MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÃO
INSTITUTO NACIONAL DE PESQUISAS ESPACIAIS

Overview: MPAS at INPE

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MONAN
Model for Ocean-laNd-Atmosphere predictioN
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Summary

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Importante details

2. Post-processing

convert_mpas
MPASSIT
diagnostic

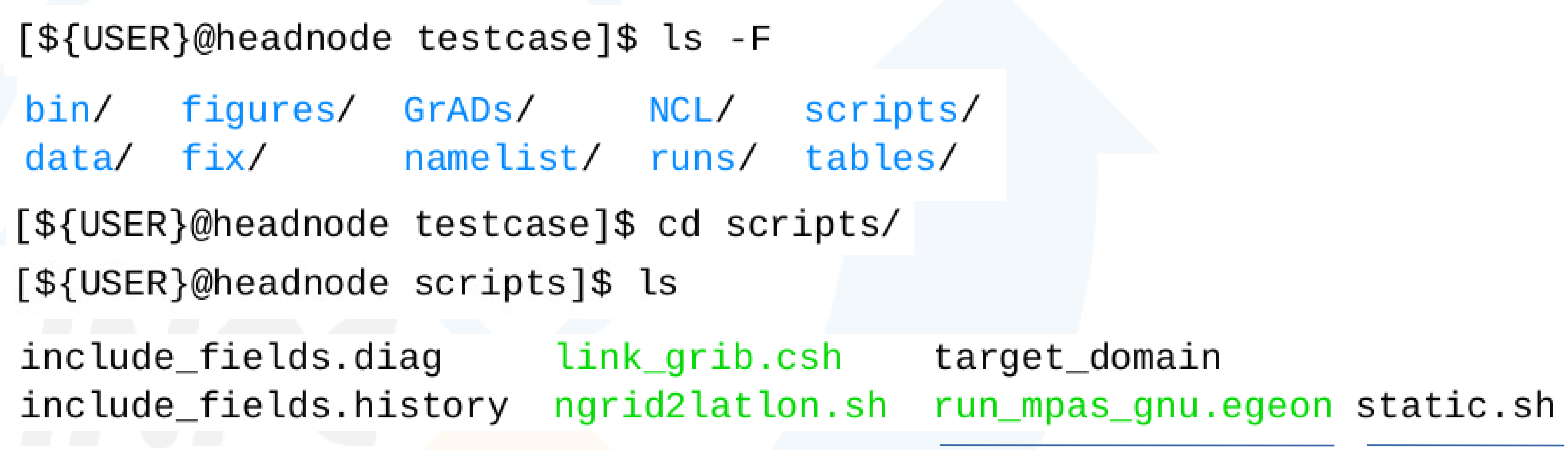
1 Guide

Latest version: 29/09/2023

Model for Prediction Across Scales-Atmosphere (MPAS-A) on INPE's EGEON System
User's Guide

This user's guide describes the procedure for installing and running the Model for Prediction Across Scales-Atmosphere (MPAS-A) on INPE's EGEON cluster.

Testcase (benchmark)



```
[${USER}@headnode testcase]$ ls -F
bin/    figures/  GrADs/     NCL/   scripts/
data/   fix/      namelist/  runs/  tables/
[${USER}@headnode testcase]$ cd scripts/
[${USER}@headnode scripts]$ ls
include_fields.diag     link_grib.csh    target_domain
include_fields.history  ngrid2latlon.sh  run_mpas_gnu.egeon  static.sh
```

Main scripts: static and model

```
# !CALLING SEQUENCE:
#
#         ./static EXP_NAME RESOLUTION
#
# For benchmark:
#         ./static ERA5 1024002
#
```

```
${USER}@headnode scripts]$ ./static.sh ERA5 1024002
```

It creates a make_static.sh script in the ../runs/$EXP_NAME/static directory:

```
${USER}@headnode scripts]$ cd ../runs/ERA5/static
```

To submit the script make_static.sh job, enter:

```
${USER}@headnode static]$ sbatch make_static.sh
```

Namelist (static fields)

namelist.init_atmosphere

```
&nhyd_model
    config_init_case = 7
    config_start_time = '2021-01-01_00:00:00'
    config_stop_time = '2021-01-01_00:00:00'
    config_theta_adv_order = 3
    config_coef_3rd_order = 0.25
/
&dimensions
    config_nvertlevels = 1
    config_nsoillevels = 1
    config_nfglevels = 1
    config_nfgsoillevels = 1
/
&data_sources
    config_geog_data_path = '../../data/WPS_GEOG/'
    config_met_prefix = 'FILE3'
    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 = 1
    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
/
```

streams.init_atmosphere

```
<streams>
<immutable_stream name= "input"
                  type= "input"
                  filename_template="x1.1024002.grid.nc"
                  input_interval="initial_only" />

<immutable_stream name= "output"
                  type= "output"
                  filename_template="x1.1024002.static.nc"
                  packages="initial_conds"
                  output_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"/>

<immutable_stream name= "lbc"
                  type= "output"
                  filename_template="lbc.$Y-$M-$D_$h.$m.$s.nc"
                  filename_interval="output_interval"
                  packages= "lbcs"
                  output_interval="3:00:00" />

</streams>
```

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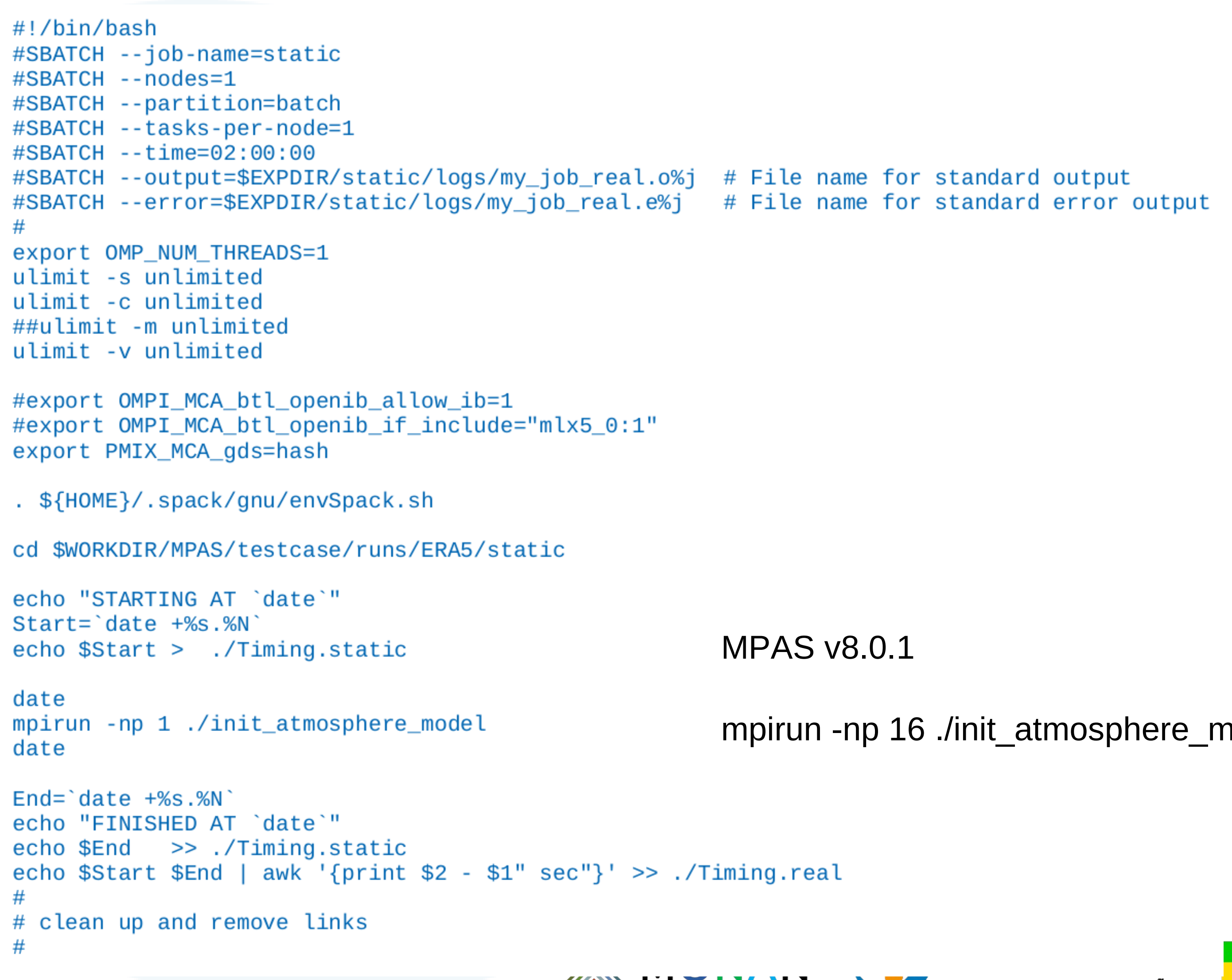
Job (static fields)

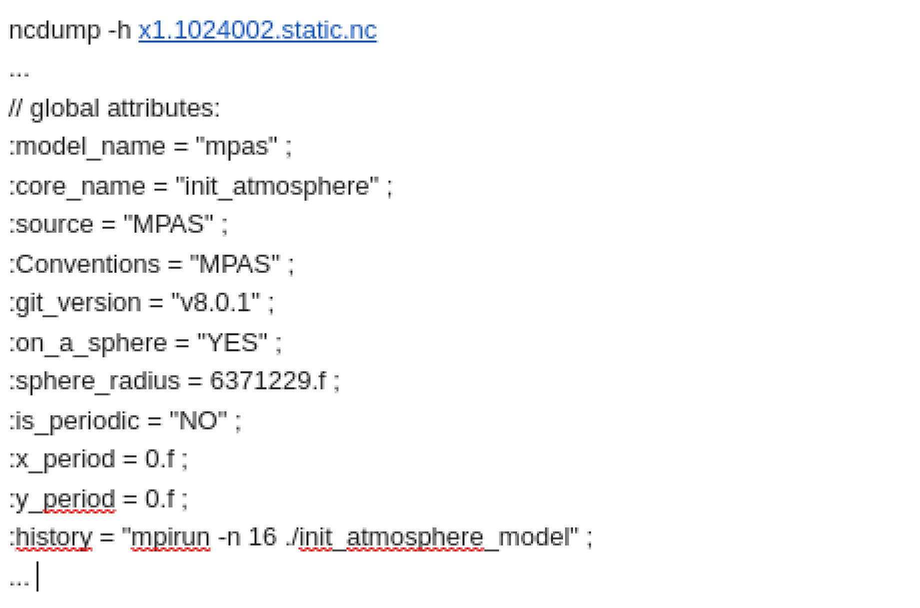


```
#!/bin/bash
#SBATCH --job-name=static
#SBATCH --nodes=1
#SBATCH --partition=batch
#SBATCH --tasks-per-node=1
#SBATCH --time=02:00:00
#SBATCH --output=$EXPDIR/static/logs/my_job_real.o%j  # File name for standard output
#SBATCH --error=$EXPDIR/static/logs/my_job_real.e%j   # File name for standard error output
#
export OMP_NUM_THREADS=1
ulimit -s unlimited
ulimit -c unlimited
##ulimit -m unlimited
ulimit -v unlimited

#export OMPI_MCA_btl_openib_allow_ib=1
#export OMPI_MCA_btl_openib_if_include="mlx5_0:1"
export PMIX_MCA_gds=hash

. ${HOME}/.spack/gnu/envSpack.sh

cd $WORKDIR/MPAS/testcase/runs/ERA5/static

echo "STARTING AT `date`"
Start=`date +%s.%N`
echo $Start >  ./Timing.static

date
mpirun -np 1 ./init_atmosphere_model
date

End=`date +%s.%N`
echo "FINISHED AT `date`"
echo $End   >> ./Timing.static
echo $Start $End | awk '{print $2 - $1" sec"}' >> ./Timing.real
#
# clean up and remove links
#
```

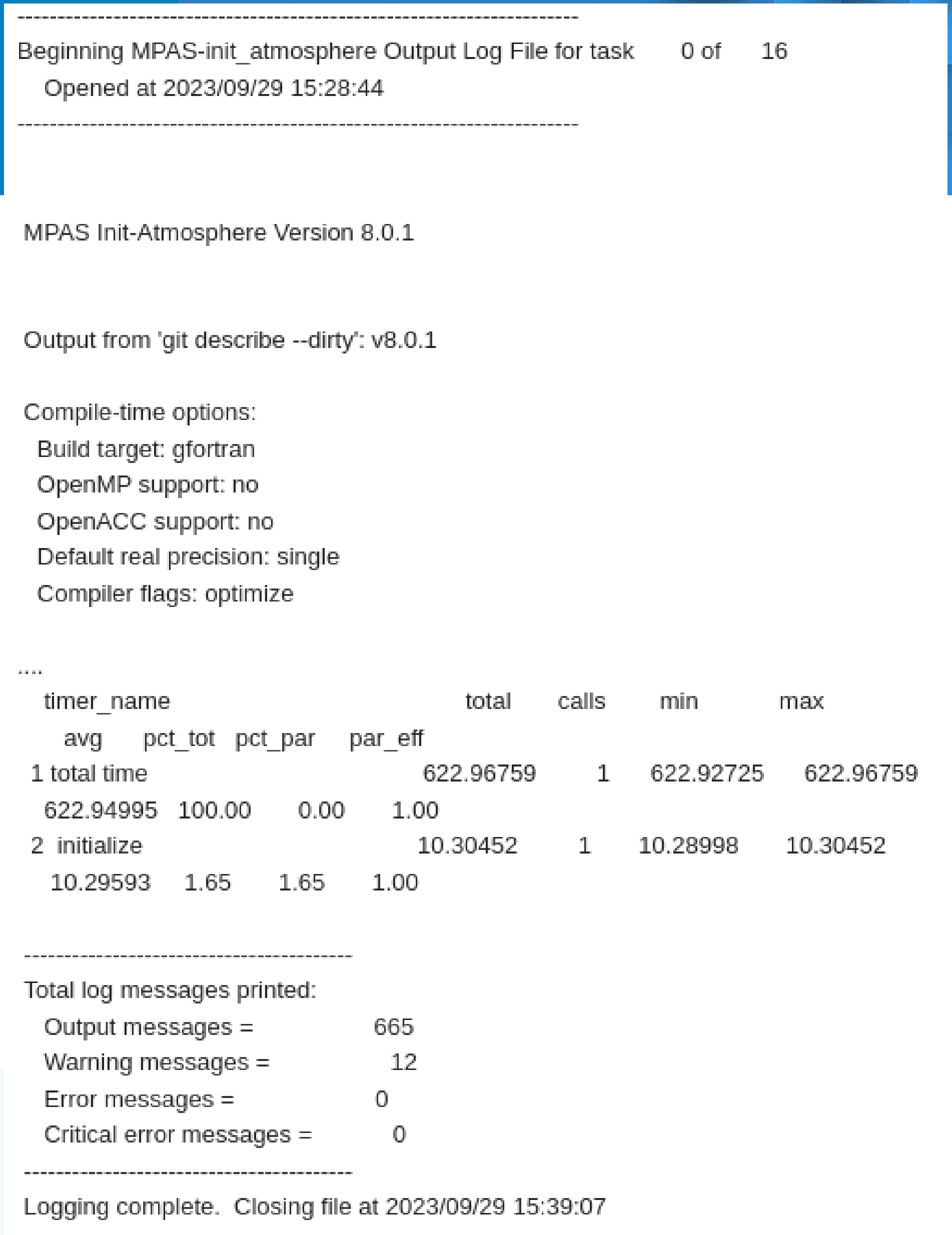
MPAS v8.0.1

mpirun -np 16 ./init_atmosphere_model

Job (static fields)

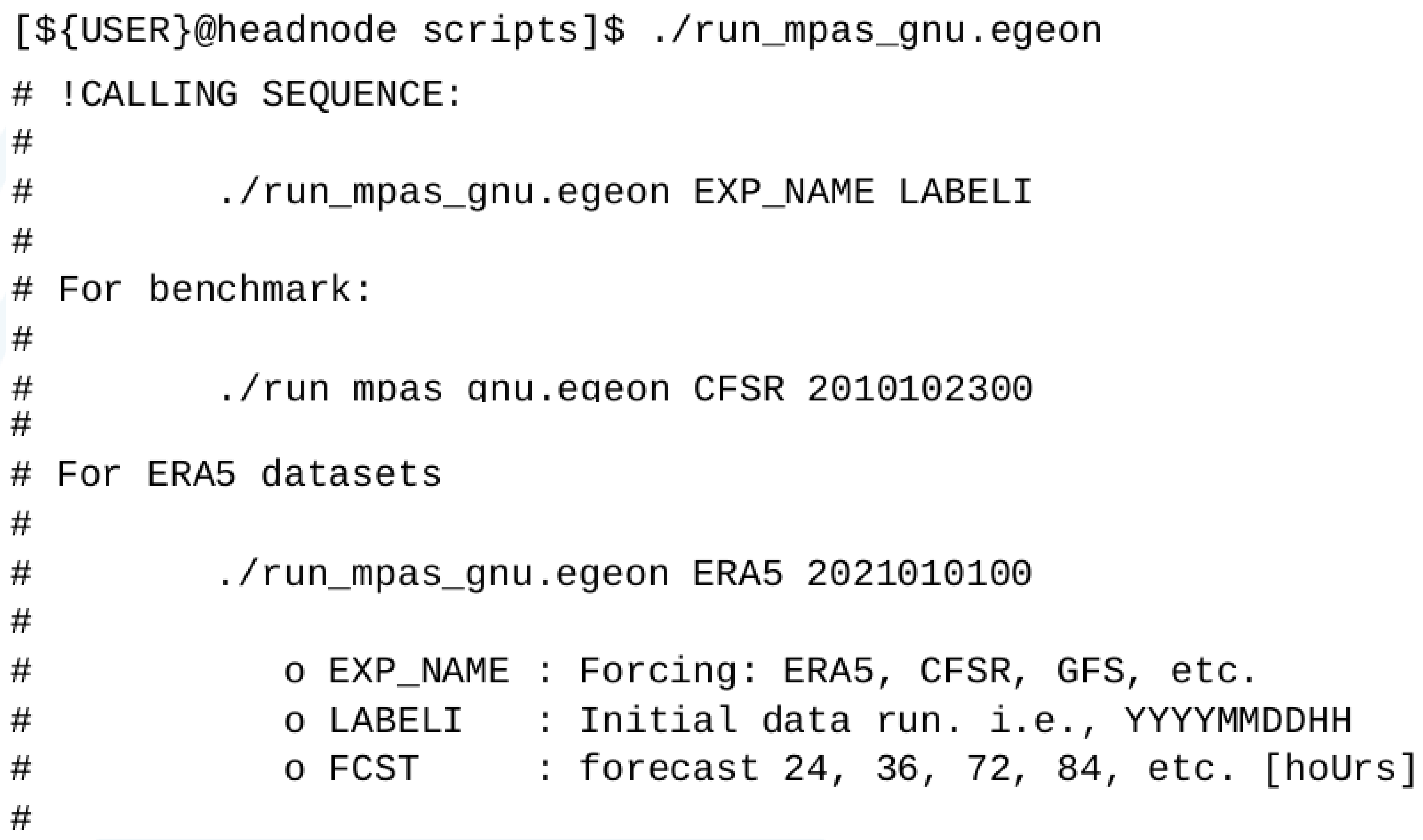


```
ncdump -h x1.1024002.static.nc
...
// global attributes:
:model_name = "mpas" ;
:core_name = "init_atmosphere" ;
:source = "MPAS" ;
:Conventions = "MPAS" ;
:git_version = "v8.0.1" ;
:on_a_sphere = "YES" ;
:sphere_radius = 6371229.f ;
:is_periodic = "NO" ;
:x_period = 0.f ;
:y_period = 0.f ;
:history = "mpirun -n 16 ./init_atmosphere_model" ;
...
```



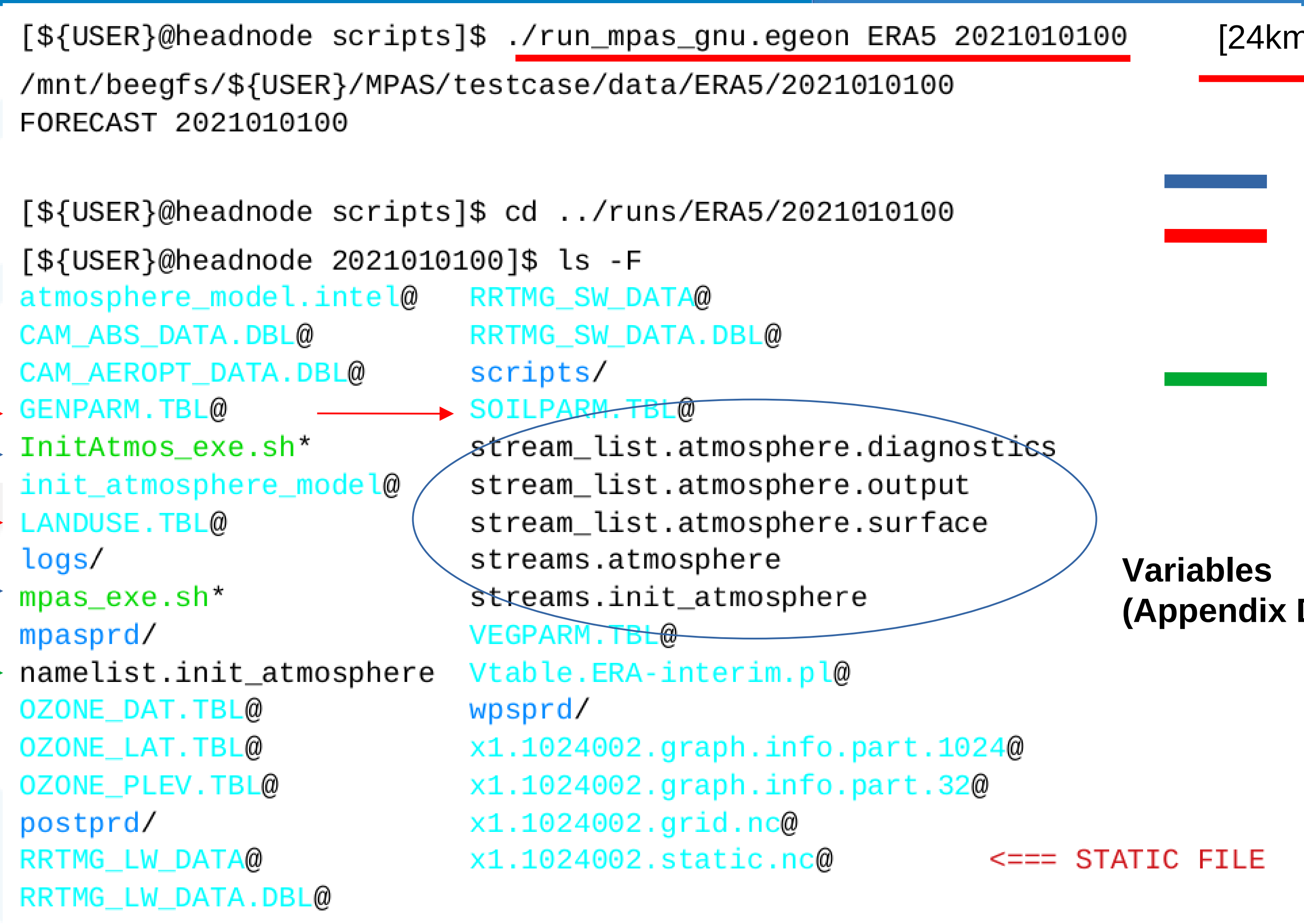
```
----------------------------------------------------------------------
Beginning MPAS-init_atmosphere Output Log File for task       0 of      16
   Opened at 2023/09/29 15:28:44
----------------------------------------------------------------------


 MPAS Init-Atmosphere Version 8.0.1


 Output from 'git describe --dirty': v8.0.1

 Compile-time options:
   Build target: gfortran
   OpenMP support: no
   OpenACC support: no
   Default real precision: single
   Compiler flags: optimize

....
   timer_name                                       total       calls        min            max
      avg        pct_tot   pct_par     par_eff
  1 total time                                 622.96759         1       622.92725       622.96759
   622.94995   100.00       0.00       1.00
  2  initialize                                  10.30452         1       10.28998       10.30452
    10.29593     1.65        1.65       1.00

 -----------------------------------------
 Total log messages printed:
    Output messages =                  665
    Warning messages =                   12
    Error messages =                     0
    Critical error messages =            0
 -----------------------------------------
 Logging complete.  Closing file at 2023/09/29 15:39:07
```

Model



```
[${USER}@headnode scripts]$ ./run_mpas_gnu.egeon
# !CALLING SEQUENCE:
#
#        ./run_mpas_gnu.egeon EXP_NAME LABELI
#
# For benchmark:
#
#        ./run_mpas_gnu.egeon CFSR 2010102300
#
# For ERA5 datasets
#
#        ./run_mpas_gnu.egeon ERA5 2021010100
#
#           o EXP_NAME : Forcing: ERA5, CFSR, GFS, etc.
#           o LABELI   : Initial data run. i.e., YYYYMMDDHH
#           o FCST     : forecast 24, 36, 72, 84, etc. [hoUrs]
#
```

Testcase (example)



```
[${USER}@headnode scripts]$ ./run_mpas_gnu.egeon ERA5 2021010100
/mnt/beegfs/${USER}/MPAS/testcase/data/ERA5/2021010100
FORECAST 2021010100

[${USER}@headnode scripts]$ cd ../runs/ERA5/2021010100
[${USER}@headnode 2021010100]$ ls -F
atmosphere_model.intel@    RRTMG_SW_DATA@
CAM_ABS_DATA.DBL@          RRTMG_SW_DATA.DBL@
CAM_AEROPT_DATA.DBL@       scripts/
GENPARM.TBL@               SOILPARM.TBL@
InitAtmos_exe.sh*          stream_list.atmosphere.diagnostics
init_atmosphere_model@     stream_list.atmosphere.output
LANDUSE.TBL@               stream_list.atmosphere.surface
logs/                      streams.atmosphere
mpas_exe.sh*               streams.init_atmosphere
mpasprd/                   VEGPARM.TBL@
namelist.init_atmosphere   Vtable.ERA-interim.pl@
OZONE_DAT.TBL@             wpsprd/
OZONE_LAT.TBL@             x1.1024002.graph.info.part.1024@
OZONE_PLEV.TBL@            x1.1024002.graph.info.part.32@
postprd/                   x1.1024002.grid.nc@
RRTMG_LW_DATA@             x1.1024002.static.nc@        <=== STATIC FILE
RRTMG_LW_DATA.DBL@
```

[24km, 7d, …]

🟦 jobs

🟥 New tables V8.0.1

🟩 namelist

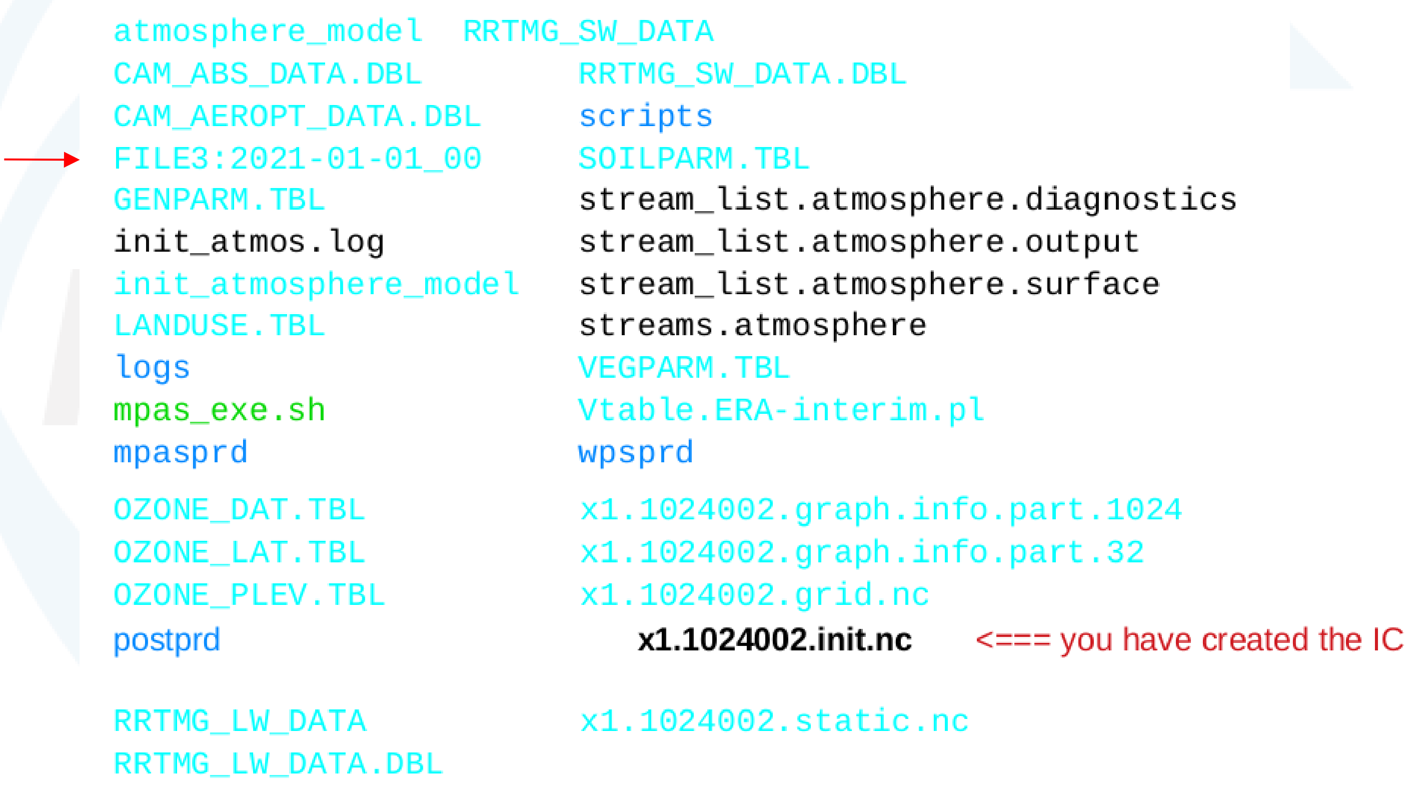
Variables (Appendix D)

Testcase (example)

```
[${USER}@headnode wpsprd]$ sbatch degrib_exe.sh
```

CFSR, NCEP, ERA5, etc.

```
[${USER}@headnode 2021010100]$ sbatch InitAtmos_exe.sh
```

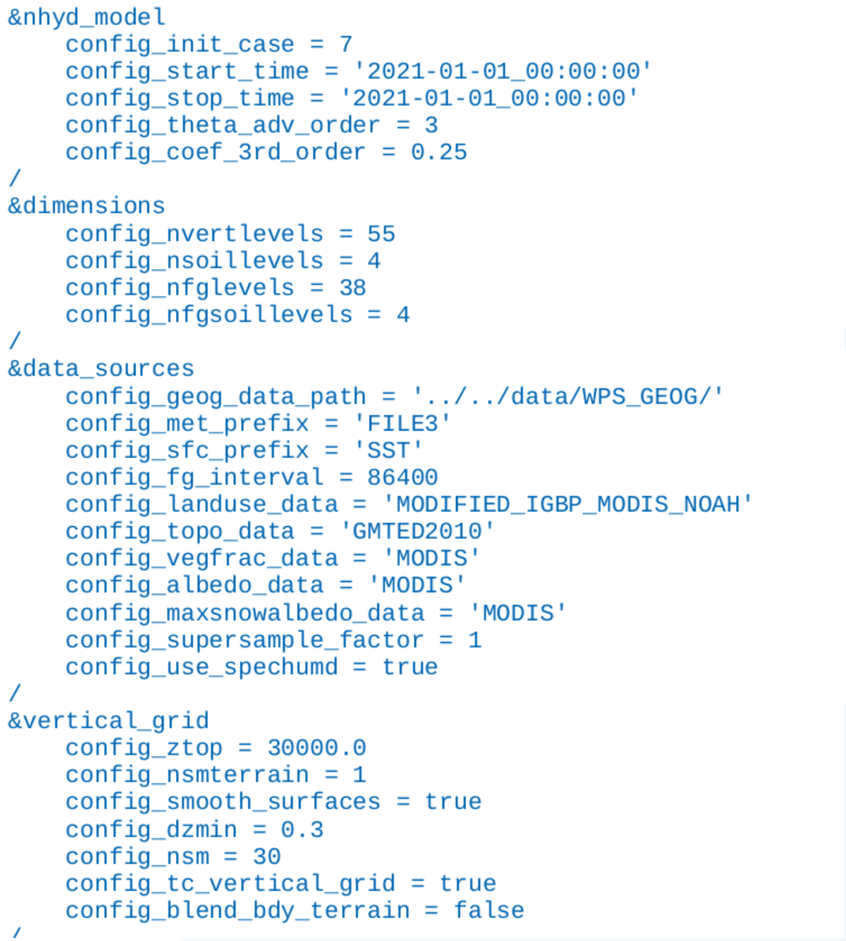


```
atmosphere_model   RRTMG_SW_DATA
CAM_ABS_DATA.DBL         RRTMG_SW_DATA.DBL
CAM_AEROPT_DATA.DBL      scripts
FILE3:2021-01-01_00      SOILPARM.TBL
GENPARM.TBL              stream_list.atmosphere.diagnostics
init_atmos.log           stream_list.atmosphere.output
init_atmosphere_model    stream_list.atmosphere.surface
LANDUSE.TBL              streams.atmosphere
logs                     VEGPARM.TBL
mpas_exe.sh              Vtable.ERA-interim.pl
mpasprd                  wpsprd

OZONE_DAT.TBL            x1.1024002.graph.info.part.1024
OZONE_LAT.TBL            x1.1024002.graph.info.part.32
OZONE_PLEV.TBL           x1.1024002.grid.nc
postprd                     x1.1024002.init.nc

RRTMG_LW_DATA            x1.1024002.static.nc
RRTMG_LW_DATA.DBL
```

<=== you have created the IC

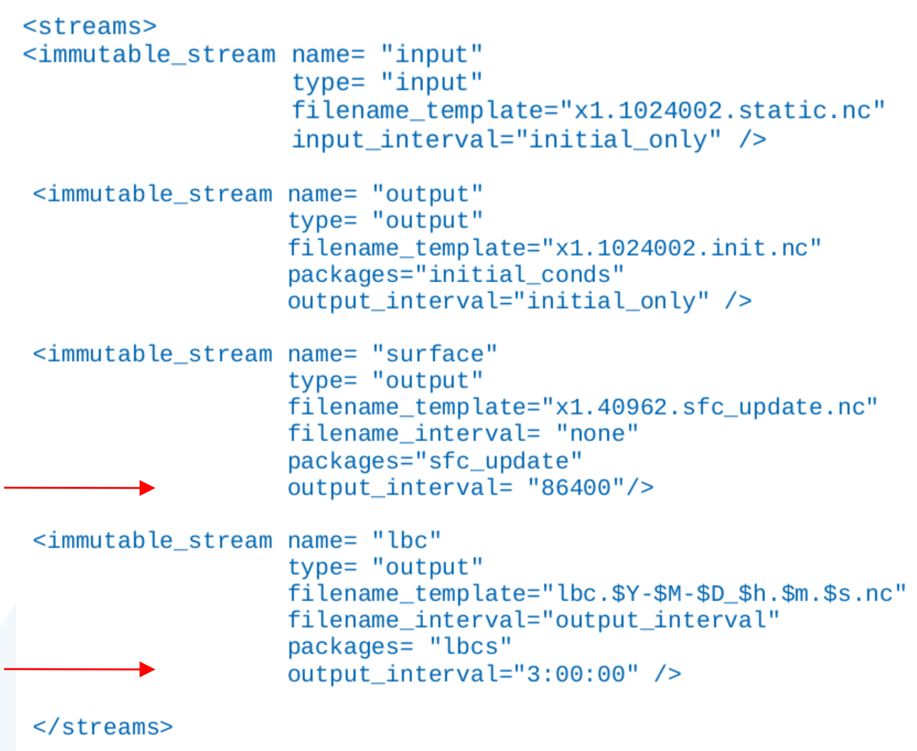
Namelist (init_atmosphere)

namelist.init_atmosphere



```
&nhyd_model
    config_init_case = 7
    config_start_time = '2021-01-01_00:00:00'
    config_stop_time = '2021-01-01_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 = '../../data/WPS_GEOG/'
    config_met_prefix = 'FILE3'
    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 = 1
    config_use_spechumd = true
/
&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
/
```

streams.init_atmosphere



```
<streams>
<immutable_stream name= "input"
                  type= "input"
                  filename_template="x1.1024002.static.nc"
                  input_interval="initial_only" />

 <immutable_stream name= "output"
                  type= "output"
                  filename_template="x1.1024002.init.nc"
                  packages="initial_conds"
                  output_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"/>

 <immutable_stream name= "lbc"
                  type= "output"
                  filename_template="lbc.$Y-$M-$D_$h.$m.$s.nc"
                  filename_interval="output_interval"
                  packages= "lbcs"
                  output_interval="3:00:00" />

 </streams>
```

Duda et al. (2019) describe in Appendix D all variables available in the MPAS model. Before running the model, check if all variables of interest are listed in stream_list.atmosphere.* files. Add or remove these variables in the associate stream_list file.

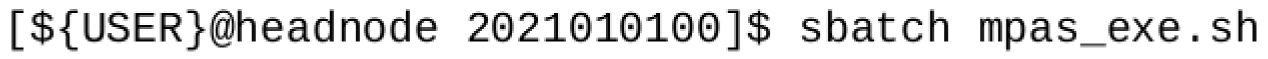
```
olrtoa
rainc
rainnc
u10
v10
q2
t2m
th2m
mslp
relhum_200hPa
relhum_250hPa
relhum_500hPa
relhum_700hPa
...
```

stream_list.atmosphere.diagnostic

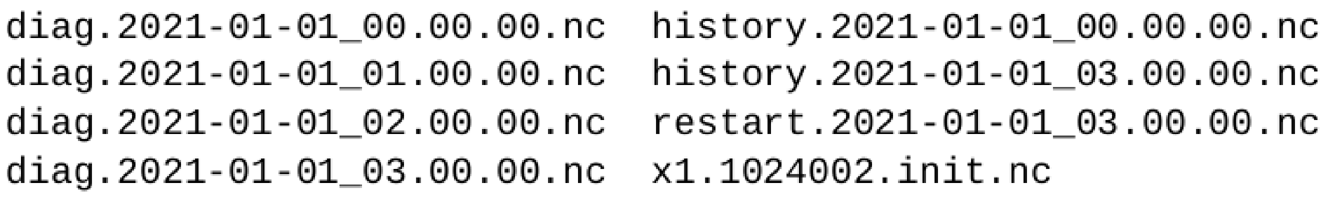
```
...
verticesOnEdge
edgesOnVertex
cellsOnVertex
kiteAreasOnVertex
meshDensity
zgrid
pressure
surface_pressure
rho
theta
relhum
w
pressure
surface_pressure
rho
theta
relhum
divergence
vorticity
ke
uReconstructZonal
uReconstructMeridional
```

stream_list.atmosphere.output

Testcase (example)



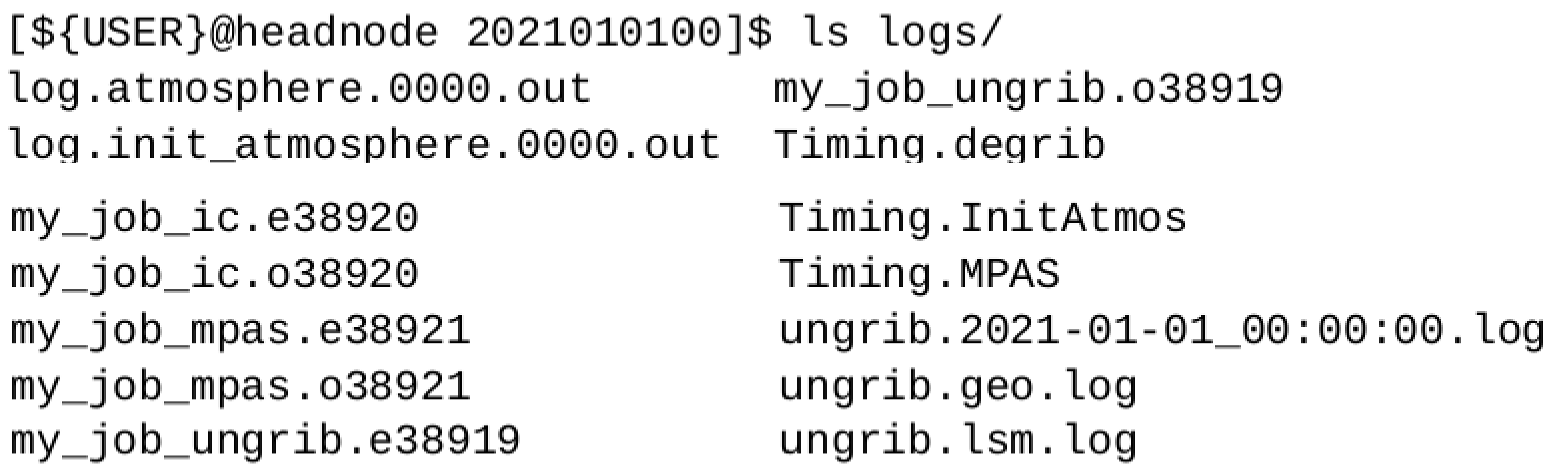
```
[${USER}@headnode 2021010100]$ sbatch mpas_exe.sh
```



```
diag.2021-01-01_00.00.00.nc  history.2021-01-01_00.00.00.nc
diag.2021-01-01_01.00.00.nc  history.2021-01-01_03.00.00.nc
diag.2021-01-01_02.00.00.nc  restart.2021-01-01_03.00.00.nc
diag.2021-01-01_03.00.00.nc  x1.1024002.init.nc
```

diag = var2D
history = var2D+ 3D
restart = big file

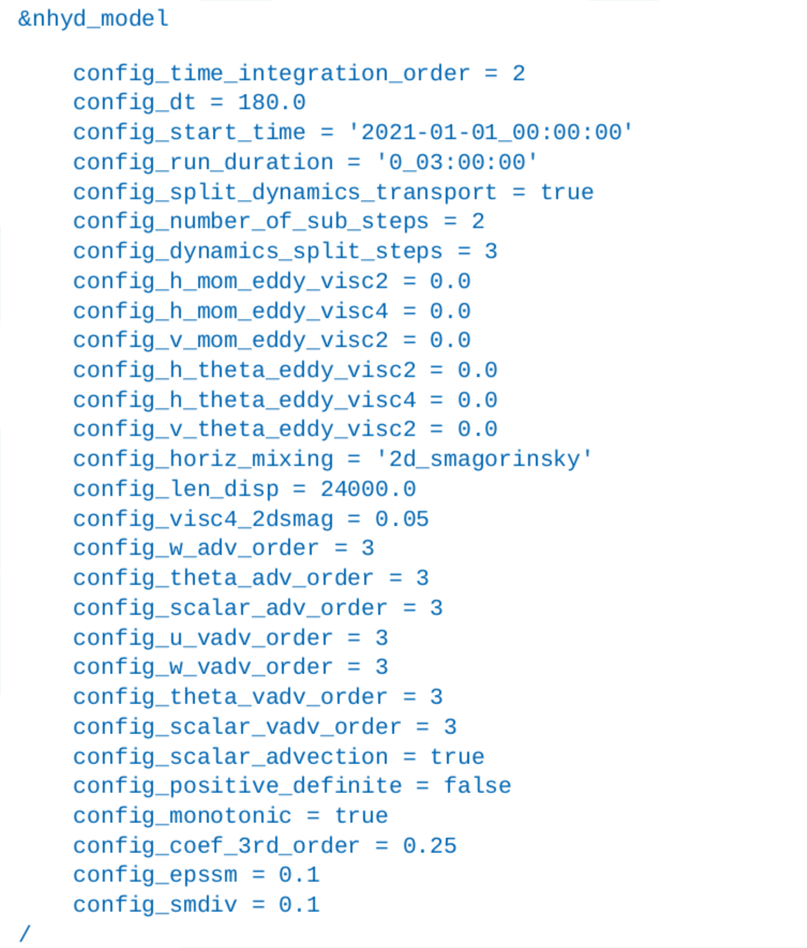
Check the size of the output files; select the more important variables for your application.



```
[${USER}@headnode 2021010100]$ ls logs/
log.atmosphere.0000.out        my_job_ungrib.o38919
log.init_atmosphere.0000.out   Timing.degrib
my_job_ic.e38920               Timing.InitAtmos
my_job_ic.o38920               Timing.MPAS
my_job_mpas.e38921             ungrib.2021-01-01_00:00:00.log
my_job_mpas.o38921             ungrib.geo.log
my_job_ungrib.e38919           ungrib.lsm.log
```

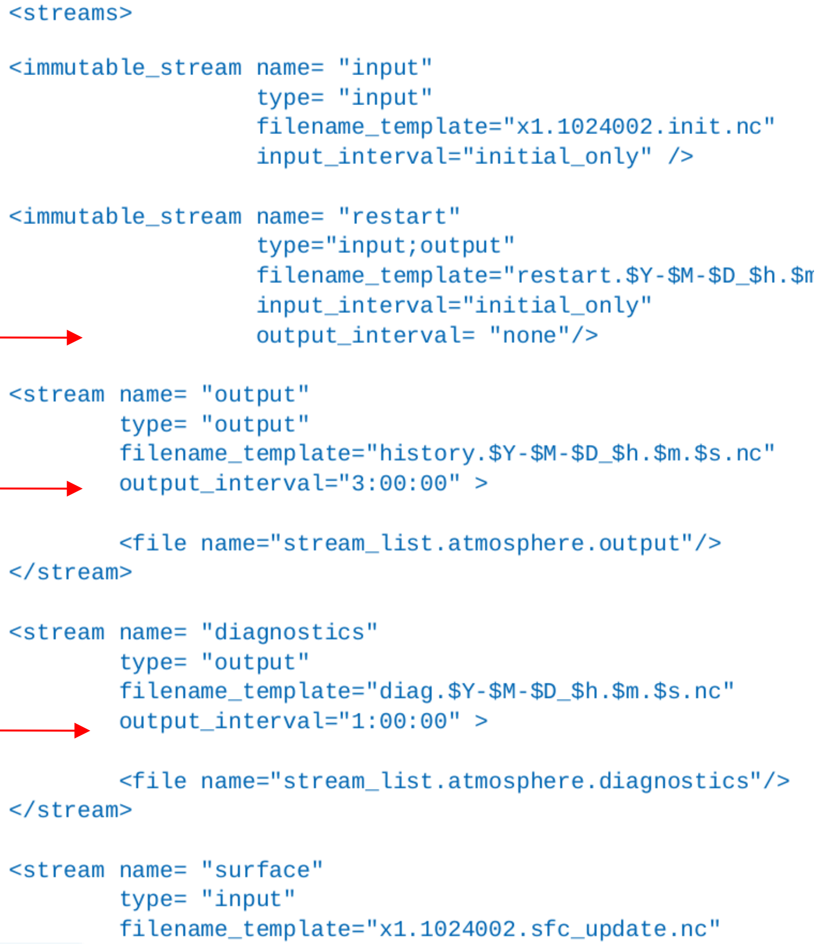
Namelist (atmosphere)

namelist.atmosphere



```
&nhyd_model

    config_time_integration_order = 2
    config_dt = 180.0
    config_start_time = '2021-01-01_00:00:00'
    config_run_duration = '0_03:00:00'
    config_split_dynamics_transport = true
    config_number_of_sub_steps = 2
    config_dynamics_split_steps = 3
    config_h_mom_eddy_visc2 = 0.0
    config_h_mom_eddy_visc4 = 0.0
    config_v_mom_eddy_visc2 = 0.0
    config_h_theta_eddy_visc2 = 0.0
    config_h_theta_eddy_visc4 = 0.0
    config_v_theta_eddy_visc2 = 0.0
    config_horiz_mixing = '2d_smagorinsky'
    config_len_disp = 24000.0
    config_visc4_2dsmag = 0.05
    config_w_adv_order = 3
    config_theta_adv_order = 3
    config_scalar_adv_order = 3
    config_u_vadv_order = 3
    config_w_vadv_order = 3
    config_theta_vadv_order = 3
    config_scalar_vadv_order = 3
    config_scalar_advection = true
    config_positive_definite = false
    config_monotonic = true
    config_coef_3rd_order = 0.25
    config_epssm = 0.1
    config_smdiv = 0.1
/
```

streams.atmosphere



```
<streams>

<immutable_stream name= "input"
                  type= "input"
                  filename_template="x1.1024002.init.nc"
                  input_interval="initial_only" />

<immutable_stream name= "restart"
                  type="input;output"
                  filename_template="restart.$Y-$M-$D_$h.$m
                  input_interval="initial_only"
                  output_interval= "none"/>

<stream name= "output"
        type= "output"
        filename_template="history.$Y-$M-$D_$h.$m.$s.nc"
        output_interval="3:00:00" >

        <file name="stream_list.atmosphere.output"/>
</stream>

<stream name= "diagnostics"
        type= "output"
        filename_template="diag.$Y-$M-$D_$h.$m.$s.nc"
        output_interval="1:00:00" >

        <file name="stream_list.atmosphere.diagnostics"/>
</stream>

<stream name= "surface"
        type= "input"
        filename_template="x1.1024002.sfc_update.nc"
```

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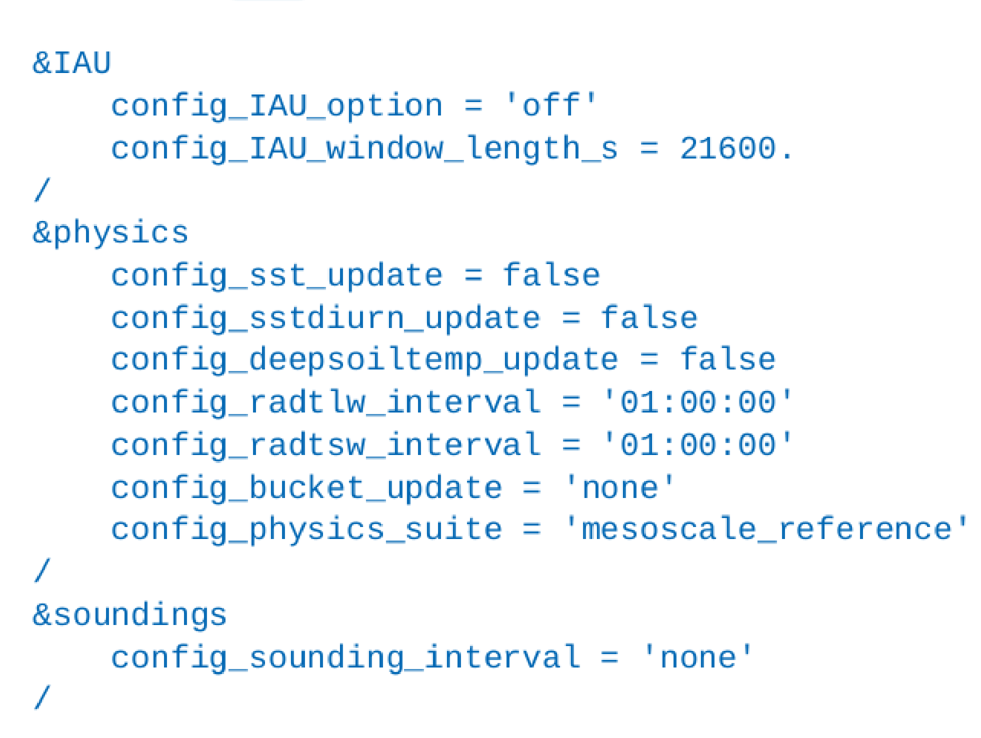
Namelist (atmosphere)

namelist.atmosphere



```
&IAU
    config_IAU_option = 'off'
    config_IAU_window_length_s = 21600.
/
&physics
    config_sst_update = false
    config_sstdiurn_update = false
    config_deepsoiltemp_update = false
    config_radtlw_interval = '01:00:00'
    config_radtsw_interval = '01:00:00'
    config_bucket_update = 'none'
    config_physics_suite = 'mesoscale_reference'
/
&soundings
    config_sounding_interval = 'none'
/
```

config_convection_scheme = 'cu_grell_freitas'
config_convection_scheme = 'cu_kain_fritsch'

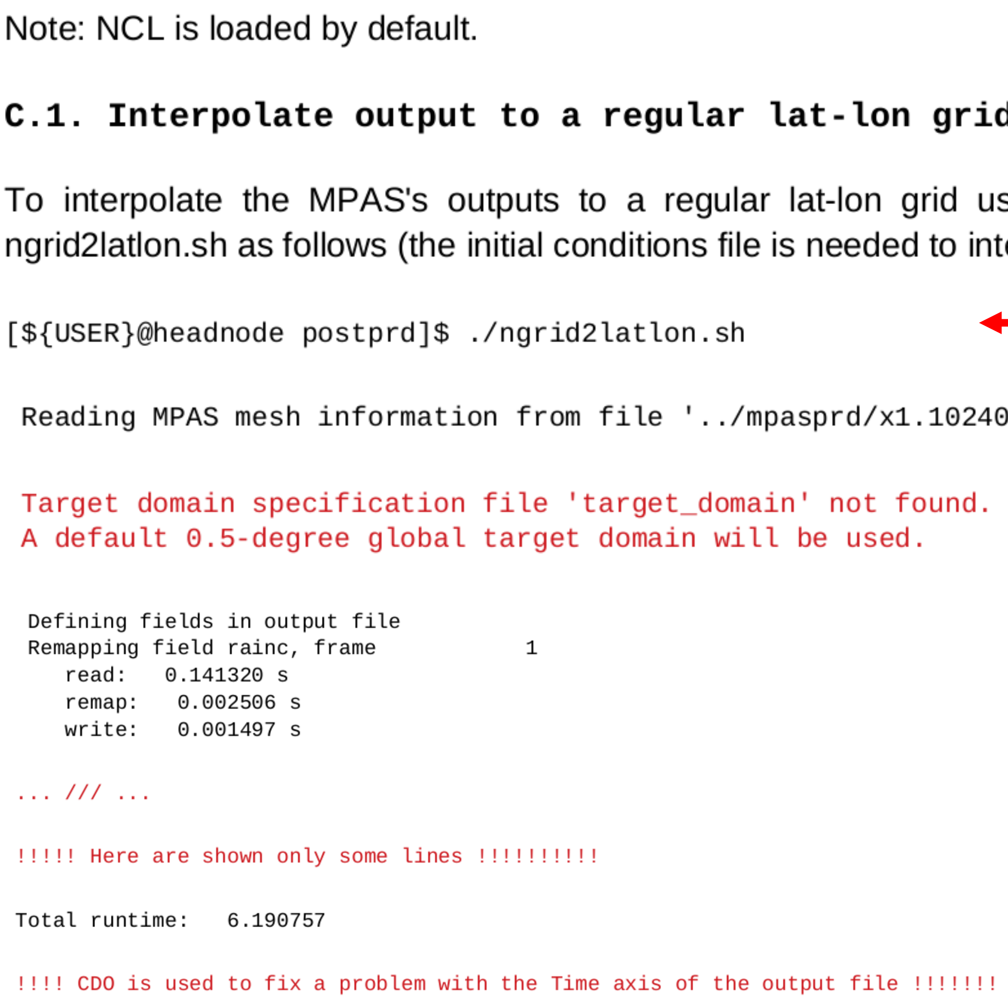
```
[$USER@headnode logs]$ grep "integration step" log.atmosphere.0000.out

   ...
   Timing for integration step: 0.712327 s
   Timing for integration step: 0.710022 s
   Timing for integration step: 0.720861 s
   Timing for integration step: 0.715116 s
   Timing for integration step: 0.728367 s
  ...
```

Check on-fly

```
[$USER@headnode logs]$ more Timing.MPAS
1695838205.037464144
1695842456.644519817
4251.61 sec
```

MPAS-A v8.0.1
FCST 10 days
8 x 128 = 1024 cores
~ 7 min x day

Testcase (example)



Note: NCL is loaded by default.

C.1. Interpolate output to a regular lat-lon grid using convert_mpas

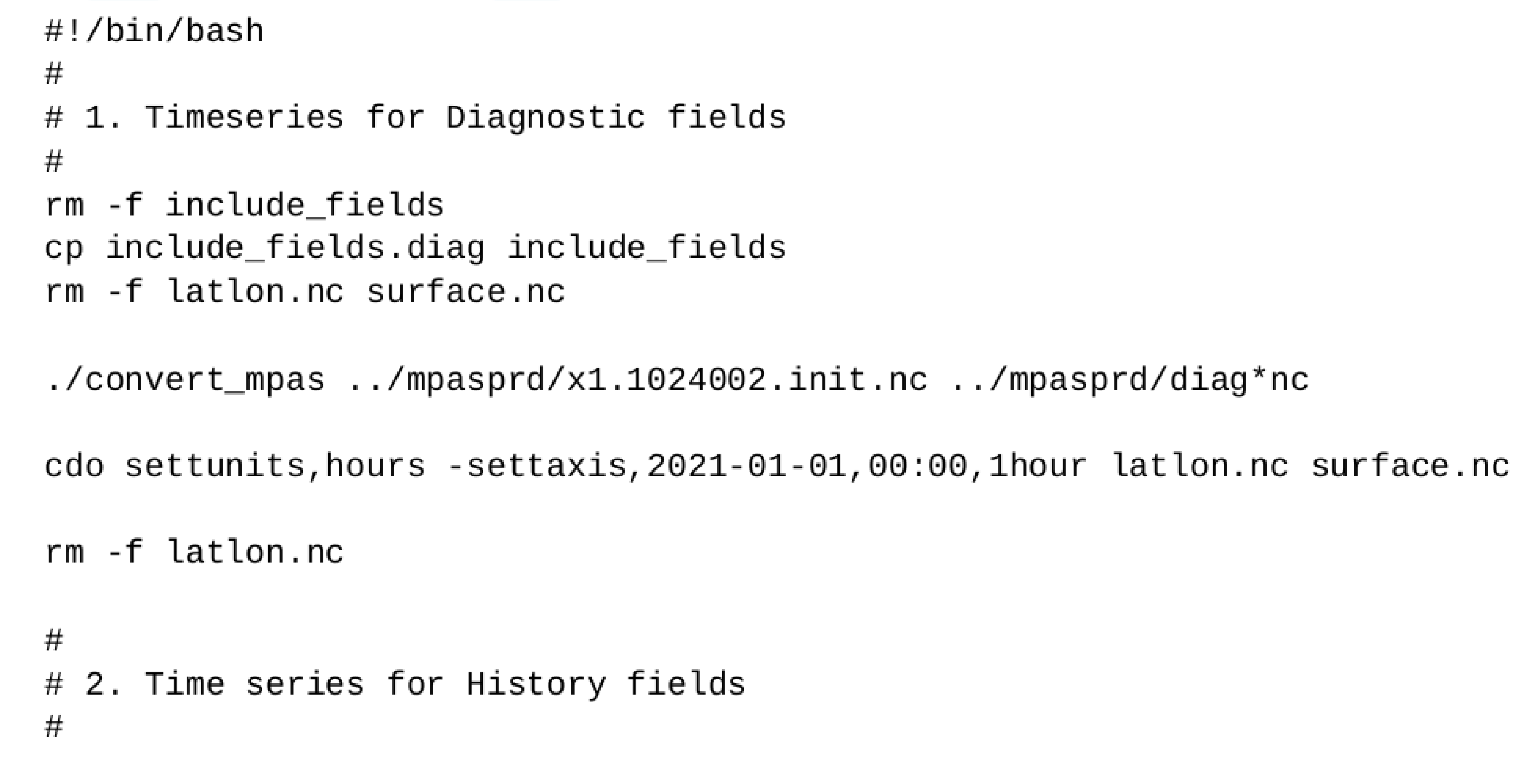
To interpolate the MPAS's outputs to a regular lat-lon grid using convert_mpas, execute the script ngrid2latlon.sh as follows (the initial conditions file is needed to interpolate the output):

```
[${USER}@headnode postprd]$ ./ngrid2latlon.sh

 Reading MPAS mesh information from file '../mpasprd/x1.1024002.init.nc'

 Target domain specification file 'target_domain' not found.
 A default 0.5-degree global target domain will be used.

 Defining fields in output file
 Remapping field rainc, frame           1
    read:   0.141320 s
    remap:   0.002506 s
    write:   0.001497 s

... /// ...

!!!!! Here are shown only some lines !!!!!!!!!!

Total runtime:   6.190757

!!!! CDO is used to fix a problem with the Time axis of the output file !!!!!!!
```

diag.* files,
history.*files

GrADs, NCL, python

Testcase (example)



```
#!/bin/bash
#
# 1. Timeseries for Diagnostic fields
#
rm -f include_fields
cp include_fields.diag include_fields
rm -f latlon.nc surface.nc

./convert_mpas ../mpasprd/x1.1024002.init.nc ../mpasprd/diag*nc

cdo settunits,hours -settaxis,2021-01-01,00:00,1hour latlon.nc surface.nc

rm -f latlon.nc

#
# 2. Time series for History fields
#
```

II Part

https://github.com/mgduda/convert_mpas/blob/master/README.md

To-do:

Transfer 'xtime' variable from input files to output file

Ensure that, for cell fields, the interpolation location lies within the triangle used for interpolation

Make sure that, when dealing with existing output files, the target mesh matches what is found in the output file

Experiment with OpenMP directives to speed up interpolation

Allow locations of 'include_fields', 'exclude_fields', and 'target_domain' files to be specified with environment variables

Decide what to do if input file contains no unlimited dimension

Testcase (example)

Fig. 1b and c shown below were generated using prec.gs script. The MPAS-A was integrated for 10 days using gnu and intel fortran compiler in this case.

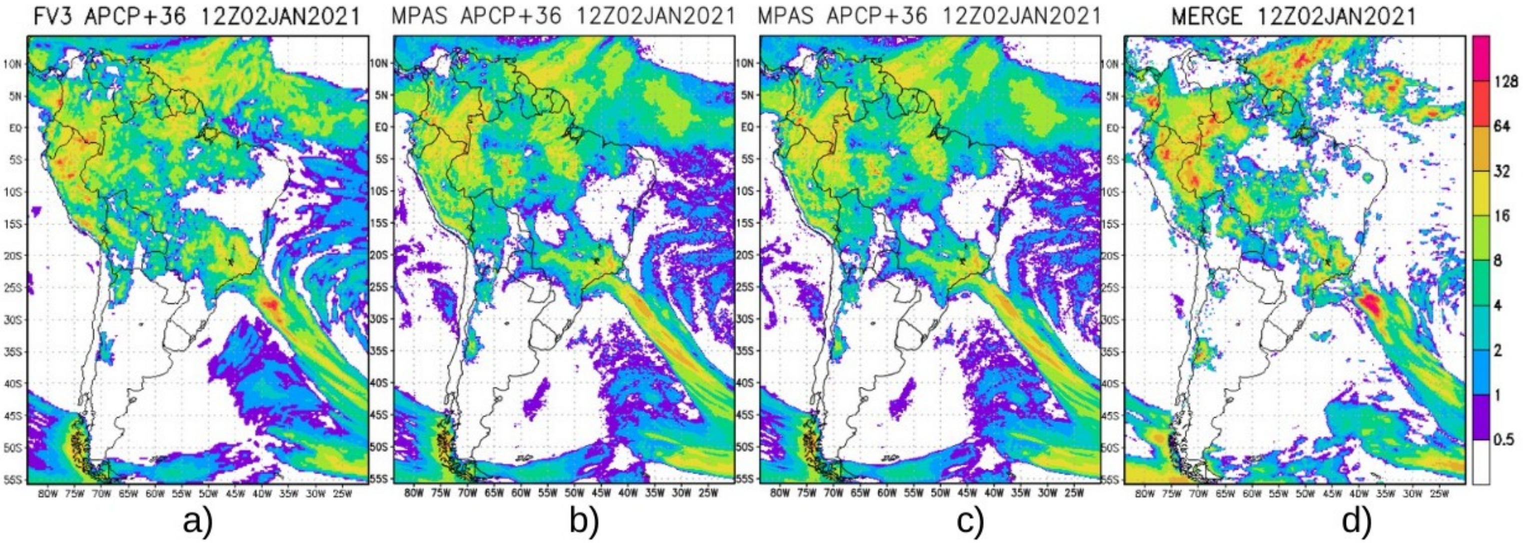


Figure 1. Forecast last 24-h accumulated rainfall (T+36) from a) FV3GFS NCEP operational model (13 km); from INPE b) MPAS-gnu (24 km); c) MPAS-intel (24 km) and observed from MERGE (d). MPAS uses initial conditions for 00Z 01JAN2021 from ERA5.

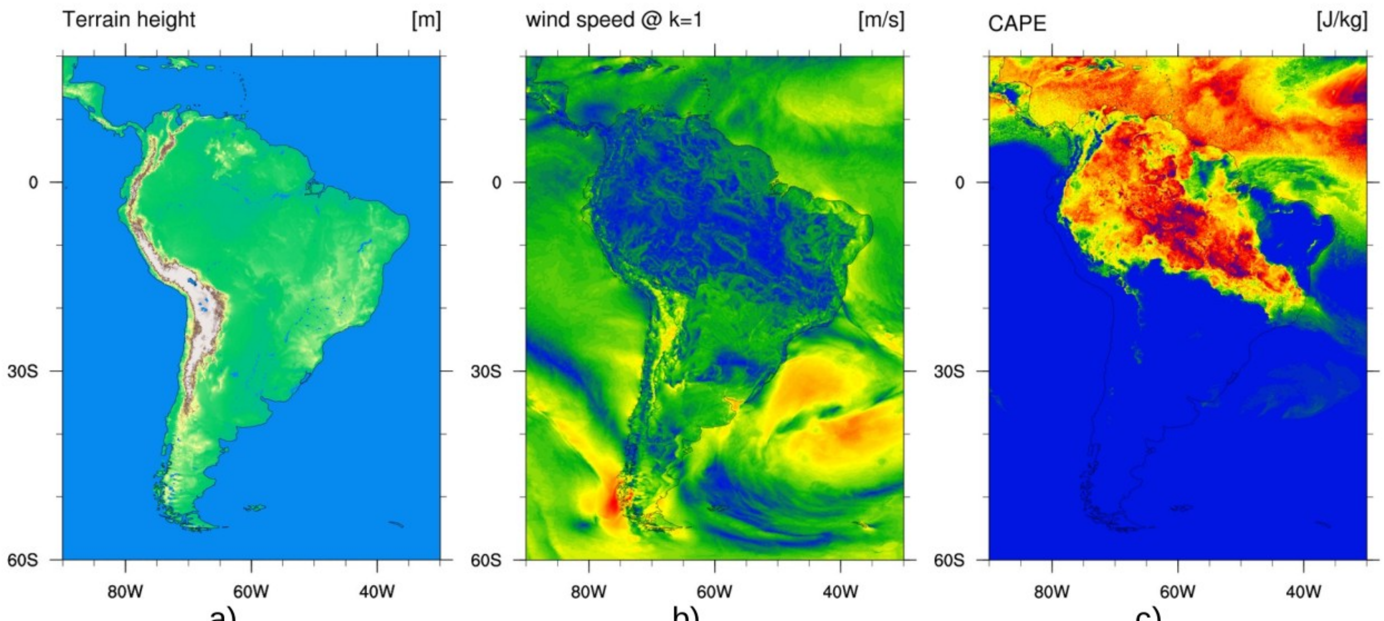
Also, utilities such as CDO and/or NCO can be used to manipulate MPAS output data. For example, to calculate the average in an area or time, select variables, remap, etc.

Testcase (example)

C.2. Visualize output directly with NCL (also ncview)

Using the available NCL scripts could generate Fig. 2. For example, to create Fig. 2a:

```
[${USER}@headnode postprd]$  export FNAME=../mpasprd/x1.1024002.init.nc

[${USER}@headnode postprd]$ ncl plot_terrain.ncl
```



a) b) c)

Figure 2. Using script NCL (direct from the output). a) Topography; b) surface wind at 10m, and c) CAPE

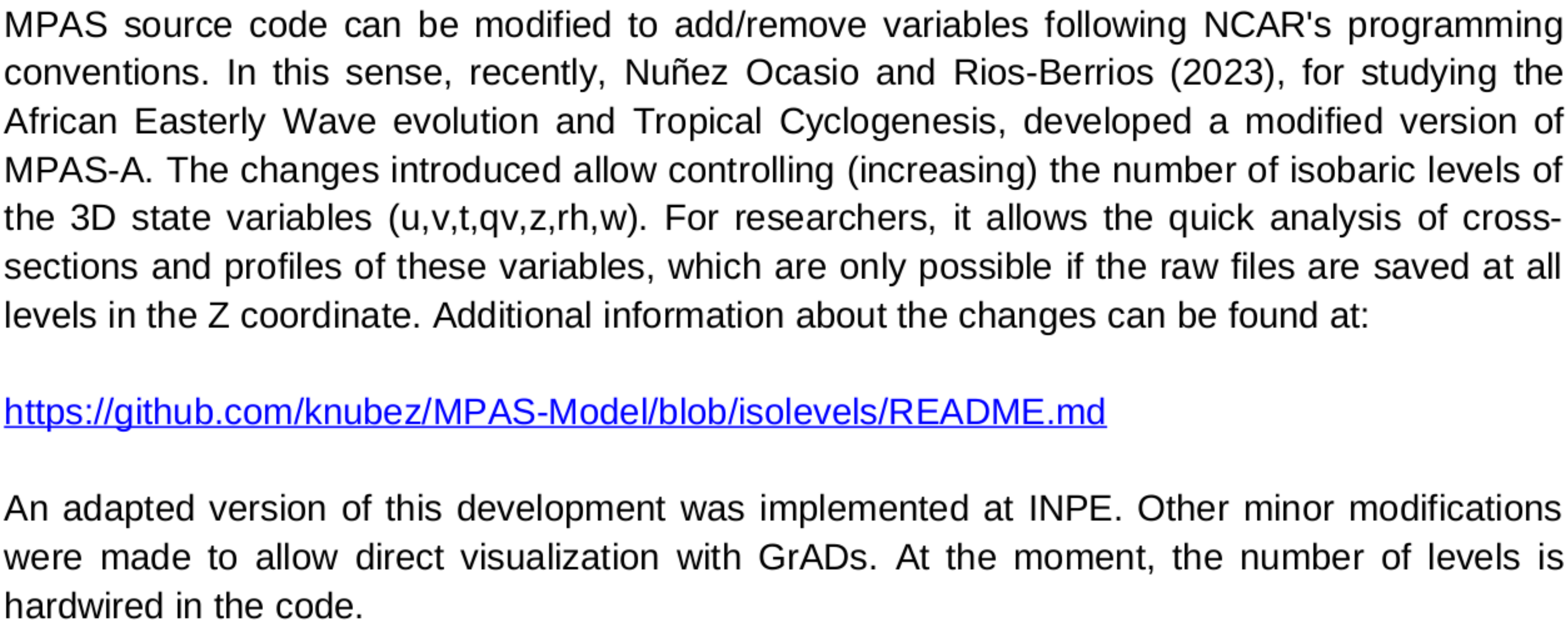
Post-processing

C.3. Other post-processing ways

The use/modification of MPAS-A outputs can be done internally or externally, implying the changes needed or not in the model's source code. As shown previously, different utilities can be used to visualize and manipulate the variables and if it was generated during the model integration process. Most of the time, this is not an obstacle (i.e., research, for example). However, it can involve the generation of large volumes of data, which can exceed the local storage capacity, especially when it is required to run the model in high resolution and/or in an operational mode. Post-processing code is required to efficiently manipulate the model outputs without modifying the source code. In this sense, a system that can be improved is represented by MPASSIT, created by Dr. Reames. This code converts MPAS outputs to a format similar to that recognized by Unified Post-Processing (UPP), which converts from NetCDF to grib2 format (compressing data). It also is helpful as it allows one to choose the vertical levels of the 3D variables. Currently, it is in the implementation stage at INPE. More information about this system can be found at:

https://github.com/LarissaReames-NOAA/MPASSIT

Post-processing



MPAS source code can be modified to add/remove variables following NCAR's programming conventions. In this sense, recently, Nuñez Ocasio and Rios-Berrios (2023), for studying the African Easterly Wave evolution and Tropical Cyclogenesis, developed a modified version of MPAS-A. The changes introduced allow controlling (increasing) the number of isobaric levels of the 3D state variables (u,v,t,qv,z,rh,w). For researchers, it allows the quick analysis of cross-sections and profiles of these variables, which are only possible if the raw files are saved at all levels in the Z coordinate. Additional information about the changes can be found at:

https://github.com/knubez/MPAS-Model/blob/isolevels/README.md

An adapted version of this development was implemented at INPE. Other minor modifications were made to allow direct visualization with GrADs. At the moment, the number of levels is hardwired in the code.

MPASv7.3/src/core_atmosphere/diagnostics

isobaric_diagnostics.F

Register_isobaric.xml

Post-processing

Also, Nuñes Ocasio (https://code.mpimet.mpg.de/boards/1/topics/11223) describes creating weights to interpolate MPAS's data to a regular grid conservatively. For example, to create the weights to interpolate the MPAS-A 15km outputs to a 0.25 x 0.25 grid:

```
cdo -P 1 --cellsearchmethod spherepart -gencon,r1440x720 -setgrid,mpas:x1.2621442.grid.nc -
selgrid,1 diag.2021-06-23_00.00.00.nc weights_.25.nc
```

Interpolating a variable from MPAS-A 15km to 0.25 x 0.25 grid:

```
cdo -P 1 -f nc4 remap,r1440x720,weights_.25.nc -setgrid,mpas:x1.2621442.grid.nc -selname,olrtoa
diag.2021-07-08_00.00.00.nc olr.p25.nc
```

Post-processing

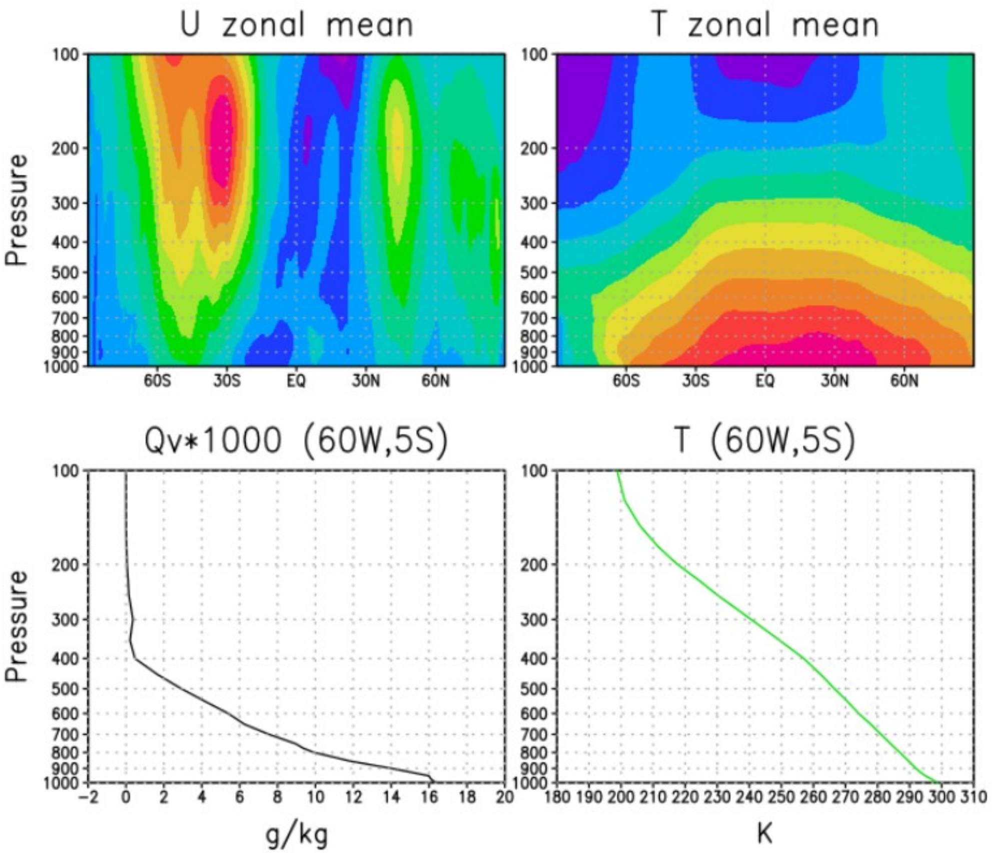
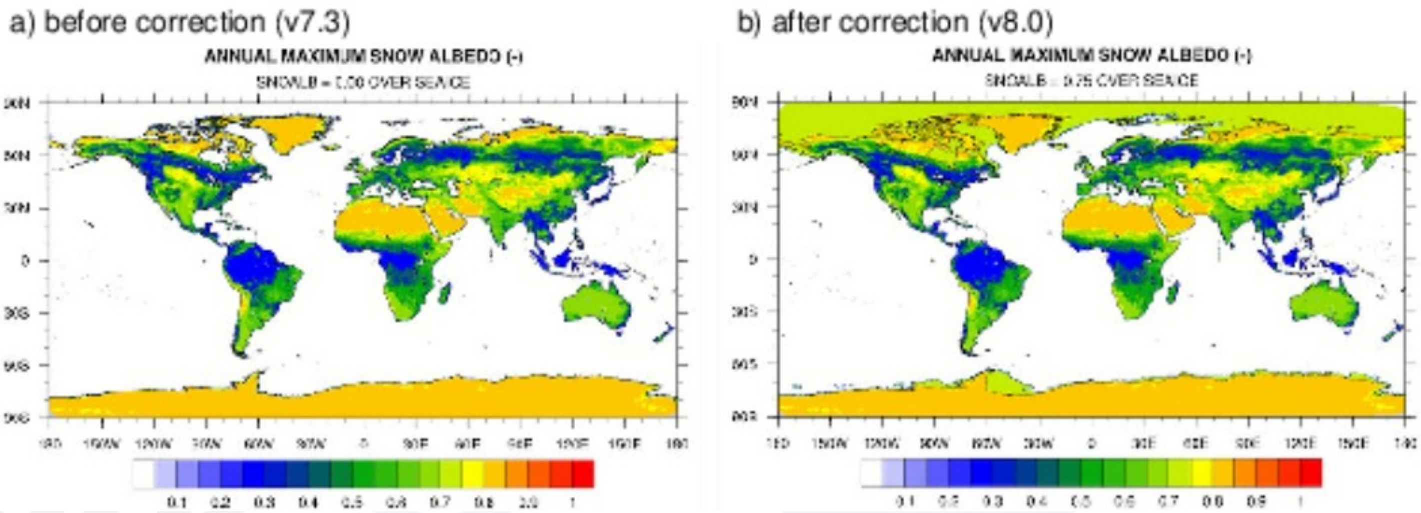


Figure 3. Example of cross-section and profiles using modified outputs.

MPAS v8.0.1 differences



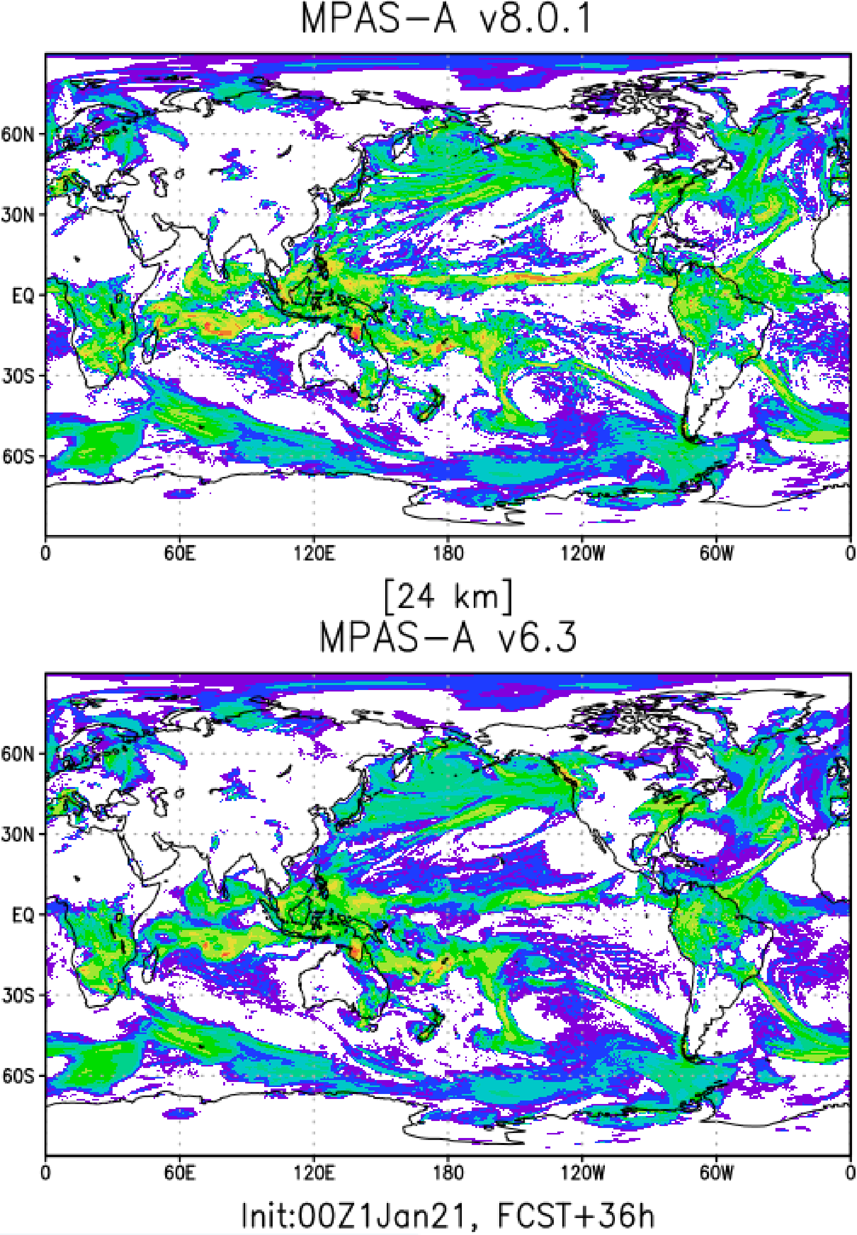
a) before correction (v7.3)

b) after correction (v8.0)

ANNUAL MAXIMUM SNOW ALBEDO (-)
SNOWALB = 0.00 OVER SEAICE
ANNUAL MAXIMUM SNOW ALBEDO (-)
SNOALB = 0.75 OVER SEAICE
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Bug fix: fraction sea-ice, physics

Updates: different physics versions: NOAHMP Framework

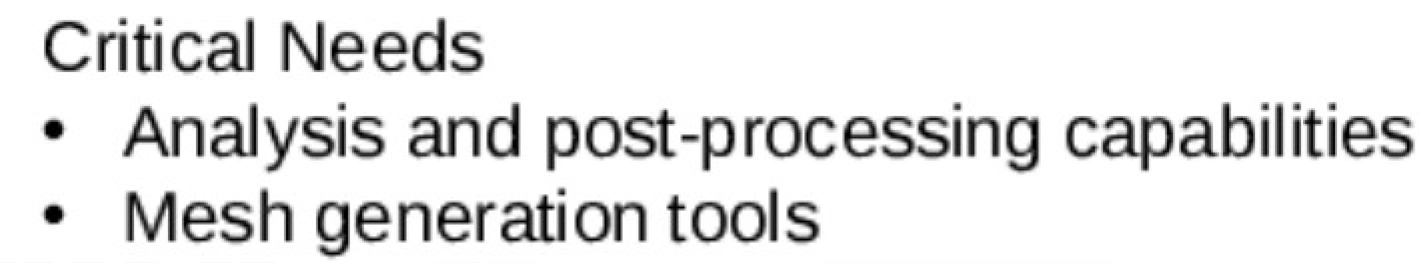


MPAS–A v8.0.1

[24 km]

MPAS–A v6.3

Init:00Z1Jan21, FCST+36h



Critical Needs

- Analysis and post-processing capabilities
- Mesh generation tools

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Obrigado

MONAN
Model for Ocean-laNd-Atmosphere predictioN

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