlon.nc
```

After launching noview we can, e.g., view the qv field, which may look something like the plot below at the lowest model level.



Feel free to browse some of the other fields in the file by selecting them from the "2d vars" and "3d vars" buttons. All of the fields are described in Appendix D of the User's Guide.

When we're done viewing the latlon.nc file, we'll delete it. The convert\_mpas utility attempts to append to existing latlon.nc files when converting a new MPAS netCDF file, and this often doesn't work as expected, so to avoid confusion, it's best to remove the latlon.nc file we just created with

```
$ rm latlon.nc
```

before converting another MPAS output file.

As we just saw, it can take upwards of a minute to interpolate a single MPAS "history" file. If we are only interested in a small subset of the fields in an MPAS file, we can restrict the interpolation to just those fields by providing a file named include fields in our working directory.

Using an editor of your choice, create a new text file named include\_fields with the following contents:

u10 v10 precipw

After saving the file, we can re-run the convert\_mpas program as before to produce a latlon.nc file with just the 10-meter surface winds and precipitable water:

```
$ convert_mpas history.2014-09-15_00.00.00.nc
```

\$ ncview latlon.nc

The convert\_mpas program should have taken just a few seconds to run; if not, make sure the latlon.nc file was deleted before re-running convert\_mpas. The only fields in the new latlon.nc file should be "precipw", "u10", and "v10".

Rather than converting just a single file at a time, we can convert multiple MPAS output files and write the results to the same latlon.nc file. The key to doing this is to use the first command-line argument to convert\_mpas to specify a file that contains horizontal (SCVT) mesh information, and to let subsequent command-line arguments specify MPAS netCDF files that contain fields to be remapped.

To interpolate the "precipw", "u10", and "v10" fields for our entire 5-day simulation, we can use the following commands:

```
$ rm latlon.nc
```

- \$ convert mpas x1.10242.init.nc history.\*.nc
- \$ ncview latlon.nc

Note, again, that the first command-line argument to <code>convert\_mpas</code> is only used to obtain SCVT mesh information by the <code>convert\_mpas</code> program when multiple command-line arguments are given, and all remaining command-line arguments specify netCDF files with fields to be interpolated!

When viewing a netCDF file with multiple time records, you can step through the time periods in neview with the "forward" and "backward" buttons to the right and left of the "pause" button:



As a final exercise in viewing MPAS output via the convert\_mpas and noview programs, we'll zoom in on a part of the globe, looking at the 250 hPa vertical vorticity field over East Asia on a 1/10-degree lat-lon grid.

To do this, we will first need to edit the include\_fields file so that it contains just the following line:

```
vorticity_250hPa
```

Then, we'll create a new file named target\_domain with the editor of our choice. This file should contain the following lines:

```
startlat=30
endlat=60
startlon=90
endlon=150
nlat=300
nlon=600
```

After editing the include\_fields file and creating the target\_domain file, we can remove the old latlon.nc file and use the convert\_mpas program to interpolate the 250 hPa vorticity field from our diag.\*.nc files:

```
$ rm latlon.nc
$ convert_mpas x1.10242.init.nc diag*nc
$ ncview latlon.nc
```

If the processing of the static, geographical fields for the 240km – 48km variable-resolution mesh has not finished, yet, you can feel free to experiment more with the convert mpas program!

## 3.4 Interpolating real-data initial conditions

Once the processing of the static, geographical fields has completed in the 240-48km\_variable directory, we should have a new "static" file as well as a log.init\_atmosphere.0000.out file. In our example, the static file is named SouthAmerica.static.nc, but your file should have whatever name was specified in the definition of the "output" stream in the streams.init atmosphere file.

Before proceeding, it's a good idea to verify that there were no errors reported in the log.init\_atmosphere.0000.out file. We can also make a plot of the terrain height field as we did for the 240-km quasi-uniform simulation:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/python_scripts/plot_terrain.py .
$ ./plot_terrain.py SouthAmerica.static.nc
```

Once we have convinced ourselves that the static, geographical processing was successful, we can proceed as we did for the 240-km quasi-uniform simulation. We'll create a symbolic link to the ERA5 intermediate file valid at 0000 UTC on 10 September 2014:

```
$ ln -s /glade/campaign/mmm/wmr/mpas tutorial/met data/ERA5:2014-09-10 00 .
```

As before, we'll set up the namelist.init\_atmosphere file to instruct the init\_atmosphere\_model program to interpolate meteorological and land-surface initial conditions:

```
config init case = 7
   config_start_time = '2014-09-10_00:00:00'
&dimensions
   config nvertlevels = 55
   config_nsoillevels = 4
   config nfglevels = 38
   config_nfgsoillevels = 4
&data sources
   config_met_prefix = 'ERA5'
   config use spechumd = false
&vertical grid
   config ztop = 30000.0
   config_nsmterrain = 1
   config smooth surfaces = true
   config_dzmin = 0.3
   config nsm = 30
   config tc vertical grid = true
   config_blend_bdy_terrain = false
&interpolation control
   config_extrap_airtemp = 'lapse-rate'
&preproc stages
   config static interp = false
   config_native_gwd_static = false
   config vertical grid = true
   config met interp = true
```

```
config_input_sst = false
  config_frac_seaice = true
/
&decomposition
  config_block_decomp_file_prefix = 'x5.30210.graph.info.part.'
/
```

Besides the namelist.init\_atmosphere file, we must also edit the XML I/O configuration file, streams.init\_atmosphere, to specify the name of the static file that will serve as input to the init\_atmosphere\_model program, as well as the name of the MPAS-Atmosphere initial condition file to be created. Specifically, we must set the filename\_template for the "input" stream to the name of our static file:

and we must set the name of the initial condition file to be created in the "output" stream:

After editing the namelist.init\_atmosphere and streams.atmosphere files, and linking the intermediate file to our run directory, we can run the init\_atmosphere\_model program by submitting the init real.pbs script to the queuing system again:

```
$ qsub init real.pbs
```

The init\_atmosphere\_model program should take just a few minutes to run. Once the init\_atmosphere\_model program finishes, as always, it is best to verify that there were no error messages reported in the log.init\_atmosphere.0000.out file. We should also have a file whose name matches the filename we specified for the "output" stream in the streams.init\_atmosphere file. In our example, we should have a file named SouthAmerica.init.nc.

If all was successful, we are ready to run a variable-resolution MPAS simulation. For this simulation, we won't prepare an SST and sea-ice surface update file for the model; however, if you would like to try doing so following what was done in Section 2.2, feel free to do so!

## 3.5 Model integration

Assuming that an initial condition file, and, optionally, a surface update file have been created, we're ready to run a variable-resolution, 240km – 48km simulation with refinement over a part of the globe that interests us.

As a first step, you may recall that we need to create symbolic links to the atmosphere\_model executable, as well as to the physics look-up tables, into our working directory:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/src/core_atmosphere/physics/physics_wrf/file
```

We will also need *copies* of the namelist.atmosphere, streams.atmosphere, and stream list.atmosphere.\* files:

```
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/stream_list.atmosphere.* .
```

Next, we will need to edit the namelist.atmosphere file. Recall from before that the default namelist.atmosphere is set up for a 120-km mesh; in order to run the model on a different mesh, there is one key key parameter that depends on the model resolution:

• config dt — the model integration time step (delta-t), in seconds.

The model timestep, <code>config\_dt</code> must be set to a value that is appropriate for the smallest grid distance in the mesh. In our case, we need to choose a time step that is suitable for a 48-km grid distance; a value of 240 seconds is reasonable. In the lecture on MPAS dynamics we will say more about how to choose the model timestep.

To tell the model the date and time at which integration will begin, and to specify the length of the integration to be run, there are two other parameters that must be set for each simulation:

- config\_start\_time the start time of the integration.
- config\_run\_duration the length of the integration.

In order to make maximal use of the time between this practical session and the next, we'll try to run a 5-day simulation starting on 2014-09-10\_00.

Lastly, when running the MPAS-Atmosphere model in parallel, we must tell the model the prefix of the filenames that contain mesh partitioning information for different MPI task counts:

• config\_block\_decomp\_file\_prefix — the file prefix (to be suffixed with processor count) of the file containing mesh partitioning information.

For the 240km - 48km variable-resolution mesh, we can find a mesh partition file with 128 partitions at /glade/campaign/mmm/wmr/mpas\_tutorial/meshes/x5.30210.graph.info.part.128. Let's symbolically link that file to our run directory now before specifying a value of 'x5.30210.graph.info.part.' for the config\_block\_decomp\_prefix in our namelist.atmosphere file.

```
$ ln -s /glade/campaign/mmm/wmr/mpas_tutorial/meshes/x5.30210.graph.info.part.128 .
```

Before reading further, you may wish to try making the changes to the namelist.atmosphere yourself. Once you've done so, you can verify that the options highlighted below match the changes you have made.

```
&nhyd_model
    config_dt = 240.0
    config_start_time = '2014-09-10_00:00:00'
    config_run_duration = '5_00:00:00'
/
&decomposition
    config_block_decomp_file_prefix = 'x5.30210.graph.info.part.'
/
```

After changing the parameters shown above in the namelist.atmosphere file, we must also set the name of the initial condition file in the streams.atmosphere file:

Optionally, if you decided to create an SST update file for this variable-resolution simulation in the previous section, you can also edit the "surface" stream in the streams.atmosphere file to specify the name of that surface update file, as well as the interval at which the model should read updates from it:

Having set up the namelist.atmosphere and streams.atmosphere files, we're ready to run the model in parallel. We can copy the same job script as we used for the quasi-uniform 240-km simulation and submit it as usual with qsub.

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/run_model.pbs .
$ qsub run_model.pbs
```

Once the model begins to run, you may like to "tail" the log.atmosphere.0000.out file with the "-f" option to follow the progress of the MPAS simulation:

```
$ tail -f log.atmosphere.0000.out
```

If the model has started up successfully and begun to run, we should see messages like this:

```
Begin timestep 2014-09-10_00:12:00
--- time to run the LW radiation scheme L_RADLW =F
--- time to run the SW radiation scheme L_RADSW =F
--- time to run the convection scheme L_CONV =T
--- time to apply limit to accumulated rainc and rainnc L_ACRAIN =F
--- time to apply limit to accumulated radiation diags. L_ACRADT =F
--- time to calculate additional physics_diagnostics =F
split dynamics-transport integration 3

global min, max w -1.06611 0.722390
global min, max u -117.781 118.251
Timing for integration step: 4.18681 s
```

This simulation will take about half an hour to run. Now may be a convenient time to ask any questions that you may have!

# 4. Running limited-area simulations

Having gained experience in running global simulations, we are now well positioned to run a limited-area (i.e., a regional) simulation with MPAS-Atmosphere. We will begin by defining the simulation domain using the MPAS-Limited-Area tool to cover any part of the globe that interests us. Then, we will subset the "static" fields from an existing 60-km quasi-uniform static file.

Once we are satisfied with the geographic coverage of our regional static fields, we will interpolate initial and lateral boundary conditions from the 0.5-degree CFSv2 datset. Given ICs and LBCs for our regional domain, we can begin running a 3-day regional simulation from 2019-09-01 0000 UTC through 2019-09-04 0000 UTC.

After our simulation has run (or, even after the first few model output files are available), we will practice using NCL and the convert\_mpas tool to visualize the regional output.

# 4.1 Defining a regional domain and subsetting static fields

To begin the work of defining a regional simulation domain for MPAS-Atmosphere, we will first obtain a copy of the MPAS-Limited-Area tool. As with the MPAS model code and MPAS-Tools code, we will clone the MPAS-Limited-Area repository from GitHub. From within our

/glade/derecho/scratch/\${USER}/mpas\_tutorial directory, we can do this with the following commands:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ git clone https://github.com/MPAS-Dev/MPAS-Limited-Area.git
```

After changing to the MPAS-Limited-Area directory that should have been created by the git clone command, we can prepare a file describing our desired regional domain. Depending on the type of region that we intend to define (circular, elliptical, channel, or polygon), we can use any of the example region definition files in the docs/points-examples/ sub-directory as a starting point.

For the purpose of illustration, we'll use the japan.ellipse.pts file from docs/points-examples/ as a starting point to set up an elliptical domain over the Mediterranean Sea; however, you may set up your regional domain over any other part of the globe using any of the available region types. After copying this file to a file named mediterranean.pts in our current working directory with

\$ cp docs/points-examples/japan.ellipse.pts mediterranean.pts

we can edit the file so that its contents look like the following:

Name: Mediterranean Type: ellipse Point: 37.9, 18.0 Semi-major-axis: 3200000 Semi-minor-axis: 1700000 Orientation-angle: 100

Again, you can set up any alternative regional domain as you prefer — the Mediterranean domain is only used here as an example!

To aid in locating your regional domain, it may be helpful to use <a href="OpenStreetMap">OpenStreetMap</a>, where you can right-click anywhere on a map and choose "Show address" to find the latitude and longitude of a point.

Having prepared a region definition file, we can use the <code>create\_region</code> tool to create a subset of an existing global "static" file for our specified region. We can symbolically link a global, quasi-uniform, 60-km static file to our working directory with:

Then, we can create a regional static file with a command like:

\$ ./create\_region mediterranean.pts x1.163842.static.nc

The create\_region tool should take just a few seconds to run, and the result should be a new static file and a new graph.info file, named according to the "Name" we specified in our region defintion file, e.g,:

```
Mediterranean.static.nc
Mediterranean.graph.info
```

At this point, we may like to plot one of the time-invariant, terrestrial fields from our new regional static file. We can plot the terrain height field using an NCL script, regional\_terrain.ncl, which we will first copy to our working directory:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/ncl_scripts/regional_terrain.ncl .
```

This NCL script uses a custom color map. In order for NCL to find this color map, we'll need to set the NCARG\_COLORMAPS environment variable as follows:

Before running the script, we will also need to set the latitude and longitude view point for the orthographic projection used by the script. In the regional\_terrain.ncl script, locate the section that looks like the following, and modify the cenlat and cenlon values so that they coincide roughly with the center of your regional domain.

Additionally, we will need to set the **GNAME** environment variable to the name of our regional static file; e.g., for our Mediterranean example:

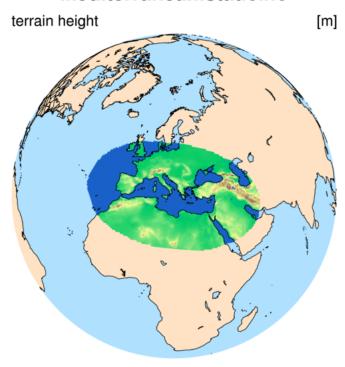
\$ export GNAME=Mediterranean.static.nc

We can then run the script with

\$ ncl regional\_terrain.ncl

to produce a PNG image that should look something like the following:

# Mediterranean.static.nc



Before proceeding to the next section, you may need to iterate between (1) modifying your region definition file, (2) running the create\_region tool to create a new netCDF file, and (3) plotting the new regional terrain field with the regional\_terrain.ncl script.

## 4.2 Interpolating regional initial conditions (ICs)

Now that we have a regional static file for our domain of interest, we can prepare initial conditions for this domain in essentially the same way as we prepared initial conditions for global simulations. The key difference is that we will blend the terrain field along the regional domain boundaries with the terrain from our initial conditions data.

Let's create a new directory in /glade/derecho/scratch/\${USER}/mpas\_tutorial to run our regional simulation:

- \$ mkdir /glade/derecho/scratch/\${USER}/mpas tutorial/regional
- \$ cd /glade/derecho/scratch/\${USER}/mpas tutorial/regional

We can then move the regional static file and graph.info files that we created in Section 4.1 to this directory:

```
$ mv /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Limited-Area/Mediterranean.static.nc .
$ mv /glade/derecho/scratch/${USER}/mpas tutorial/MPAS-Limited-Area/Mediterranean.graph.info .
```

As with the global simulations from earlier sections, we will need to link the <code>init\_atmosphere\_model</code> executable to our run directory, and we will also need to <code>copy</code> the <code>namelist.init\_atmosphere</code> and <code>streams.atmosphere</code> files, which we will modify for our regional domain.

```
$ In -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/init_atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.init_atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.init_atmosphere .
```

For our regional simulation, we will use 0.5-degree CFSv2 data valid on 2019-09-01 0000 UTC for initial conditions. We can symbolically link the CFSV2 intermediate file to our run directory as follows:

```
$ ln -s /glade/campaign/mmm/wmr/mpas tutorial/met data/CFSV2:2019-09-01 00 .
```

Recall that we use the Metis tool to create mesh partition files for a specified number of MPI tasks. Using Metis's <code>gpmetis</code> tool, we can create a partition file for 128 MPI tasks from the <code>Mediterranean.graph.info</code> file that was generated by MPAS-Limited-Area. The following command should be work:

```
$ gpmetis -minconn -contig -niter=200 Mediterranean.graph.info 128
```

Even if we choose not to interpolate the initial conditions in parallel, we will ultimately need the mesh partition file to run the model in parallel.

Now, we are ready to edit our namelist.init\_atmosphere and streams.init\_atmosphere files. To test your understanding, you may like to first try preparing these files yourself for the creation of initial conditions for your regional domain. Once you've finished editing these files, you can compare against the changes highlighted below (click on the light blue header bars). Remember that your static file and graph.info file may have different names, depending on where your regional domain is located.

#### The edited namelist.init\_atmosphere file

```
&nhyd model
   config_init_case = 7
   config start time = '2019-09-01 00:00:00'
   config_stop_time = '2010-10-23 00:00:00'
    config theta adv order = 3
   config_coef_3rd_order = 0.25
&dimensions
   config nvertlevels = 55
   config nsoillevels = 4
    config_nfglevels = 38
    config nfgsoillevels = 4
&data sources
    config geog data path = '/glade/campaign/mmm/wmr/mpas tutorial/mpas static/'
   config_met_prefix = 'CFSV2'
    config sfc prefix = 'SST'
    config_fg_interval = 86400
    config landuse data = 'MODIFIED IGBP MODIS NOAH'
    config topo data = 'GMTED2010'
   config_vegfrac_data = 'MODIS'
    config albedo data = 'MODIS'
   config_maxsnowalbedo_data = 'MODIS'
    config_supersample_factor = 3
    config use spechumd = false
&vertical grid
   config_ztop = 30000.0
    config nsmterrain = 1
   config smooth surfaces = true
   config_dzmin = 0.3
    config nsm = 30
   config tc vertical grid = true
    config blend bdy terrain = true
&interpolation control
    config_extrap_airtemp = 'lapse-rate'
&preproc stages
   config static interp = false
    config_native_gwd_static = false
    config vertical grid = true
```

```
config_met_interp = true
  config_input_sst = false
  config_frac_seaice = true

/
&io
   config_pio_num_iotasks = 0
    config_pio_stride = 1

/
&decomposition
   config_block_decomp_file_prefix = 'Mediterranean.graph.info.part.'
//
```

#### The edited streams.init\_atmosphere file

For namelist and streams settings that were not modified, either the default value of the setting is acceptable, or the setting is not used when interpolating time-varying initial conditions. Now is also a good time to check that you understand why we needed to modify the settings that we did in the namelist.init\_atmosphere and streams.init\_atmosphere files.

After checking your modifications to the namelist.init\_atmosphere and streams.init\_atmosphere files, above, we can run the init\_atmosphere\_model program with 128 MPI tasks to create regional initial conditions. To do this, we can copy a prepared job script to run the init\_atmosphere\_model program and submit it with qsub.

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/init_parallel.pbs .
$ qsub init_parallel.pbs
```

Once the job completes, as always, it's important to verify that there were no errors during the execution of the init\_atmosphere\_model program; the end of the log.init\_atmosphere.0000.out file should report zero errors:

```
Total log messages printed:

Output messages = 464

Warning messages = 6

Error messages = 0

Critical error messages = 0
```

If there were no errors, we should now have a regional initial conditions file; for our example regional domain the file should be named Mediterranean.init.nc. We're now ready to generate lateral boundary conditions for our domain in the next section!

# 4.3 Interpolating regional lateral boundary conditions (LBCs)

The interpolation of lateral boundary conditions for a regional simulation domain is conceptually similar to the interpolation of initial conditions: the key differences are: (1) fields are interpolated at several time periods, and (2) the set of fields to be interpolated are a subset of those required for initial conditions (they include: theta, rho, u, w, and moisture species).

We will use the CFSv2 reanalyses for lateral boundary conditions. Three days' worth of six-hourly CFSv2 fields are available in the /glade/campaign/mmm/wmr/mpas\_tutorial/met\_data directory, and we can symbolically link all of these CFSv2 files to our run directory with the following command:

```
$ ln -sf /glade/campaign/mmm/wmr/mpas tutorial/met data/CFSV2* .
```

All that is needed now is to once again edit the namelist.init\_atmosphere and streams.init\_atmosphere files to set up the interpolation of LBCs using "init case" 9. The relevant settings are highlighted in the sections, below (click the light blue headers to expand each edited file).

#### The edited namelist.init\_atmosphere file

#### The edited streams.init\_atmosphere file

There are a few points worth making about the changes in the streams.init\_atmosphere file.

- Because the interpolation of LBCs is not only a horizontal interpolation to the regional mesh, but also
  a vertical interpolation to the vertical coordinate surfaces, the "input" stream must read from a file
  that contains a valid "zgrid" field. The initial conditions file contains horizontal and vertical mesh
  information, and so we use it as the file from which the "input" stream reads.
- The MPAS stream manager infrastructure will complain if an input stream and an output stream share the same filename\_template, so the filename\_template for the "output" stream must be set to some other filename; since "init case" 9 only writes the "lbc" stream, we can make up any filename we like for the "output" stream.

• The output\_interval for the "lbc" stream must match the value of the config\_fg\_interval namelist option. In this regional example, using "21600" or "6:00:00" are equivalent (we could even specify "360:00" if we would like!).

After having edited our namelist.init\_atmosphere and streams.init\_atmosphere files, we are ready to run the init\_atmosphere\_model program again using 128 MPI tasks. We can submit the init parallel.pbs script again with qsub:

```
$ qsub init_parallel.pbs
```

After the init\_atmosphere\_model program completes, it is a good idea (as always!) to verify that there were no errors reported at the end of the log.init\_atmosphere.0000.out file:

```
Total log messages printed:
Output messages = 2742
Warning messages = 0
Error messages = 0
Critical error messages = 0
```

If there were no errors, we should now have "lbc" files in our run directory:

```
$ 1s -1 lbc*nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-01_00.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-01_10.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-01_12.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-01_18.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-02_00.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-02_00.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-02_06.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-02_12.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-02_18.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_00.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_00.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_18.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_18.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_18.00.00.nc
-rw-r--r- 1 class112 cbet 15469296 Sep 5 16:37 lbc.2019-09-03_18.00.00.nc
```

We're now ready to run a regional simulation in the next section!

## 4.4 Running a regional simulation

Given regional initial conditions and lateral boundary conditions, we are almost ready to run a regional simulation. The only differences from running a global simulation are: (1) we need to set a namelist option to enable the application of LBCs in each model timestep, and (2) we need to set up an LBC input stream for the model.

As in previous exercises, we will need to symbolically link the atmosphere\_model executable, as well as the look-up tables used by physics schemes, into our run directory. We can do this with the following commands:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/src/core_atmosphere/physics/physics_wrf/file
```

We also need copies of the default namelist.atmosphere, streams.atmosphere, and stream\_list.atmosphere.\* files, which we will edit for our simulation.

```
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/stream_list.atmosphere.* .
```

As with global simulations, the key namelist parameters that must be modified are:

- config\_dt the model integration timestep; roughly six times the minimum grid distance in km is a reasonable first guess
- config start time the starting time for the simulation
- config\_run\_duration the duration of the simulation
- config\_block\_decomp\_file\_prefix the prefix (excluding the final number) of the file providing mesh partition information

Different from global simulations, we must also set the namelist option config apply lbcs = true!

You may like to try editing the namelist.atmosphere file yourself before checking your changes against those highlighted, below (click on the light blue header).

#### The edited namelist.atmosphere file

In the streams.atmosphere file, we will need to set the filename\_template for the "input" stream to the name of our regional initial conditions file. We will also need to set the input\_interval for the "lbc\_in" stream to the interval at which we have prepared lateral boundary conditions files.

After editing the streams.atmosphere file, you can compare your changes against those highlighted, below (click on the light blue header).

#### The edited streams.atmosphere file

Once we have finished editing the namelist.atmosphere and streams.atmosphere files, we're ready to run a simulation. We can copy the same job script as we used for the quasi-uniform 240-km simulation and submit it as usual with qsub.

- \$ cp /glade/campaign/mmm/wmr/mpas\_tutorial/job\_scripts/run\_model.pbs .
  \$ qsub run model.pbs
- This simulation will take a while to run. Once the first few netCDF output files have been produced, even before the full simulation has completed, we can proceed to the next section to practice visualizing the initial regional model output.

## 4.5 Visualizing regional output

If the regional simulation ran successfully — or even if it has just begun running and has produced several time periods of output — we can visualize the output using two different methods.

In order to take a quick first look at the output, we can use the convert\_mpas tool to interpolate our output to a regular latitude-longitude grid, after which we can view the interpolated fields using noview.

Let's first check whether the path to the convert\_mpas program is in our \$PATH environment variable with:

\$ which convert\_mpas

If the "which" command prints something like

/usr/bin/which: no convert\_mpas ...

we can set our \$PATH environment variable by typing:

\$ export PATH=/glade/derecho/scratch/\${USER}/mpas\_tutorial/convert\_mpas:\$PATH

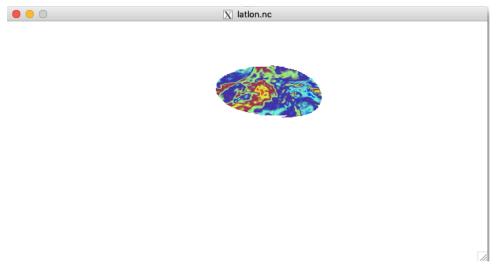
To start, we can simply interpolate the full set of fields from all diagnostics output files to a global 0.5-degree lat-lon grid with the following command:

\$ convert mpas Mediterranean.static.nc diag\*nc

We can then view the resulting latlon.nc file with ncview:

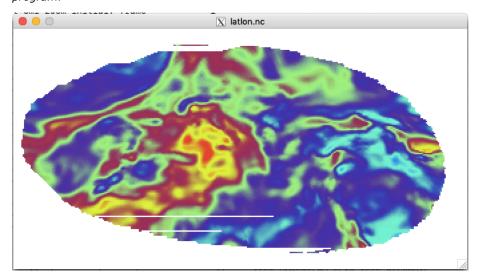
\$ ncview latlon.nc

Because the default target grid for the convert\_mpas program is a global, 0.5-degree grid, viewing, e.g., the "precipw" field might look like the image below.



As we did in Section 3.3, we can try to interpolate to a lat-lon grid that is windowed around our regional domain. Following Section 3.3 to prepare a target\_domain file, can you produce a latlon.nc file that looks something like the following?

Remember: it's generally best to remove any existing latlon.nc file before re-running the convert\_mpas program!



As mentioned in the lectures, the <code>convert\_mpas</code> program may produce some interpolation artifacts as of the time of this tutorial. We expect to have this fixed in the near future, but for now, we can ignore any interpolation artifacts and animate through all time slices of several model diagnostic fields in <code>neview</code> to gain confidence that our regional simulation is producing plausible results.

After we've taken some time to browse the interpolated diagnostic fields with ncview, we can make use of NCL to produce figures more suitable for use in publications or presentations.

In /glade/campaign/mmm/wmr/mpas\_tutorial/ncl\_scripts is a template script, regional\_cells.ncl, for plotting the individual cell values from a regional MPAS netCDF file. We can copy this script to our run directory with the following command:

\$ cp /glade/campaign/mmm/wmr/mpas\_tutorial/ncl\_scripts/regional\_cells.ncl .

By default, this script plots the vegetation type field, <code>ivgtyp</code>, with the view-point set to 20.0 N latitude, 80.0 E longitude. With the editor of your choice, open the <code>regional\_cells.ncl</code> file and locate the section of the script with the following (it should be around line 68):

```
; Center latitude and longitude; cenlat = 20.0 cenlon = 80.0
```

Let's change the center latitude and longitude values for the view-point to the approximate center of our regional domain. For our example Mediterranean domain, the following settings might be reasonable, but if your regional domain is located over a different part of the globe, you should modify these values as necessary.

```
;
; Center latitude and longitude
;
cenlat = 38.0
cenlon = 20.0
```

In general, the regional cells.ncl script reads three environment variables:

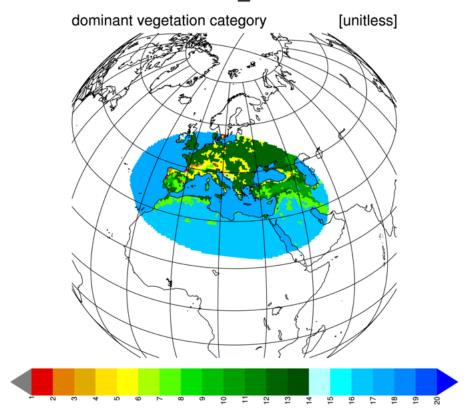
- FNAME the name of the file containing the field to be plotted
- GNAME the name of the file containing the mesh information
- T for time-varying fields, the time period to plot (0 is the first time in a file)

In order to plot the vegetation type field from our initial conditions files, the following settings of these variables will work:

- FNAME=Mediterranean.init.nc
- GNAME=Mediterranean.init.nc
- T=0

After setting these environment variables and running the NCL script, we should have a plot equivalent to the one below in a file named "cells.png".

# 2019-09-01\_00:00:00



The part of the regional\_cells.ncl script that handles the actual plotting is general enough to handle any field — we just need to set an appropriate plotting range and color table in the script when changing fields. Next, we can try to modify the script to plot the precipitable water ("precipw") field using a different color map.

Before proceeding, you may like to open  $\underline{\text{the NCL Color Table Gallery}}$  in a new tab to see the available NCL color tables.

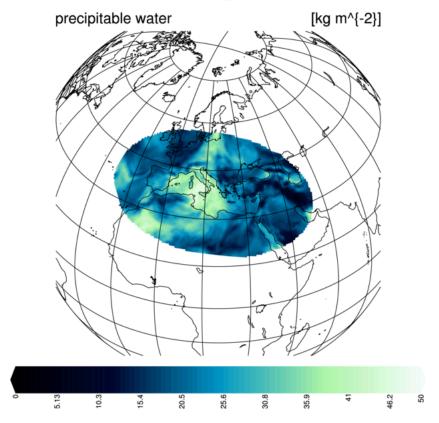
With the editor of your choice, open the regional\_cells.ncl file and locate the section of the script (beginning around line 84) where the field to be plotted, the color map, and the contour levels are set. Let's modify this section of the script so that it looks like the following:

We located the "GMT\_ocean" color table from the NCL Color Table Gallery link, above. Before re-running the script, we will need to set the **fname** environment variable to the name of one of our diagnostics model output files. If our regional simulation has progressed through at least forecast hour 24, we could use the following:

```
$ export FNAME=diag.2019-09-02_00.00.00.nc
```

We can then re-run the script to produce a plot like the one below.

# 2019-09-02\_00:00:00



With the remaining time in this session, feel free to experiment with plotting other fields from any of the netCDF output files. Browsing the model output that has been converted to a latitude-longitude grid with the convert\_mpas before deciding on the field to plot and the range of values to set in the regional cells.ncl script may be helpful.

# 5. Defining new output streams, and visualization

In this section, we'll restart a simulation from the end of the five-day, global 240-km simulation that we started in the second section. Before restarting the simulation, though, we'll define new output streams.

Optionally, before restarting the simulation, we can also try adding a list of sounding locations for the simulation.

After launching the restart simulation with new output streams (and perhaps some sounding output), we'll practice using some NCL scripts to visualize the first five days of output from the variable-resolution 240-km – 48-km simulation

# 5.1 Setting up the restart simulation

As we saw in the lectures, setting up a simulation to restart from a previously run simulation is relatively simple. We'll begin by making sure that we're in the directory where we ran the original, 5-day 240-km global simulation:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform
```

Before making any changes to the namelist.atmosphere file, we will first check to see which restart files are available; if our original simulation completed successfully, we should have one restart file per day, valid at the end of each of the five days of the simulation:

```
$ 1s -1 restart*nc
-rw-r--r- 1 duda ncar 197382136 Apr 8 23:57 restart.2014-09-11_00.00.00.nc
-rw-r--r- 1 duda ncar 197382136 Apr 8 23:57 restart.2014-09-12_00.00.00.nc
-rw-r--r- 1 duda ncar 197382136 Apr 8 23:58 restart.2014-09-13_00.00.00.nc
-rw-r--r- 1 duda ncar 197382136 Apr 8 23:59 restart.2014-09-14_00.00.00.nc
-rw-r--r- 1 duda ncar 197382136 Apr 8 23:59 restart.2014-09-15_00.00.00.nc
```

In principle, we could restart our simulation from any of these files, but we'll begin from the last available file, valid at 0000 UTC on 15 September.

There are just two changes that need to be made to the namelist.atmosphere file: we need to set the starting time of the simulation to 2014-09-15\_00:00:00 and we need to set the config\_do\_restart

We can keep all of the other namelist options as they were, including the <code>config\_run\_duration</code> option — restarting the simulation and running for another five days should be fine, since we had a total of 10 days of SST and sea-ice information in our surface update file.

Before running the model, we'll make a few other changes as described in the next sections!

### 5.2 Defining new output streams

We may also like to write out some additional fields from our restart simulation at a higher temporal frequency. You may recall from the lectures that we can define new output streams in the streams.atmosphere file.

We will provide an example here of writing out the 10-meter AGL horizontal winds every 60 minutes, but you can feel free to look through Appendix D of the MPAS-Atmosphere Users' Guide to see if there are any other fields that you may like to write out.

Let's define a new output stream named "sfc\_winds" in the streams.atmosphere file:

This new stream must be defined somewhere between the opening <streams> and closing </streams> tags in the streams.atmosphere file.

Note in the stream definition above that the files that will be written will have names like surface\_winds.2014-09-15\_00.nc, surface\_winds.2014-09-15\_01.nc, etc. by our choice of the
"filename\_template". Also, MPAS will create new files at each output time, rather than packing many
time records into the same file; this is controlled by the "filename\_interval" option. Finally, note that the
stream will be written every 60 minutes. Since our simulation starts at 00:00:00 UTC, the minutes and
seconds part of the output files is unnecessary. Of course, we may want to add \$m and \$s to our filename
template if we were writing this stream more frequently than once per hour.

In the next section, we'll describe the steps to write out vertical profiles at specific (lat,lon) locations before we run our restart simulation.

# 5.3 Adding soundings to the simulation

It may at times also be helpful to write out vertical profiles of basic model fields at specified (lat,lon) locations from a model simulation. In MPAS terminology, this is described as writing "soundings" from the simulation.

In principle, we can write out soundings for as many locations as we would like. Here, we'll describe how to write out soundings from three locations: Boulder, Colorado; McMurdo Station, Antarctica; and New Delhi, India.

We will need to specify the locations for the soundings in a text file named sounding\_locations.txt in our model run directory:

```
40.0 -105.25 Boulder
28.7 77.2 NewDelhi
-77.85 166.67 McMurdo
```

The three columns of the file contain the latitude, longitude, and name of the sounding. The latitude and longitude are given as decimal degrees, and the name cannot contain whitespace (since it will be used to name output files).

For this exercise, if you would prefer to write out soundings for different locations, feel free to change the list of locations as you would like!

Lastly, we need to specify how frequently these soundings will be written during the model simulation. This is done through the config sounding interval option in the namelist.atmosphere file. By

default, this option can be found near the bottom of the file. Let's choose to write soundings every three hours:

```
&soundings
    config_sounding_interval = '3:00:00'
/
```

Having set the output interval for soundings, we're ready to make a restart simulation.

## 5.4 Running the restart simulation

Now that we've edited our namelist.atmosphere file for our restart run, we've added a new output stream with surface winds to the streams.atmosphere file, and we've specified a list of locations for which profiles will be written every three hours, we can restart the model and simulate an additional five days by submitting our existing run\_model.pbs script with qsub:

```
$ qsub run_model.pbs
```

Once the job has started to run, it's a good idea to check several points:

- Does running tail -f log.atmosphere.0000.out show timesteps being taken by the model?
- Do you see new output files named surface winds.2014-09-15 00.nc, etc.?
- Do you see sounding files for Boulder, New Delhi, and McMurdo Station as files with the .snd suffix?

If all of the above check out, our restart simulation is successfully running! In the next section, we'll look at a couple of new NCL scripts for plotting model output.

### 5.5 Using NCL to visualize output

Now that our restart simulation is running, we can examine in more detail an example NCL script for plotting horizontal fields as individual cells. To try out this script, we can work with output from our 240km – 48km variable-resolution simulation.

In order to plot horizontal fields, we can begin by ensuring that we are in the 240-48km\_variable directory before copying over the latlon cells.ncl script:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/240-48km_variable
$ cp /glade/campaign/mmm/wmr/mpas tutorial/ncl scripts/latlon cells.ncl .
```

This script reads the name of the MPAS NetCDF file with SCVT mesh information from an environment variable named GNAME (roughly, "G" means "grid"). The MPAS NetCDF file that contains the actual field to be plotted is identified by the environment variable FNAME (roughly, "F" means "field").

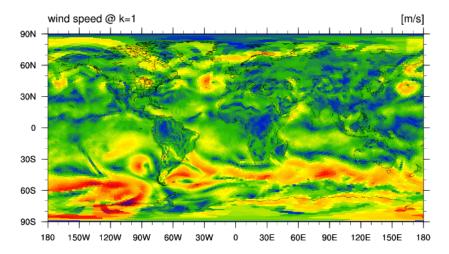
We'll plot a field from the diag.2014-09-11\_00.00.00.nc file. The mesh information can be found in the MPAS initial conditions file, which may be named SouthAmerica.init.nc, though you may have chosen a different name corresponding to a different location of refinement. We'll set the GNAME and FNAME environment variables before proceeding:

```
$ export GNAME=SouthAmerica.init.nc
$ export FNAME=diag.2014-09-11_00.00.00.nc
```

Remember, your initial conditions file may have a different name!

By default, the latlon\_cells.ncl script plots the lowest-model-level wind speed, and the output is saved to a PNG image in a file named cell\_plot.png. Running the script should produce this plot, which you can view with the display command.

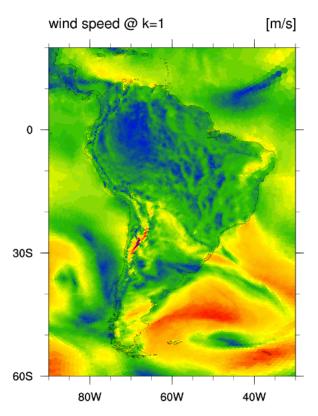
```
$ ncl latlon_cells.ncl
$ display cell_plot.png
```



Since we are working with a variable-resolution mesh, we may like to set a plotting window to cover only part of the refined region in our simulation. We can set a plotting window in the latlon\_cells.ncl script by editing the section of the script that looks like this:

```
; The bounding box for the plot mapLeft = -180.0 mapRight = 180.0 mapBottom = -90.0 mapTop = 90.0
```

Feel free to set the plotting window however you would like for your variable-resolution simulation. For example, if we were to set the plotting window to cover South America before re-running the script, the result might look like the following:



Finally, we may like to plot other fields. We can see which fields were written to the diag.\*.nc files using ncdump:

```
$ ncdump -h diag.2014-09-11_00.00.00.nc
```

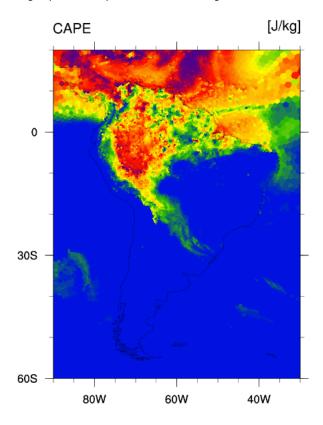
If, for example, we would like to plot Convective Available Potential Energy (CAPE), we could edit the latlon\_cells.ncl script near the comment "The field to be plotted" so that it looked like the following:

```
; The field to be plotted
h = f->cape(0,:)
```

```
; The field name
field_name = "CAPE"
field_units = "[J/kg]"

; The range of field values to plot (start, stop, number)
cnLevels = fspan(0,3000,50)
```

Generally, we will need to assign the variable to be plotted, specify the plotting name and units for the field, and specify a range of value for the field. Making these changes and re-running the NCL script might produce a plot like the following:



Now that you have a feel for how to edit the latlon\_cells.ncl script, feel free to try plotting other fields!

# 6. Adding new passive tracers

In this section, we'll get some experience in making source-code changes to add a passive tracer to the model. Although the exercises in this section are independent of those in other section, it may be best to finish the exercises from the previous section first, since we will be changing the model source code and recompiling the model executable.

# 6.1 Creating initial conditions for the tracer

We'll begin by defining our new passive tracer in the Registry.xml file for the init\_atmosphere core. Let's change directories to the copy of the MPAS-Model source code in our /glade/derecho/scratch/\${USER}/mpas tutorial directory:

\$ cd /glade/derecho/scratch/\${USER}/mpas\_tutorial/MPAS-Model

Opening up the src/core\_init\_atmosphere/Registry.xml file with our editor of choice, we will look for the var\_array section named "scalars"; it should look something like this:

As we saw in the lectures, we will need to add our new passive tracers here. Let's add a new passive tracer named "mytracer1". The array\_group that we assign to this tracer can be anything other than "moist". By convention, we'll call the array group for this new tracer "passive". After adding our new tracer, the "scalars" var\_array should look like this:

After making this change to the Registry.xml file, we'll clean and re-compile the init\_atmosphere core. Recall that, after we make changes to the Registry.xml file, we need to "clean" the build first so that the changes take effect. Later, when we modify only Fortran source code, there will be no need to "clean" before re-compiling. The following two commands should suffice:

```
$ make clean CORE=init_atmosphere
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=init atmosphere
```

If compilation was successful, we should now have a new init\_atmosphere\_model executable. At this point, if we were to create new initial conditions, the "mytracer1" field would be present in the initial conditions, but it would be zero everywhere. We next need to add code to define the initial conditions for "mytracer1".

To define the initial value of our new tracer, use your preferred editor to open the src/core\_init\_atmosphere/mpas\_init\_atm\_cases.F file. Search for these two lines of code that call the routine to initialize real-data test cases:

An appropriate place to add a call to our tracer initialization routine would be directly after the call to init\_atm\_case\_gfs. Let's add a new line of code below this to call a new subroutine, which we'll name init tracers.

Notice that this new routine (which we have yet to define!) takes as input two arguments; as we will see, these two arguments are MPAS "pools", which we discussed in the lectures.

As a start, we will define the init\_tracers function so that it simply writes a message to the log file. At the bottom of the src/core\_init\_atmosphere/mpas\_init\_atm\_cases.F, but before the line "end module init atm cases", let's add the following Fortran code:

```
subroutine init_tracers(mesh, state)
  implicit none
  type (mpas_pool_type), intent(in) :: mesh
  type (mpas_pool_type), intent(inout) :: state
  call mpas_log_write('====== Handling tracer initialization =======')
end subroutine init_tracers
```

After saving our code changes, we can re-compile the init\_atmosphere core with:

```
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=init atmosphere
```

Again, because we have not changed the Registry.xml file since we last re-compiled, there's no need to "make clean".

Compilation should take just a minute, and if it completes successfully, we're ready to try out our modified code, even though it won't actually create initial conditions for our passive tracer, yet. So that we don't overwrite files from any of our previous sessions, we'll work in a new directory, passive tracer:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial
$ mkdir passive_tracer
```

<sup>\$</sup> cd passive\_tracer

We'll test out our passive tracer on the 240-km uniform mesh, for which we have already created a "static" file. Now that we have experience in creating initial conditions, the following procedure should seem familiar:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/x1.10242.static.nc .
$ ln -s /glade/campaign/mmm/wmr/mpas_tutorial/met_data/ERA5:2014-09-10_00 .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/init_atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.init_atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.init_atmosphere .
```

As in Section 2.1, we'll edit the namelist.init atmosphere so that it looks like the following:

```
&nhyd model
   config_init_case = 7
   config_start_time = '2014-09-10_00:00:00'
&dimensions
   config nvertlevels = 55
   config_nsoillevels = 4
   config_nfglevels = 38
   config_nfgsoillevels = 4
&data sources
   config_met_prefix = 'ERA5'
   config_use_spechumd = false
&vertical_grid
   config_ztop = 30000.0
   config_nsmterrain = 1
   config_smooth_surfaces = true
   config_dzmin = 0.3
   config nsm = 30
   config_tc_vertical_grid = true
   config_blend_bdy_terrain = false
&interpolation_control
   config_extrap_airtemp = 'lapse-rate'
&preproc_stages
   config static interp = false
   config_native_gwd_static = false
   config_vertical_grid = true
   config_met_interp = true
   config_input_sst = false
   config_frac_seaice = true
```

We'll then edit the filename that will be read by the "input" stream in the streams.init\_atmosphere file so that it matches the name of our "static" file:

Also as in Section 2.1, we'll change the name of the initial conditions file to be created:

We should now be able to run the init\_atmosphere\_model executable to produce an x1.10242.init.nc file:

```
$ qcmd -A UMMM0006 -- ./init_atmosphere_model
```

If there were no errors in the log.init\_atmosphere.0000.out file, we can check for the presence of our passive tracer in the x1.10242.init.nc file:

```
$ ncdump -h x1.10242.init.nc | grep mytracer1
```

Besides the creation of the x1.10242.init.nc file, we should also look for this message in the log.init\_atmosphere.0000.out file:

```
===== Handling tracer initialization ======
```

If all was successful, we can go back to the MPAS-Model directory and add code to provide initial conditions for our passive tracer. Let's change back to the MPAS source code directory:

Using our favorite editor, let's open the src/core\_init\_atmosphere/mpas\_init\_atm\_cases.F file and change the code for our init\_tracers subroutine so that it looks like the following:

```
subroutine init_tracers(mesh, state)
    implicit none
    type (mpas_pool_type), intent(in) :: mesh
    type (mpas pool type), intent(inout) :: state
    integer, pointer :: index mytracer1
    integer, pointer :: nCells
    integer, pointer :: nVertLevels
    integer :: k, iCell
    real (kind=RKIND), dimension(:), pointer :: latCell
    real (kind=RKIND), dimension(:), pointer :: lonCell
    real (kind=RKIND), dimension(:,:,:), pointer :: scalars
    call mpas_log_write('====== Handling tracer initialization =======')
    call mpas_pool_get_dimension(mesh, 'nCells', nCells)
call mpas_pool_get_dimension(mesh, 'nVertLevels', nVertLevels)
    call mpas_pool_get_dimension(state, 'index_mytracer1', index_mytracer1)
    call mpas_pool_get_array(state, 'scalars', scalars)
    call mpas_pool_get_array(mesh, 'latCell', latCell)
call mpas_pool_get_array(mesh, 'lonCell', lonCell)
    do iCell = 1, nCells
         do k = 1, nVertLevels
             scalars(index mytracer1,k,iCell) = &
                        0.0001 * 0.5 * (sin(latCell(iCell)*4.0) * &
                                          sin(lonCell(iCell)*8.0) + 1.0)
         end do
    end do
end subroutine init tracers
```

Based on what was discussed in the MPAS software lecture about Registry, pools, and logging, you have the necessary information at your disposal to make sense of the code for the <code>init\_tracers</code> routine!

After saving our changes, we can re-compile the init\_atmosphere core once again:

```
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=init_atmosphere
```

We can now try creating new initial conditions with our updated init\_tracers routine. Let's change back
to the passive\_tracer directory, remove the old x1.10242.init.nc file, and create a new initial
conditions file:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/passive_tracer
$ rm x1.10242.init.nc
$ qcmd -A UMMM0006 -- ./init_atmosphere_model
```

If the creation of the new x1.10242.init.nc file was successful, you may like to try using the convert\_mpas utility to see what our new "mytracer1" field looks like. For a quick reminder of how the convert\_mpas tool works, you may find it helpful to refer back to Section 3.3.

### 6.2 Adding the tracer to the model

Now that we have a new passive tracer in our initial conditions, we'll need to edit the Registry.xml file for the atmosphere core so that the model itself will know about the new tracer.

Let's begin by changing back to the model source code directory:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model
```

We can edit the src/core\_atmosphere/Registry.xml file, recalling from the lectures that we not only need to define the tracer, but we also need to define an array that will hold the tendencies for the tracer. Even if we don't supply any sources or sinks, the model needs memory to be allocated for the tracer tendency, e.g., for use in the scalar transport routines.

In the src/core\_atmosphere/Registry.xml file, search for the word "var\_array" several times until you come to the definition of the scalars var\_array tag, which should begin with lines that look like this:

Let's add a new XML var tag inside the var\_array tag to define our new "mytracer1" tracer; this new tag may look something like the following:

```
<var name="mytracer1" array_group="passive" units="kg kg^{-1}"
    description="Our first passive tracer"/>
```

Remember: it's important that the passive tracer belongs to an array\_group other than "moist"; here, we've just used the string "passive", though in principle you could choose another name.

Similarly, we need to define a tendency array for our new passive tracer. Searching for the word "scalars\_tend", we should find a section of XML for the scalars\_tend var\_array that begins with the following lines:

We'll define a new var entry in this var\_array for our passive tracer tendency; this new entry might look something like the following:

<var name="tend\_mytracer1" name\_in\_code="mytracer1" array\_group="passive" units="kg m^{-3} s^{-1}"
 description="Tendency of our first tracer mass per unit volume divided by d(zeta)/dz"/>

Don't forget to set the value for array\_group to "passive"!

With these changes to the Registry.xml file, we can re-compile the atmosphere core. But, we'll first need to "clean" the code, since the last core that we compiled was the init atmosphere core.

```
$ make clean CORE=atmosphere
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=atmosphere
```

If compilation was successful, we can change directories to our passive\_tracer directory and prepare to run MPAS:

\$ cd /glade/derecho/scratch/\${USER}/mpas\_tutorial/passive\_tracer

You may recall from Section 2.3 that we need the MPAS executable, atmosphere\_model, as well as a number other files in order to run a simulation. Let's link or copy these files as we did in Section 2.3:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/namelist.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/streams.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/stream_list.atmosphere.* .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/src/core_atmosphere/physics/physics_wrf/file
```

In order to run the model in parallel with 128 MPI tasks, we'll need to link the /glade/campaign/mmm/wmr/mpas\_tutorial/meshes/x1.10242.graph.info.part.128 mesh partition file into our working directory:

```
$ In -s /glade/campaign/mmm/wmr/mpas_tutorial/meshes/x1.10242.graph.info.part.128 .
```

Now, we can proceed to set up the namelist.atmosphere and streams.atmosphere files as we did in Section 2.3 before running the model simulation.

#### Hints:

- (1) When editing the namelist.atmosphere file, there are three key changes to make:
  - The model time step, config\_dt, must be set based on the minimum grid distance in the mesh
  - The starting time of the simulation must be specified with the config\_start\_time variable
  - If running with multiple MPI tasks, config\_block\_decomp\_file\_prefix must be set to the prefix of the graph partition file
- (2) In the streams.atmosphere file, there is only one change that needs to be made:
  - The filename\_template for the "input" stream must be set to the name of the netCDF file with initial conditions

When running the model, we can copy the run\_model.pbs batch script before submitting the job with qsub:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/run_model.pbs .
$ qsub run model.pbs
```

The entire set of scalars is written to the default "history" files, so as soon as the first several output files are available, we can try making plots of our new "mytracer1" passive tracer. Then, we can stop the model simulation and proceed to the next sub-section, where we will add sources and sinks for our new tracer before running a longer simulation.

To terminate a running job on Derecho, we first need to find its job ID from qstat:

We just need the numeric part of the job ID in order to cancel the job with qdel:

```
$ qdel 4153631
```

You can verify that the job has been terminated by waiting a minute or so before running qstat again.

# 6.3 Adding sources and sinks

Having added a passive tracer to our initial conditions and defined the tracer in the model so that it will be transported during a simulation, it's not much additional work to define sources and sinks for the tracer. Here, we will define time-invariant sources and sinks that are set up when the model begins running, but we could in principle define time-varying sources and sinks that are periodically updated from an input file, for example.

To add time-invariant sources and sinks, we can change to our MPAS-Model source directory and edit the src/core\_atmosphere/Registry.xml file with the editor of our choice. Searching for the section of the file that begins the definition of the "tend" var\_struct around line 1751 we should see the following:

```
<var_struct name="tend" time_levs="1">
    <!-- tendencies for prognostic variables -->
```

Just below the tendencies for prognostic variables comment line, let's add a definition for our passive tracer's sources/sinks:

```
<var name="mytracer1_sources" type="real"
    dimensions="nVertLevels nCells Time"
    units="kg m^{-2} s^{-1}"
    description="Our first passive tracer areal production rate" />
```

As in the lecture on adding passive tracers, our example tracer will be produced and destroyed at the surface of the model.

Next, we can add code to set the "mytracer1\_sources" field when the model starts up. In the src/core\_atmosphere/mpas\_atm\_core.F source file in the atm\_mpas\_init\_block subroutine (around line 368), we will add declarations of two new array pointers at the end of the variable declarations (around line 418) as in the highlighted code, below:

```
integer, pointer :: nThreads
integer, dimension(:), pointer :: cellThreadStart, cellThreadEnd
integer, dimension(:), pointer :: cellSolveThreadStart, cellSolveThreadEnd
integer, dimension(:), pointer :: edgeThreadStart, edgeThreadEnd
integer, dimension(:), pointer :: edgeSolveThreadStart, edgeSolveThreadEnd
integer, dimension(:), pointer :: vertexThreadStart, vertexThreadEnd
integer, dimension(:), pointer :: vertexSolveThreadStart, vertexSolveThreadEnd
integer, dimension(:), pointer :: vertexSolveThreadStart, vertexSolveThreadEnd
logical, pointer :: config_do_restart, config_do_DAcycling
real (kind=RKIND), dimension(:,:), pointer :: mytracer1_sources
integer, dimension(:), pointer :: ivgtyp
call atm compute signs(mesh)
```

Then, near the end of the atm\_mpas\_init\_block subroutine, around line 585, we can add code to set the production/destruction of our tracer based on whether a model cell is land or water:

```
call mpas_pool_get_array(tend, 'mytracer1_sources', mytracer1_sources)
call mpas_pool_get_array(sfc_input, 'ivgtyp', ivgtyp)

mytracer1_sources(:,:) = 0.0_RKIND
do iCell=1,nCells
   ! Assume that vegetation category 17 is water
   ! (true for MODIS land use, not true for USGS)
   if (ivgtyp(iCell) == 17) then
       ! 2 g/m^2/day destruction over water
```

```
mytracer1_sources(1,iCell) = -0.002 / 86400.0
else
    ! 4 g/m^2/day production over land
    mytracer1_sources(1,iCell) = 0.004 / 86400.0
end if
end do
end subroutine atm_mpas_init_block
```

real(kind=RKIND), dimension(:,:), allocatable:: theta, tend th

Finally, we can add our source terms to the tendency array for our new tracer. In src/core\_atmosphere/physics/mpas\_atmphys\_todynamics.F at the bottom of the variable declarations in the physics get tend subroutine, we can add the following variable declarations around line 124:

Then, near the bottom of the subroutine before several arrays are deallocated, we can add code to include our source terms in the tendency for our passive tracer:

Since we have modified the Registry.xml file, we will need to clean the code before re-compiling the model:

```
$ make clean CORE=atmosphere
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=atmosphere
```

After the model has been successfully re-compiled, we can change directories to our run directory, remove any existing model output files, and re-run the model:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/passive_tracer
$ rm -f diag*nc history*nc restart*nc
$ qsub run model.pbs
```

Once the model has started to run and has produced several history files — which should now contain our new "mytracer1" field — we can use, e.g., convert\_mpas to interpolate the model history files to a lat-lon grid for quick visualization of our new tracer with sources and sinks in the lowest model layer!

# 7. Computing new diagnostic fields

In this final section, we will add a new diagnostic field to the model: an approximation to the radiative energy balance computed as the integrated difference between the outgoing and incoming radiation fluxes (both long-wave and short-wave) at the top of the model. The integration will occur between output times of the new diagnostic field.

Disclaimer: this exercise was developed by a software engineer; if the diagnostic described here makes no physical sense or otherwise contains errors, please don't let this negatively affect your views of MPAS-Atmosphere as a scientifically credible model!

## 7.1 Defining the diagnostic field and adding place-holder code

The MPAS-Atmosphere model contains a framework for organizing new diagnostic computations into their own modules, which contain routines to perform different stages of the computation of the diagnostic (e.g., accumulation, averaging, and resetting). To separate the complications of computing the diagnostic from those of implementing the diagnostic in the MPAS-Atmosphere code, we can begin by simply defining a variable for our new energy balance diagnostic along with some placeholder code with print

statements. We can then verify that the model compiles correctly and prints the expected lines to the log.atmosphere.0000.out file, demonstrating that at a technical level we have successfully connected our new diagnostic module with the MPAS-Atmosphere diagnostic framework. In the next section, then, we will be free to focus on the correct computation of the diagnostic itself.

Let's begin by changing to the directory containing our MPAS-Model source code:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model
```

All of the changes for our energy balance diagnostic will be confined to the src/core\_atmosphere/diagnostics subdirectory; we can change to that sub-directory now:

```
$ cd src/core_atmosphere/diagnostics
```

There are just three files in this directory that serve as the interface between the rest of the MPAS-Atmosphere model and our new diagnostic:

- Makefile changes here will ensure that our new Fortran code will be used when we recompile MPAS
- Registry\_diagnostics.xml changes here will allow any new variables defined by our diagnostic code to be available to the rest of the MPAS code (in particular, to the stream manager, which allows our diagnostic field to be written to output files)
- mpas\_atm\_diagnostics\_manager.F changes here will ensure that the different stages of computation required by our new diagnostic are called at the correct points in each model timestep

Before modifying the three files listed above, we can first define a new variable in an XML file for our diagnostic. With the editor of your choice, create a new file named Registry\_energy\_balance.xml With the following contents (click the light blue header):

#### Registry\_energy\_balance.xml

We can also create a new Fortran module with place-holder code, in which each subroutine simply prints a message to the log file. With the editor of your choice, create a new file named mpas\_energy\_balance\_diagnostics.F with the following contents (click the light blue header):

### mpas\_energy\_balance\_diagnostics.F

Having defined a variable to store our diagnostic as well as placeholder code in a new Fortran module, we can edit the Makefile, Registry\_diagnostics.xml, and mpas\_atm\_diagnostics\_manager.F files to connect our diagnostic. The required changes to each of these files are highlighted in the code, below.

#### Makefile

### Registry\_diagnostics.xml

## mpas\_atm\_diagnostics\_manager.F

Now, we can try re-compiling MPAS-Atmosphere. When making changes to diagnostic Registry files, it's generally necessary to clean the code before recompiling. Let's change to the top-level MPAS-Model directory, and clean and re-compile with the following commands:

```
$ cd ../../..
$ make clean CORE=atmosphere
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=atmosphere
```

After the model has been successfully compiled, we can create a new directory to run a short test simulation, through which we can verify that our diagnostic is being invoked by the model by looking for our print statements in the log file. Let's first make a new sub-directory in /qlade/derecho/scratch/\${USER}/mpas tutorial for our new diagnostic simulations:

```
$ mkdir -p /glade/derecho/scratch/${USER}/mpas_tutorial/energy_balance
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/energy_balance
```

Rather than create new initial conditions, we can simply re-run the 240-km quasi-uniform simulation, this time with our new diagnostic. We can therefore symbolically link the initial conditions, surface update, and mesh partition file from that simulation into our new run directory, and copy the namelist.atmosphere, streams.atmosphere, and stream\_list.atmosphere.\* files, too:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/x1.10242.init.nc .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/x1.10242.sfc_update.nc .
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/x1.10242.graph.info.part.128 .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/namelist.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/streams.atmosphere .
$ cp /glade/derecho/scratch/${USER}/mpas_tutorial/240km_uniform/stream_list.atmosphere.* .
```

Additionally, we will need to symbolically link to our newly recompiled atmosphere\_model executable as well as the physics look-up tables with the following commands:

```
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/atmosphere_model
$ ln -s /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model/src/core_atmosphere/physics/physics_wrf/file
```

Lastly, we will edit the namelist.atmosphere file to run a non-restart (i.e., a "cold-start") simulation from 2019-09-10 0000 UTC for just one hour. Our only goal with this initial simulation is to verify that our place-holder diagnostic code is being called!

```
config_start_time = '2014-09-10_00:00:00'
config_run_duration = '1:00:00'
config do restart = false
```

After verifying that the variables above are set correctly in the namelist.atmosphere file, we can copy the run model.pbs batch script before submitting the job with qsub:

```
$ cp /glade/campaign/mmm/wmr/mpas_tutorial/job_scripts/run_model.pbs .
$ qsub run model.pbs
```

This simulation should take just a minute or so to run. After the model completes, you can check the log.atmosphere.0000.out file for the print statements from our dignostic routines. Do you see lines like the following?

```
min/max of meshScalingDel2 = 1.00000 1.00000
min/max of meshScalingDel4 = 1.00000 1.00000
Sounding location file 'sounding_locations.txt' not found.
TESTING: energy_balance_setup
TESTING: energy_balance_reset
TESTING: energy_balance_update
TESTING: energy_balance_compute
Timing for diagnostic computation: 6.03111 s
Timing for stream output: 1.10848 s
TESTING: energy_balance_reset
```

If our diagnostic prints appear in the log file, we can proceed to the next section, where we will focus on the computation of the diagnostic without having to worry about the software details that were dealt with in this section.

## 7.2 Adding code to compute the diagnostic

In order to compute the accumulated net radiative energy between output times for our 'accradflux' field, we will need to implement three functions in our new mpas\_energy\_balance\_diagnostics.f module. Let's begin by changing directories to our MPAS-Model source directory, and then to the diagnostics subdirectory:

```
$ cd /glade/derecho/scratch/${USER}/mpas_tutorial/MPAS-Model
$ cd src/core atmosphere/diagnostics
```

Conceptually, we will need to implement changes to the following routines:

- ullet energy\_balance\_setup here we need to set the initial accradflux field to zero
- energy\_balance\_update here we need to add in the net energy flux for the current model time step
- energy\_balance\_reset here we need to reset the accradflux field after it has been written to an
  output stream

The expandable headers, below, highlight the changes that we need to make in each of these three subroutines.

subroutine energy\_balance\_setup

subroutine energy\_balance\_update

## subroutine energy\_balance\_reset

After editing the file, we can change back to the top-level MPAS-Model directory and recompile the model. Because we did not change any Registry XML files, there is no need to "make clean", first.

```
$ cd ../../..
$ qcmd -A UMMM0006 -- make -j8 gnu CORE=atmosphere
```

If the model compilation was successful, we are ready to try a model simulation with our new *accradflux* diagnostic in the next section!

# 7.3 Testing the diagnostic with a short simulation

To test our our diagnostic field, we can use a short, 12-hour simulation in which we write our "accradflux" field every six hours to its own output stream. All code changes have been completed, so we can change directories to /glade/derecho/scratch/\${USER}/mpas tutorial/energy balance:

```
$ cd /glade/derecho/scratch/${USER}/mpas tutorial/energy balance
```

Let's begin by adding a new stream like the following to our streams.atmosphere file:

```
<stream name="toa_energy_balance"
    type="output"
    clobber_mode="overwrite"
    filename_template="accradflux.$Y-$M-$D_$h.$m.$s.nc"
    filename_interval="output_interval"
    output_interval="6:00:00" >
        <var name="accradflux"/>
</stream>
```

Remember: the new stream must be defined between the opening <streams> and closing </streams> tags!

Next, we can set the duration of our model simulation to just 12 hours by setting config\_run\_duration to '12:00:00' in our namelist.atmosphere file:

```
config_run_duration = '12:00:00'
```

Finally, we can remove any existing output files from our earlier test run with

```
$ rm diag*nc history*nc surface_winds*nc
```

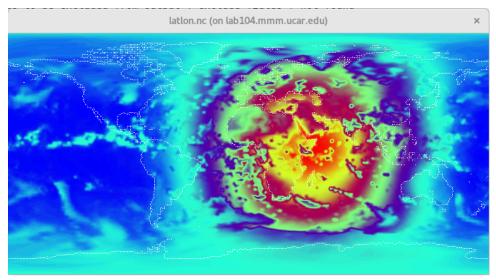
before running our short simulation with 128 MPI tasks:

```
$ qsub run_model.pbs
```

This simulation should take just a couple of minutes to complete, and when it has finished, we should have "accradflux" files in our run directory:

```
$ ls -1 accradflux*
-rw-r--r- 1 class104 cbet 46088 Sep 10 17:56 accradflux.2014-09-10_00.00.00.nc
-rw-r--r- 1 class104 cbet 46088 Sep 10 17:57 accradflux.2014-09-10_06.00.00.nc
-rw-r--r- 1 class104 cbet 46088 Sep 10 17:58 accradflux.2014-09-10 12.00.00.nc
```

If you interpolate the "accradflux" files to a 0.5-degree latitude-longitude grid with the <code>convert\_mpas</code> tool, does the last time period for the field (valid 12 hours after our initial time) look like the following?



Now that we have the top-of-the-atmosphere accumulated net radiative energy flux integrated over two six-hour periods from our 12-hour simulation, we can compute a radiation budget (in W / m^2) for these time periods with a Python script. Using an editor of your choice, create a file named compute budget.py with the following contents:

```
import numpy as np
from netCDF4 import Dataset

f = Dataset('accradflux.2014-09-10_12.00.00.nc')
accradflux = f.variables['accradflux'][:]
```

```
g = Dataset('x1.10242.init.nc')
areaCell = g.variables['areaCell'][:]
print(np.sum(accradflux * areaCell) / np.sum(areaCell) / 21600.0)
```

We can run this script with:

```
$ python compute_budget.py
```

You can try changing the time perdiod for which this radiation budget is computed by changing 'accradflux.2014-09-10\_12.00.00.nc' to 'accradflux.2014-09-10\_06.00.00.nc' in the script.

Positive values indicate more incoming radiation at the top of the atmosphere than outgoing radiation.

With the remaining time in this session, you may like to try one of the following:

- Run a multi-day simulation, writing the "toa\_energy\_balance" stream only once per day; then, compute the radiation budget for 24-hour periods using a modified version of the Python script described above
- Run a two-day simulation, writing the "toa\_energy\_balance" stream every three hours; then, compute the radiation budget for these three-hour periods and note how the resulting values change during the simulation.

**IMPORTANT NOTE:** By default the MPAS stream manager will refuse to overwrite any existing output files. Before re-running simulations, you will generally need to remove previous model output files with:

```
$ rm diag*nc history*nc surface winds*nc accradflux*nc restart*nc
```

However, as described in Section 5.2 of the MPAS-Atmosphere User's Guide, you can set the clobber\_mode attribute for output streams so that any existing files will be overwritten.

As an example of processing multiple NetCDF files in a loop in Python, you can use the following script: