Running MPAS Part 1: Creating initial conditions and running a basic global simulation

Michael G. Duda
NCAR/MMM

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Outline

Initial conditions for "real-data" simulations

- Processing time-invariant, terrestrial fields ("static" fields)
- Interpolating atmospheric and land-surface fields
- Producing SST and sea-ice update files

Running a basic simulation

Initial conditions for "idealized" simulations

- 3-d baroclinic wave test case
- 3-d supercell test case
- 2-d mountain wave test case

There will be many digressions along the way…

Outline

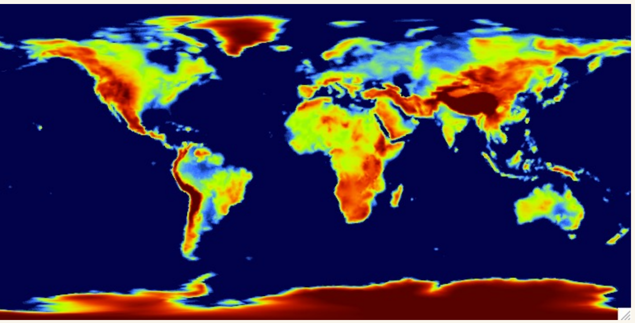
Real-data Initial Conditions
- Processing time-invariant fields ("static" file generation)
- Interpolating atmospheric and land-surface fields
- Producing SST and sea-ice update files

Running a basic simulation

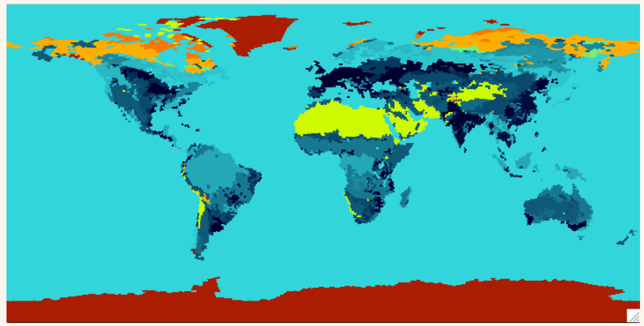
Creating idealized initial conditions
- 3-d baroclinic wave test case
- 3-d supercell test case
- 2-d mountain wave test case

Real-data ICs: processing static fields

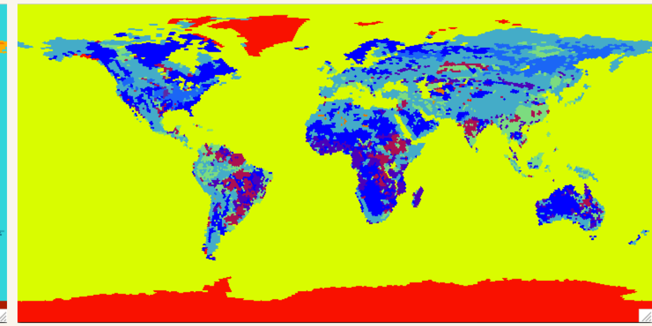
When we talk about time-invariant, “static” fields, what exactly do we mean?



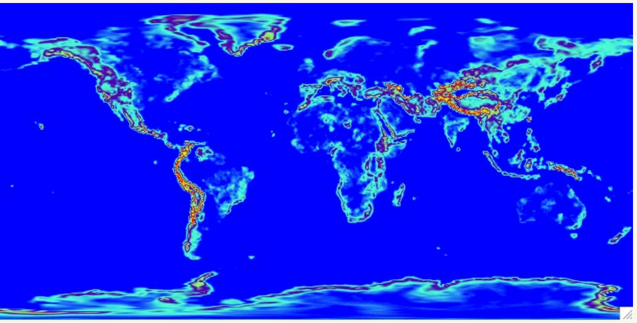
Terrain elevation



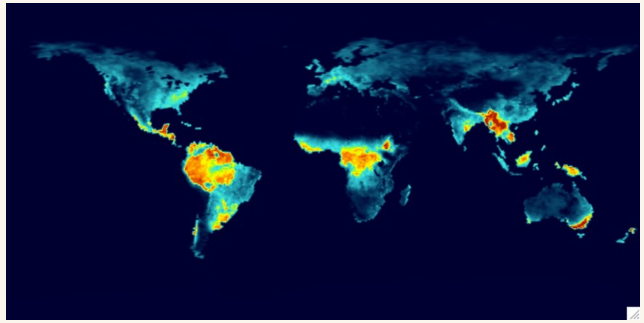
Dominant land use category



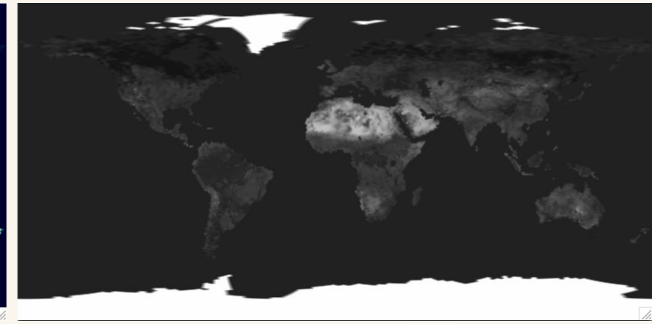
Dominant soil category



Sub-grid-scale terrain variance



Climatological monthly vegetation fraction



Climatological monthly surface albedo

These fields can be interpolated once and re-used for any real-data simulation

Real-data ICs: processing static fields

From where do we obtain the datasets for these “static” fields?

MPAS
Model for Prediction Across Scales

MPAS Atmosphere Public Releases

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MPAS Atmosphere 8.2.0 was released on 27 June 2024.

For information on the GPU-enabled MPAS-Atmosphere model, please refer to this documentation

MPAS Atmosphere 8.2.0 release notes

Source code downloads:

- MPAS v8.2.0
- GPU-enabled MPAS-Atmosphere v6.x

here Users' Guide

PAS-Atmosphere tutorial

MPAS-Atmosphere meshes

Static geographical datasets ← Next...

Monthly climatological aerosol dataset (QNWFA_QNIFA_SIGMA_MONTHLY.dat)

Configurations for idealized test cases

Sample input files for real-data simulations

Visualization and analysis tools

A variable resolution MPAS Voronoi mesh

MPAS
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Real-data ICs: processing static fields

Before creating initial conditions, we need a CVT mesh!

MPAS
Model for Prediction Across Scales

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here Users' Guide

MPAS-Atmosphere tutorial

MPAS-Atmosphere meshes ← Next...

Static geographical datasets

Monthly climatological aerosol dataset (QNWFA_QNIFA_SIGMA_MONTHLY.dat)

Configurations for idealized test cases

Sample input files for real-data simulations

Visualization and analysis tools

A variable resolution MPAS Voronoi mesh

Real-data ICs: processing static fields

The mesh download page has meshes that have been well-tested

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MPAS-Atmosphere Meshes

Several resolutions of quasi-uniform and refined meshes are available for download. Each mesh download provides an SCVT mesh on the unit sphere, the mesh connectivity (graph.info) file for the mesh, and partitionings of the mesh (e.g., graph.info.part.32) for various MPI task counts.

Additionally, for quasi-uniform meshes, "static" files using the default datasets are available. The static file downloads provide single-precision static files in CDF-5/64-bit data format and mesh connectivity files.

Creating limited-area subsets of meshes

MPAS-Atmosphere includes the capability to perform regional simulations. Regional meshes are formed as subsets of existing meshes. Currently, the MPAS-Limited-Area Python tool is the supported method for generating regional meshes as subsets of any of the meshes or static files available on this download page. Please refer to the documentation provided with MPAS-Limited-Area for details of its use.

Quasi-uniform meshes and static files

480-km mesh (2562 horizontal grid cells)

Download the 480-km mesh (1.5 MB)
Download the 480-km static file (1.0 MB)

384-km mesh (4002 horizontal grid cells)

Download the 384-km mesh (2.4 MB)
Download the 384-km static file (2.3 MB)

240-km mesh (10242 horizontal grid cells)

Download the 240-km mesh (6.3 MB)
Download the 240-km static file (4.0 MB)

120-km mesh (40962 horizontal grid cells)

Download the 120-km mesh (25.7 MB)
Download the 120-km static file (16.2 MB)

Real-data ICs: processing static fields

Filenames of the meshes that are found on the download page include:

```
x1.40962.grid.nc
x1.163842.grid.nc
x1.655362.grid.nc
x1.2621442.grid.nc
x1.5898242.grid.nc
x4.163842.grid.nc
x4.535554.grid.nc
x5.6488066.grid.nc
```

How does one interpret these cryptic names?

Real-data ICs: processing static fields

Filenames of the meshes that are found on the download page include:

```
x1.40962.grid.nc
x1.163842.grid.nc
x1.655362.grid.nc
x1.2621442.grid.nc
x1.5898242.grid.nc
x4.163842.grid.nc
x4.535554.grid.nc
x5.6488066.grid.nc
```

Refinement factor:

x1 = no refinement (quasi-uniform)

x4 = refinement by a factor of 4

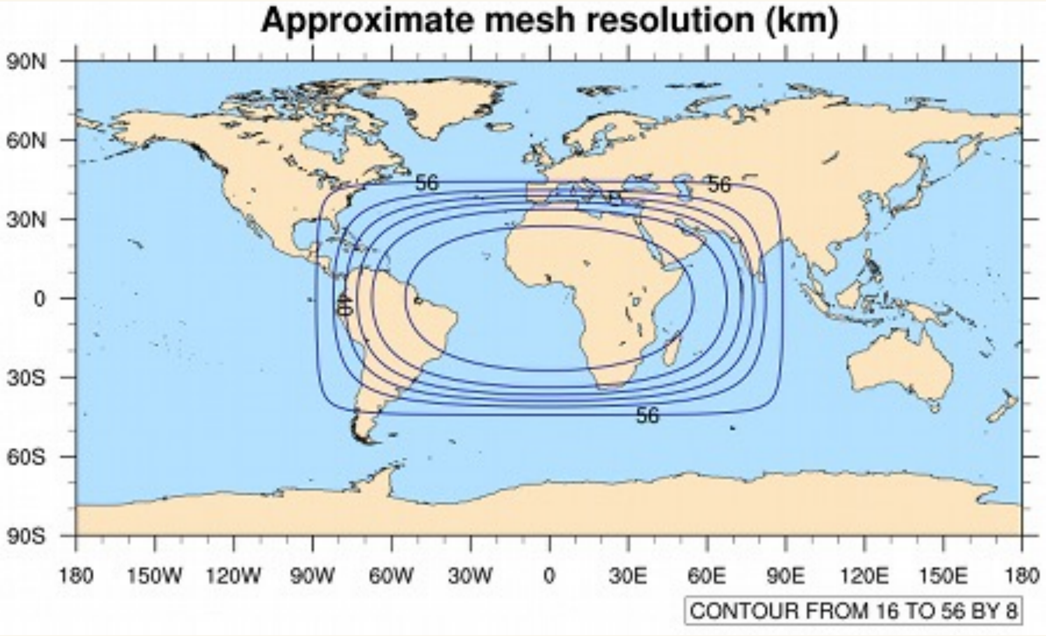
x5 = refinement by a factor of 5

Real-data ICs: processing static fields

Filenames of the meshes that are found on the download page include:

```
x1.40962
x1.163842
x1.655362
x1.2621442
x1.5898242
x4.163842
x4.535554
x5.6488066
```

Total number of cells in the mesh



Real-data ICs: processing static fields

When downloading a mesh, you'll get the mesh itself as well as various *mesh (graph) partition files*.

For example, the x1.40962 mesh (about 120-km resolution) is provided with the following files:

`x1.40962.grid.nc` – the mesh itself
`x1.40962.graph.info` – the mesh connectivity graph
`x1.40962.graph.info.part.2` – pre-computed partitioning for 2 MPI tasks
`x1.40962.graph.info.part.8` – pre-computed partitioning for 8 MPI tasks
`x1.40962.graph.info.part.16` – pre-computed partitioning for 16 MPI tasks
...

We'll say more about partition files when talking about running the model, and also when talking about MPAS meshes

Real-data ICs: processing static fields

Recall from the lecture about compiling MPAS that there are two executables we need to initialize and run an MPAS-Atmosphere simulation:

`init_atmosphere_model`

- Handles all stages of processing real-data initial conditions
- Handles processing of SST and sea-ice update files
- Handles generation of various idealized initial conditions
- Handles generation of lateral boundary conditions

`atmosphere_model`

- The model itself, responsible for performing integration/simulation given any source of initial conditions

Real-data ICs: processing static fields

How does the 'init_atmosphere' core manage to combine all of this functionality into one program?

- The key idea is that `init_atmosphere_model` may be run in stages using different options

```
&nhyd_model
    config_init_case = 7
    ...
/

&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
/
```

config_init_case:

2 = ideal baroclinic wave
4 = ideal squall line
5 = ideal supercell
6 = ideal mountain wave
7 = real-data initialization
8 = surface update file creation
9 = lateral boundary conditions

&preproc_stages: *Only used for real-data cases to control, e.g., whether we interpolate static fields, compute fields for GWDO scheme, interpolate meteorological data, etc.*

Real-data ICs: processing static fields

Generally, there are two files that must be edited every time the `init_atmosphere_model` program is run:

`namelist.init_atmosphere`

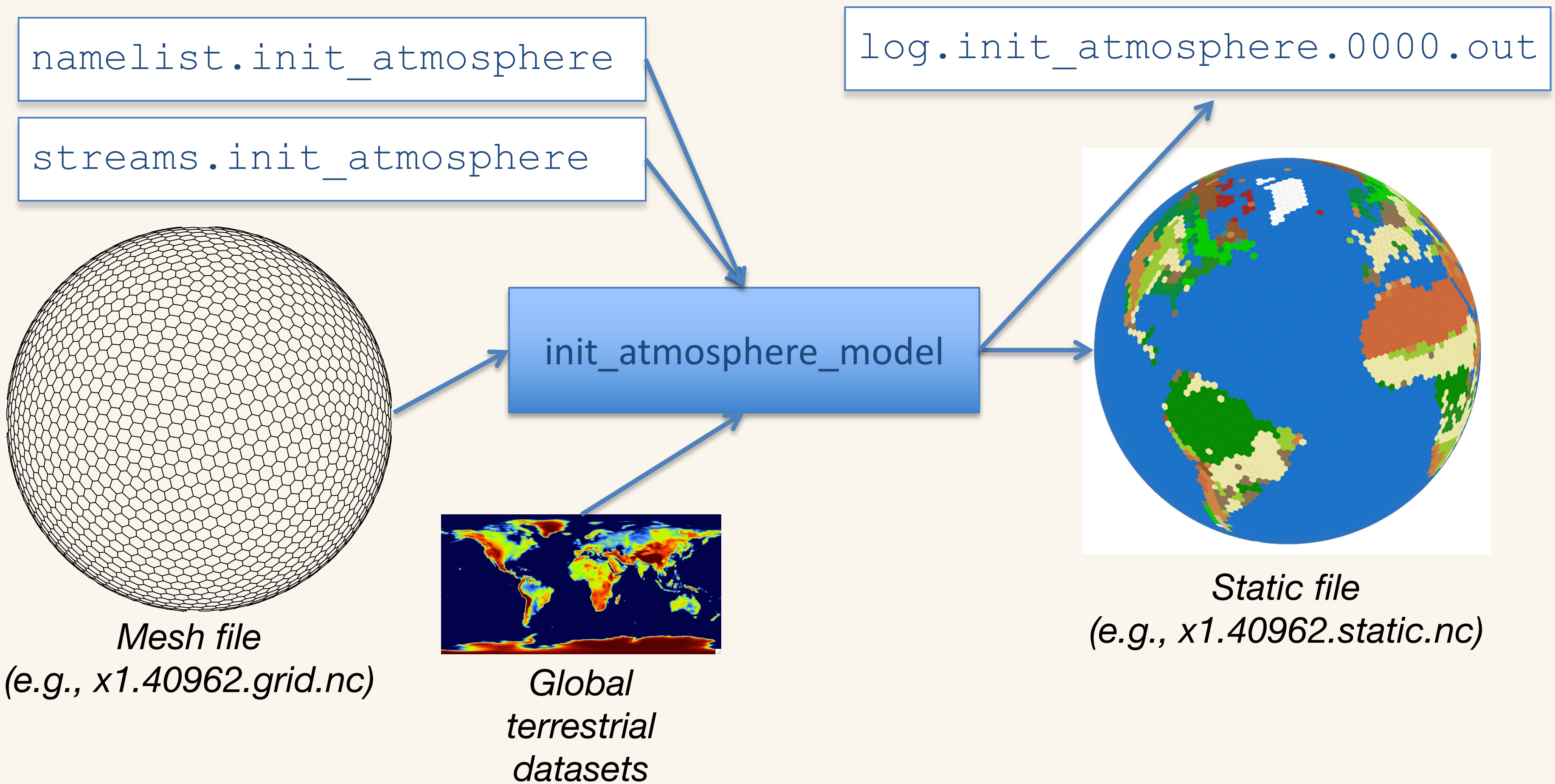
- Fortran namelist file
- Determines which "case" will be prepared (e.g., idealized cases, real-data case)
- Determines sub-options for the selected initialization case

`streams.init_atmosphere`

- XML file
- Specifies which netCDF files will be read and written by the `init_atmosphere_model` program

Real-data ICs: processing static fields

Input and output files when producing a “static” file:



Real-data ICs: processing static fields

Key settings in the `namelist.init_atmosphere` file:

```
&nhyd_model
    config_init_case = 7
/
&data_sources
    config_geog_data_path = '/glade/work/wrfhelp/WPS_GEOG/'
    config_landuse_data = 'MODIFIED_IGBP_MODIS_NOAH'
    config_topo_data = 'GMTED2010'
    config_vegfrac_data = 'MODIS'
    config_albedo_data = 'MODIS'
    config_maxsnowalbedo_data = 'MODIS'
/
&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
/
```

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Real-data ICs: processing static fields

Key settings in the `streams.init_atmosphere` file:

```
<immutable_stream name="input"
                  type="input"
                  filename_template="x1.40962.grid.nc"
                  input_interval="initial_only" />


<immutable_stream name="output"
                  type="output"
                  filename_template="x1.40962.static.nc"
                  packages="initial_conds"
                  output_interval="initial_only" />
```

Real-data ICs: processing static fields

The result should be a “static” netCDF file with

- terrain
- land use category
- soil category
- climatological albedo
- climatological vegetation fraction
- sub-grid-scale orography statistics for the GWDO scheme

Also, the radius of the SCVT mesh should be 6371229.0 m!

Real-data ICs: processing static fields

Look for messages like the following in the `log.init_atmosphere.0000.out` file:

```
--- enter subroutine init_atm_static:
Using GMTED2010 terrain dataset
/shared/WPS_GEOG/topo_gmted2010_30s/00001-01200.00001-01200
/shared/WPS_GEOG/topo_gmted2010_30s/01201-02400.00001-01200
/shared/WPS_GEOG/topo_gmted2010_30s/02401-03600.00001-01200
```

```
Computing GWDO static fields on the native MPAS mesh

--- Using GMTED2010 terrain dataset for GWDO static fields
```

```
-----------------------------------------
Total log messages printed:
   Output messages =                 3067
   Warning messages =                  10
   Error messages =                     0
   Critical error messages =            0
-----------------------------------------
```

Quasi-uniform static files

At this point, you may ask:

- If the "static" fields are independent of the starting time of a simulation,
- couldn't the MPAS developers do the preceding steps once and make the resulting static files available for everyone?

Quasi-uniform meshes and static files

480-km mesh (2562 horizontal grid cells)

Download the 480-km mesh (1.5 MB)
Download the 480-km static file (1.0 MB)

384-km mesh (4002 horizontal grid cells)

Download the 384-km mesh (2.4 MB)
Download the 384-km static file (2.3 MB)

240-km mesh (10242 horizontal grid cells)

Download the 240-km mesh (6.3 MB)
Download the 240-km static file (4.0 MB)

The mesh download page has links to "static" files for all quasi-uniform meshes

Outline

Real-data Initial Conditions
- Processing time-invariant fields (“static” file generation)
- Interpolating atmospheric and land-surface fields
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- 3-d baroclinic wave test case
- 3-d supercell test case
- 2-d mountain wave test case

Digression: "intermediate" data files

Time-varying meteorological and land-surface fields in MPAS-Atmosphere are interpolated from *intermediate* files produced by the ungrib component of the WRF Pre-processing System.

We'll assume in this tutorial that these files have already been prepared!

- Additional details may be found in the links, below

WRF Model web page: http://www2.mmm.ucar.edu/wrf/users/

WRF Users' guide:
https://www2.mmm.ucar.edu/wrf/users/wrf_users_guide/build/html/index.html

WPS source code: https://github.com/wrf-model/WPS

Tutorial slides for running ungrib:
http://www2.mmm.ucar.edu/wrf/users/tutorial/201801/wps_general.pdf

Real-data ICs: interpolating meteorological fields

Input and output files when producing an "init" file:

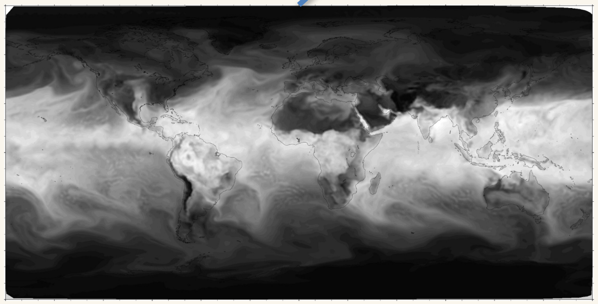
`namelist.init_atmosphere`

`streams.init_atmosphere`

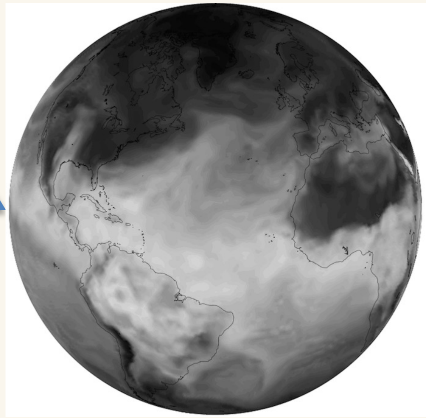
`log.init_atmosphere.0000.out`

init_atmosphere_model

Static file
(e.g., x1.40962.static.nc)



WPS "intermediate" file
(e.g., GFS:2014-09-10_00)



Initial conditions file
(e.g., x1.40962.init.nc)
The smoothed terrain following vertical grid has also been generated…

Real-data ICs: interpolating meteorological fields

Key settings in the `namelist.init_atmosphere` file:

```
&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 = 'GFS'
/
```

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Real-data ICs: interpolating meteorological fields

Key settings in the `namelist.init_atmosphere` file (*cont.*):

```
&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
/
&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
/
```

Real-data ICs: interpolating meteorological fields

Key settings in the `streams.init_atmosphere` file:

```
<immutable_stream name="input"
                  type="input"
                  filename_template="x1.40962.static.nc"
                  input_interval="initial_only" />


<immutable_stream name="output"
                  type="output"
                  filename_template="x1.40962.init.nc"
                  packages="initial_conds"
                  output_interval="initial_only" />
```

Real-data ICs: interpolating meteorological fields

The result should be a “init” netCDF file with

- *everything from the “static” file*
- 3-d vertical grid information
- 3-d potential temperature (*theta*)
- 3-d winds (*u* and *w*)
- 3-d water vapor mixing ratio (q_v)
- 3-d soil moisture
- 3-d soil temperature

Real-data ICs: interpolating meteorological fields

Look for messages like the following in the `log.init_atmosphere.0000.out` file:

```
 real-data GFS test case
Using option 'linear' for vertical extrapolation of temperature
max ter = 5393.19321458650
Setting up vertical levels as in 2014 TC experiments


--- config_tc_vertical_grid = T
--- als   = 0.750000000000000E-01
--- alt   = 1.70000000000000
--- zetal = 0.750000000000000
```

```
Interpolating TT at 27 1000.00000000000
Interpolating U at 27 1000.00000000000
Interpolating V at 27 1000.00000000000
Interpolating RH at 27 1000.00000000000
Interpolating GHT at 27 1000.00000000000
*************************************************
Found 38 levels in the first-guess data
*************************************************
```

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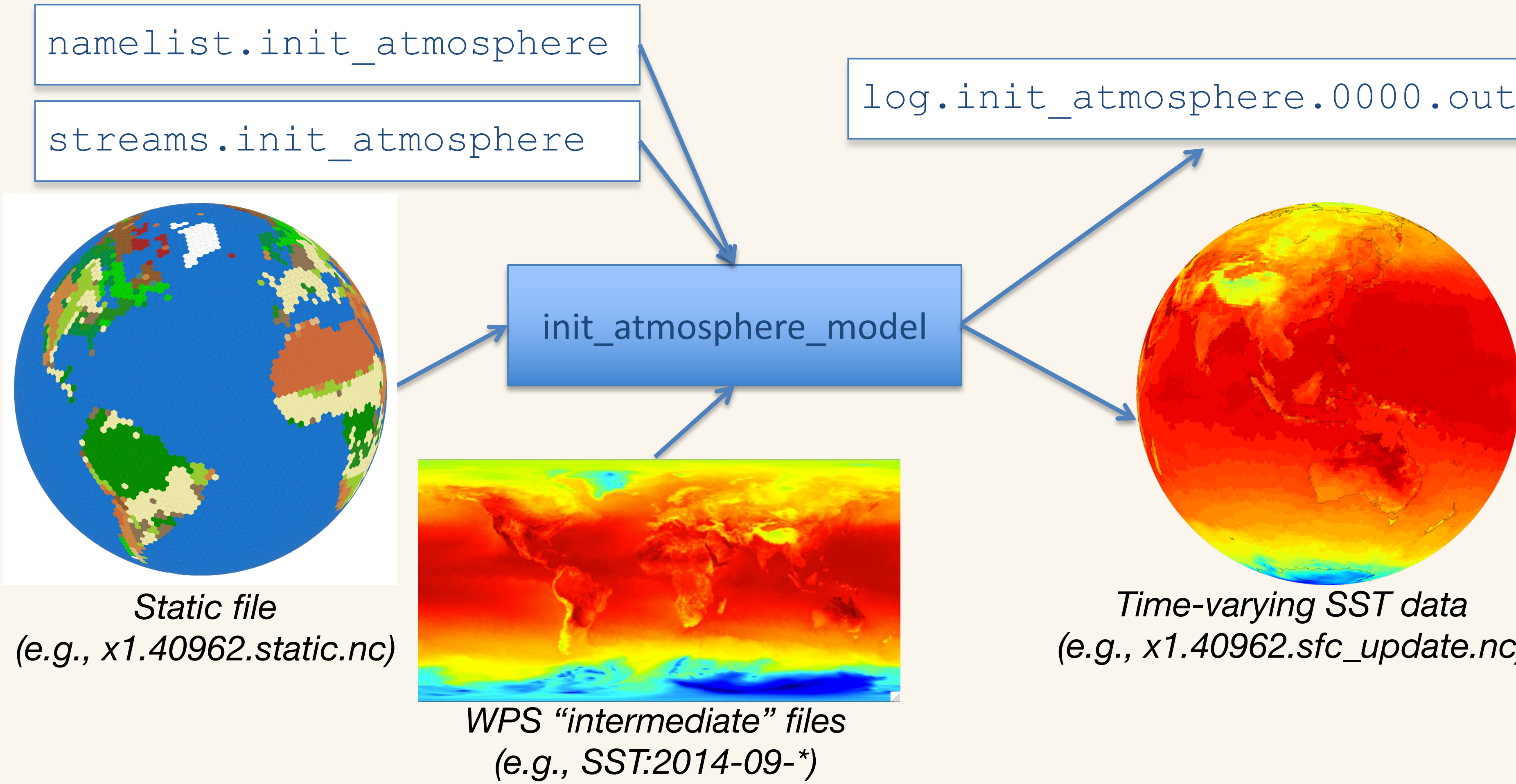
Producing SST and sea-ice update files

Input and output files when producing an SST update file:



MPAS
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Producing SST and sea-ice update files

Key settings in the `namelist.init_atmosphere` file:

```
&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
/
```

Producing SST and sea-ice update files

Key settings in the `streams.init_atmosphere` file:

```
<immutable_stream name="input"
                  type="input"
                  filename_template="x1.40962.static.nc"
                  input_interval="initial_only" />

<immutable_stream name="surface"
                  type="output"
                  filename_template="x1.40962.sfc_update.nc"
                  filename_interval="none"
                  packages="sfc_update"
                  output_interval="86400" />
```

Real-data ICs: processing static fields

Look for messages like the following in the `log.init_atmosphere.0000.out` file:

```
real-data surface (SST) update test case
Processing file SST:2014-09-10_00
Processing file SST:2014-09-11_00
Processing file SST:2014-09-12_00
Processing file SST:2014-09-13_00
Processing file SST:2014-09-14_00
Processing file SST:2014-09-15_00
Processing file SST:2014-09-16_00
Processing file SST:2014-09-17_00
Processing file SST:2014-09-18_00
Processing file SST:2014-09-19_00
Processing file SST:2014-09-20_00
```

```
-----------------------------------------
Total log messages printed:
   Output messages =                  144
   Warning messages =                   0
   Error messages =                     0
   Critical error messages =            0
-----------------------------------------
```

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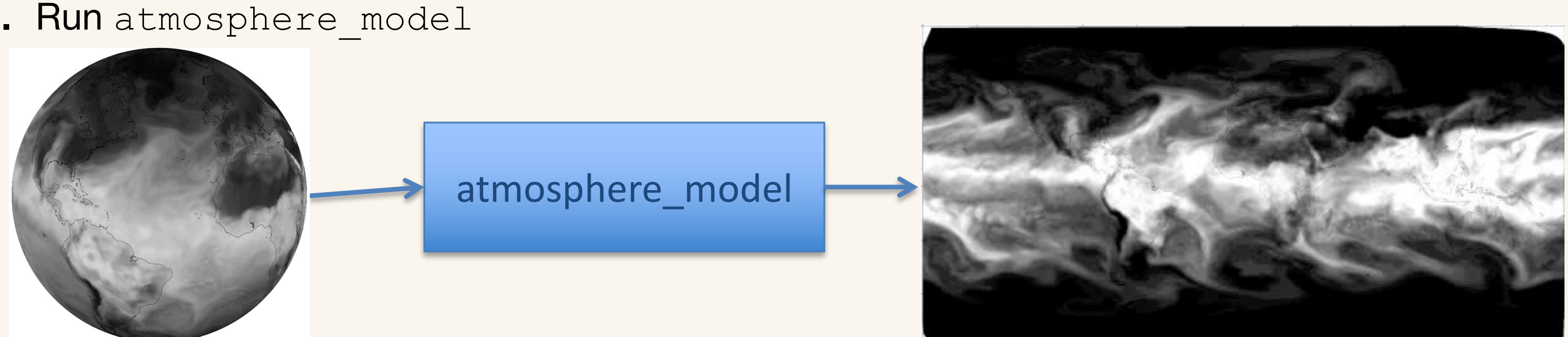
Running the MPAS-Atmosphere model

The same `atmosphere_model` executable can be used for either real-data or idealized simulations

Given initial conditions (e.g., `x1.40962.init.nc`), all that is needed to run the model is to:

1. Edit the `namelist.atmosphere` file to set model timestep, mixing and damping parameters, physics options, etc.
2. Edit the `streams.atmosphere` file to specify the name of the input initial conditions file and the frequency of model history files
3. Ensure that the proper mesh partition file (e.g., `x1.40962.graph.info.part.64`) is present
4. Run `atmosphere_model`



Running the MPAS-Atmosphere model

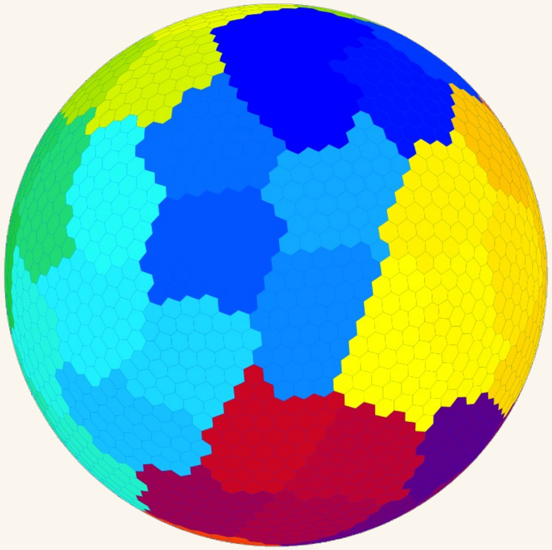
Before running the model itself (`atmosphere_model`), verify that the following namelist options have been properly set:

- **config_start_time** – The starting time of the simulation, which should either match the time in the initial conditions files or a *model restart file*.
- **config_dt** – The model timestep, in seconds; try starting with a timestep of between 5 and 6 times the minimum model grid spacing in kilometers; also ensure that model output interval is evenly divided by the timestep

Besides these crucial namelist options, ensure that the names of input and output files are correctly set in the `streams.atmosphere` file!

Digression: Mesh partition files

MPAS meshes must be partitioned using *Metis* in order for MPAS to allow simulations to run in parallel



However, the meshes available from the MPAS-Atmosphere download page are provided with several pre-computed partition files

- **In many cases, it may not be necessary for you to run Metis yourself; just use a pre-computed partitioning**

For example, the x1.40962 mesh (about 120-km resolution) is provided with the following files:

`x1.40962.grid.nc` – the mesh itself
`x1.40962.graph.info` – the mesh connectivity graph
`x1.40962.graph.info.part.2` – pre-computed partitioning for 2 MPI tasks
`x1.40962.graph.info.part.8` – pre-computed partitioning for 8 MPI tasks
`x1.40962.graph.info.part.16` – pre-computed partitioning for 16 MPI tasks
…

Running the MPAS-Atmosphere model

As the model runs, information about the progress of the model is written to the file `log.atmosphere.0000.out`

You can *tail* this file to check on model progress, e.g.,

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

```
Begin timestep 2017-06-12_01:00:00
--- 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  -0.4467210       1.098162
global min, max u   -89.13145       88.83957
Timing for integration step:    0.3368 s
```

Above: Example output for a timestep in the log file from a typical model run.

MPAS
Model for Prediction Across Scales

One final, important note…

If there are any errors reported in the `log.init_atmosphere.0000.out` or `log.atmosphere.0000.out` files, look for `log.*.err` files, and have a closer look!

```
 ----------------------------------------
 Total log messages printed:
    Output messages =                  46
    Warning messages =                  0
    Error messages =                    0
    Critical error messages =           1
 ----------------------------------------
```

```
------------------------------------------------------------------------
Beginning MPAS-init_atmosphere Error Log File for task     0 of     1
    Opened at 2018/07/27 16:35:58
------------------------------------------------------------------------



CRITICAL ERROR: Could not open input file 'x1.40926.init.nc' to read
mesh fields
Logging complete.  Closing file at 2018/07/27 16:35:58
```

Outline

Real-data Initial Conditions
- Processing time-invariant fields (“static” file generation)
- Interpolating atmospheric and land-surface fields
- Producing SST and sea-ice update files

Running a basic simulation

Creating idealized initial conditions
- 3-d baroclinic wave test case
- 3-d supercell test case
- 2-d mountain wave test case

MPAS
Model for Prediction Across Scales

Selecting among idealized cases

Creating idealized initial conditions (ICs) with the `init_atmosphere_model` program is much easier than creating real-data ICs

- No need for external datasets or multiple pre-processing steps: model fields are prescribed by formulae!
- Simply choose the appropriate initialization case

config_init_case (integer)

Units	-
Description	*Type of initial conditions to create:* *1 = Jablonowski & Williamson barolinic wave (no initial perturbation),* *2 = Jablonowski & Williamson barolinic wave (with initial perturbation),* *3 = Jablonowski & Williamson barolinic wave (with normal-mode perturbation),* *4 = squall line,* *5 = super-cell,* *6 = mountain wave,* *7 = real-data initial conditions from, e.g., GFS,* *8 = surface field (SST, sea-ice) update file for use with real-data simulations* *9 = lateral boundary conditions update file for use with real-data simulations*
Possible Values	1 – 9 *(default: 7)*

Idealized case downloads

Some idealize cases (e.g., super-cell) require doubly-periodic meshes

- Your best option is to simply download a prepared run directory for idealized cases
- After unpacking the tar file, symbolically link your `init_atmosphere_model` and `atmosphere_model` executables into the resulting directory and follow the README file

Idealized case downloads

MPAS Atmosphere Public Releases

[MPAS Home]

Overview
- MPAS-Atmosphere
- MPAS-Albany Land Ice
- MPAS-Ocean
- MPAS-Seaice
- Data Assimilation
- Publications
- Presentations

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First...

Resources
- License Information
- Wiki
- Bug Tracker
- Mailing Lists
- MPAS Developers Guide
- MPAS Mesh Specification Document

MPAS Atmosphere 8.2.0 was released on 27 June 2024.

For information on the GPU-enabled MPAS-Atmosphere model, please refer to this documentation

MPAS Atmosphere 8.2.0 release notes

Source code downloads:

- MPAS v8.2.0
- GPU-enabled MPAS-Atmosphere v6.x

...here Users' Guide

MPAS-Atmosphere tutorial

MPAS-Atmosphere meshes

Static geographical datasets

Monthly climatological aerosol dataset (QNWFA_QNIFA_SIGMA_MONTHLY.dat)

Configurations for idealized test cases

Next...

Sample input files for real-data simulations

Visualization and analysis tools

A variable resolution MPAS Voronoi mesh

Idealized case downloads

MPAS
Model for Prediction Across Scales

MPAS Home

Overview

MPAS-Atmosphere
MPAS-Albany Land Ice
MPAS-Ocean
MPAS-Seaice
Data Assimilation
Publications
Presentations

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MPAS-Seaice download

Resources

License Information

MPAS-Atmosphere Idealized Test Cases

The downloads below for MPAS-Atmosphere idealized test cases include the following:

- an MPAS mesh file to be used with the test case;
- for 3-d test cases, mesh decomposition files for several MPI task counts;
- a namelist file for creating initial conditions for the test case;
- a namelist file for running the model; and
- NCL scripts for making plots of the output.

The process of generating initial conditions and running each test case is described in further detail in the MPAS-Atmosphere Users' Guide.

Test cases on the Cartesian plane

Supercell

Download

Mountain-wave

Download

Test cases on the sphere

Jablonowski and Williamson baroclinic wave

Download

Summary

- Begin by downloading a mesh from the MPAS-A mesh download page
- For real-data initial conditions:
  - Interpolate time-invariant ("static") terrestrial fields
  - Obtain an "intermediate" file with atmospheric and soil state
  - Generate vertical grid and interpolate time-varying fields
- For idealized initial conditions:
  - Easiest to download .tar.gz file for the idealized case from MPAS webpage
- Run the simulation
  - At a minimum, set starting time and integration step in the `namelist.atmosphere` file
  - Ensure you have a mesh partition file corresponding to # of MPI tasks
  - Set input and output filenames in the `streams.atmosphere` file