# NASA Unified Weather Research and Forecasting Model (NU-WRF)

A Tutorial For NU-WRF development version (v11)

NUWRF software integration group

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## Introduction

#### What is in this tutorial?

This tutorial describes the process of downloading, compiling, and running NU-WRF (development version) for four different and representative workflows:

- Basic: Based on WRF ARW.
- WRF-LIS: The recommended non-chemistry NU-WRF workflow (LIS MERRA forcing).
- Chemistry: The recommended chemistry (non-LIS) NU-WRF workflow.
- SCM: The Single Column Model NU-WRF workflow (with LIS coupling).

Each workflow consists of a series of steps starting with the acquisition of data files followed by the execution of several NU-WRF components. Successful completion of any workflow requires that **all** steps be completed in the order presented.

For any additional information please consult the NU-WRF user's guide at: https://nuwrf.gsfc.nasa.gov/sites/default/files/docs/nuwrf\_userguide\_v11.pdf

# Special instructions

- All workflows are designed with pre-defined settings<sup>1</sup>, including datasets.
   Workflows are not guaranteed to work if you deviate from the prescribed instructions. So, please refrain from editing the inputs unless you know what you are doing.
- It is assumed that users are running on Discover or Pleiades using the bash shell. However, the steps described here should work under other shells.

**IMPORTANT**:Henceforth all lines starting with '>' are Unix commands to be executed by the users.

**Note on paths**: On Pleiades *most* paths are identical to the ones on Discover. So, in most cases just removing "/discover" from the path should be enough for the setup instructions to work on both systems.

**Note on workflows**: Only the basic and default workflows are available on Pleiades.

¹That is, compiler/MPI combination, external libraries and run-time settings.

## Useful links

- Community ARW User Guide https://www2.mmm.ucar.edu/wrf/users/docs/user\_guide\_v4/v4.3/contents.html
- Community WRF ARW Online Tutorial http://www2.mmm.ucar.edu/wrf/OnLineTutorial/index.php
- Documentation for using Discover and other NCCS systems https://www.nccs.nasa.gov/nccs-users/instructional
- Documentation for using Pleiades and other NAS systems http://www.nas.nasa.gov/hecc/support/kb/

**NOTE**: The details for building the software on Discover and Pleiades are automatically handled by NUWRF's build scripts!

# Setup

Before starting any workflow there are a few steps that must be completed:

- Download or checkout the NU-WRF code.
- Build the NU-WRF executable components.
- Set some environment variables.

#### Download the code

Tar files are available on NCCS and NAS computers for s0942 group members. Otherwise, the code must be obtained from the Git repository (see next slide). On DISCOVER:

> cp /discover/nobackup/projects/nu-wrf/releases/stable
 /<tarball> /some/path

#### On PLEIADES:

> cp /nobackupp8/nuwrf/releases/stable/<tarball> /some/
 path

where tarball is: nu-wrf\_v11-wrf44-lisf73.tgz

#### To untar type:

> tar -zxf nu-wrf\_v11-wrf44-lisf74.tgz

#### Download the code

The code can also be obtained from its Git repository (an account is required for access):

```
> cd /discover/nobackup/user_id/
```

```
> git clone -b develop https://git.mysmce.com/astg/nuwrf
    /nu-wrf-dev
```

Using Git is more advantageous. Once you clone the repository you have a "complete repository" in your local work area. Now you can change the files and commit your features using Git's branching capabilities (you would need to submit a merge request). Other developers can pull your changes from the repository and continue working with the improvements you added to the files. For more information about using our Git repository please see this Git intro or refer to the NU-WRF user's guide:

https://nuwrf.gsfc.nasa.gov/nu-wrf-user-quide

## **Build NU-WRF**

First, log in to a Discover node or Pleiades front-end node. Create environment variable **NUWRFDIR** that defines the directory path of the NU-WRF code downloaded earlier. Then, **cd** to it. For example, on Discover:

- > export NUWRFDIR=/discover/nobackup/user\_id/nu-wrf
- > cd \$NUWRFDIR

For the Basic workflow execute the build script as follows:

> ./build.sh wrf,wps &

That will print some setup information and will run the build in the background (so, just press Enter to get back to the Unix prompt). Build information will be saved in a single make.log file. To view the progress of the NU-WRF build you can run:

> tail -f make.log &

The build will take about 1-2 hours, so please be patient. If the compilation fails then you can view the make.log file to check what went wrong.

## **Build NU-WRF**

For the other workflows, use the following commands.

#### WRF-LIS workflows:

#### Chemistry workflow:

> ./build.sh chem,wps,lis,utils &

#### SCM workflow:

> ./build.sh ideal\_scm\_lis\_xy,wps,lis,ldt,lis4scm &

For more information about the NU-WRF build system run build.sh without arguments:

> ./build.sh

## **Build NU-WRF**

After compilation - assuming there are no errors - several executables will be created. Some important executables are::

```
WRF executables:
$NUWRFDIR/WRF/main/real.exe
$NUWRFDIR/WRF/main/wrf.exe

WPS executables:
$NUWRFDIR/WPS/geogrid.exe
$NUWRFDIR/WPS/metgrid.exe
$NUWRFDIR/WPS/ungrib.exe
```

For example, to see the names of all the executables created with an exe extension run:

```
> find $NUWRFDIR -name \*.exe
```

## **Environment variables**

We already set **NUWRFDIR**, but we need two more variables.

- Select a directory for running the model and set it equal to the RUNDIR environment variable. For example:
  - > export RUNDIR=/discover/nobackup/user\_id/scratch/
    basic\_workflow

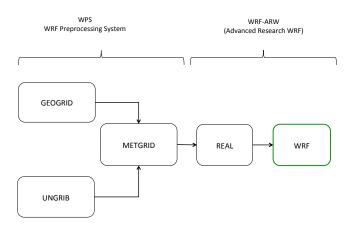
- Make sure you create RUNDIR outside of NUWRFDIR. This
  is useful when switching between NU-WRF versions or for
  updating to new changes.
- Finally, set the PROJECTDIR environment variable:
  - > export PROJECTDIR=/discover/nobackup/projects/nuwrf

## Basic Workflow

A NU-WRF workflow consists of running various pre-processing (WPS) components as well as the main NU-WRF model. The basic workflow described next is the simplest approach to running simulations with NU-WRF. It consists of running the WRF Pre-processing System (WPS) plus an additional WRF pre-processor (REAL) before running the WRF model.

Neither chemistry nor advanced land surface initialization are used.

#### NU-WRF basic workflow (similar to WRF ARW).



Note that GEOGRID and UNGRIB are independent of each other so you may choose to run one or the other first.

# Required files for basic workflow

#### Copy the basic workflow files to **RUNDIR**:

```
> cp -r $PROJECTDIR/tutorial/basic_workflow/* $RUNDIR
Where:
common.reg : shared script with settings used by other
   scripts.
*.reg : scripts to run pre-processors and model.
namelist*: namelist files required by executables.
data/ungrib/* : GRIB atmospheric data for initial
   conditions used by UNGRIB component.
```

**Note**: All workflows described in this tutorial are part of a small database of testcases used for NU-WRF regression testing. Such tests are executed using the reg script located in scripts/python/regression and can be used to generate/setup the files in each testcase (hence the reg extension of the script files). For more information see section 7.

# Required script changes

> cd \$RUNDIR

Use your favorite editor to edit **common.reg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
```

# \*\*\* Please make sure these settings are correct \*\*\*

RUNDIR Specifies the location of the temporary run directory

You may need to edit all the .reg files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:

#SBATCH --account s0942

Change if you want to change the number of nodes, mil - to run on Mila

#SBATCH --ntasks=16 --constraint=mil

Uncomment and set according to your needs and privileges:

##SBATCH --qos=high

Uncomment (if desired) and substitute your e-mail here:

##SBATCH --mail-user=user@nasa.gov
```

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# A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start\_date and end\_date
  - In namelist.input look for start\_ and end\_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - You may need to modify the namelists. For example in namelist.input, make sure end\_day - start\_day = run\_days.
- For any other changes please refer to the user's guide.

## **GEOGRID**

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For N domains (max\_dom in namelist.wps), N geo\_em files will be created.

Before running GEOGRID ensure your domain is in the right location. To do so run plotgrids\_new.ncl

- > module load ncview
- > ncl \$NUWRFDIR/WPS/util/plotgrids\_new.ncl

This is where you would edit namelist.wps to modify the domain information. Now run GEOGRID:

- > cd \$RUNDIR
- > sbatch geogrid.reg

When done, check for the "Successful completion" string in the file geogrid.slurm.out. geogrid.log.nnnn (nnnn is the cpu number) files will also be created for tracking run failures or debugging.

#### **UNGRIB**

UNGRIB unpacks GRIB1 or GRIB2 files that contain meteorological data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and writes specific fields in a WPS intermediate format.

- Input: namelist.wps and GRIB input data.
- Output: Several FNL\* files corresponding to the number of intervals (interval\_seconds) in simulation length (start/end dates).

#### Notes:

- The GRIB input is referenced in the run script, ungrib.reg: ./link\_grib.csh data/ungrib/fnl\_\*
- The UNGRIB output (FNL) is determined by the settings in the WPS namelist (namelist.wps).
- makes use of Vtables that list the fields and their GRIB codes that must be unpacked from the GRIB files.

#### To run:

- > cd \$RUNDIR
- > ./ungrib.reg

## **METGRID**

METGRID horizontally interpolates the output from UNGRIB to the WRF domains and combines it with the output from GEOGRID/UNGRIB.

- Input: namelist.wps, UNGRIB output, geo\_em\* files.
- Output: Several met\_em\* files corresponding to the number of intervals (interval\_seconds) in simulation length (start/end dates).

#### To run:

- > cd \$RUNDIR
- > sbatch metgrid.reg

When done, check for "Successful completion" string in the file metgrid.slurm.out. metgrid.log.nnnn (nnnn is the cpu number) files also be created for tracking run failures or debugging.

## **REAL**

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input, met\_em\* files, geo\_em\* files.
- Output: wrfinput\* files (one for each domain), wrfbdy\_d01.

#### To run:

- > cd \$RUNDIR
- > sbatch real.reg

Check real.slurm.out for run completion. If necessary check the real\_logs directory for real.rsl.out.nnnn and real.rsl.error.nnnn files.

## **WRF**

This program will perform a numerical weather prediction simulation using the data from REAL.

- Input: namelist.input, wrfinput\* files (one for each domain), wrfbdy\_d01.
- Output: wrfout\* files (one for each domain).

#### To run:

- > cd \$RUNDIR
- > sbatch wrf.reg

Check wrf.slurm.out for run completion. If necessary check the wrf\_logs directory for wrf.rsl.out.nnnn and wrf.rsl.error.nnnn files.

# Post-processing on Discover

#### Using NCVIEW:

- > module load ncview
- > ncview <filename>

# Post-processing on Discover

## Using RIP (NCAR graphics). Submit the rip job:

```
> cd $RUNDIR
> ./rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename
rip.bash will run ripdp_wrfarw and rip to generate NCAR
   Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin -
   where $NCARG ROOT is
$PROJECTDIR/lib/sles12/ekman/intel-intelmpi/ncarg
Sample RIP plot specification tables are in $NUWRFDIR/
```

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on customizing plots with RIP.

scripts/rip and are looped through by rip.bash

Minor changes to rip.bash may be necessary.

# Post-processing on Discover

Other available community software packages are ARWPOST (for GRADS), UPP (for GRIB), and MET (for atmospheric verification)

For more information on community post-processing packages available with WRF, see

```
https://www2.mmm.ucar.edu/wrf/users/docs/user_guide_v4/v4.3/users_guide_chap9.html
```

#### ARW user homepage:

```
http://www2.mmm.ucar.edu/wrf/users
```

NUWRF specific post-processors are GSDSU (simulates satellite data) and LVT (land surface verification).

# Adjustments for Pleiades

#### On Pleiades set PROJECTDIR to:

> export PROJECTDIR=/nobackupp8/nuwrf

Revise all the \*.reg files and edit as needed. The scripts should work with minor modifications - if any at all, but make sure you check the following anyway:

```
Change s0942 to the appropriate SBU charge code:

#PBS -W group_list=s0942

Change if you want to change number of nodes and nodes:

#PBS -l select=6:ncpus=16:mpiprocs=16:model=san

Set according to your needs and privileges:

#PBS -q devel
```

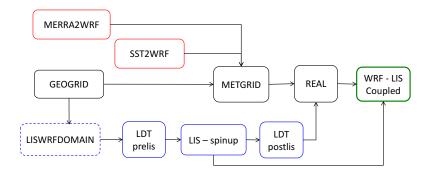
## **Default Workflow**

The default workflow is a more advanced approach to running simulations with NU-WRF. Instead of using land surface fields interpolated from a coarser model or reanalysis, a custom-made land surface state is created by LIS on the same grid and with the same terrestrial data and land surface physics as WRF. WRF then calls LIS on each advective time step, and provides atmospheric forcing data, and receives land surface data (fluxes, albedo, etc) in return.

No chemistry is used.

#### NU-WRF default workflow.

#### MERRA2WRF, SST2WRF, LIS spin up & WRF-LIS coupled workflow



This NU-WRF default workflow uses MERRA/MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS-SST (Remote Sensing Systems SST product), LIS land surface model initial conditions, and runs WRF coupled with LIS.

## Required files for default workflow

#### Copy the following files to **RUNDIR**:

```
> export RUNDIR=/discover/nobackup/<my_user_id>/scratch/
    default_workflow
> cp -r $PROJECTDIR/tutorial/default_workflow/* $RUNDIR
Where:
common.reg : shared script with settings used by other
    scripts.
*.reg : scripts to run pre-processors and model.
namelist* : namelist files required by executables.
```

**Note**: Unlike the "basic" workflow, we have no ungrib data. The reason is that this workflow uses MERRA2 reanalysis data as the source of the meteorological fields.

# Required script changes

> cd \$RUNDIR

Use your favorite editor to edit **common.reg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# *** Please make sure these settings are correct ***
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
```

# RUNDIR specifies the location of the temporary run directory RUNDIR=<CHANGE THIS>

You may need to edit all the \*.reg files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code: 
#SBATCH --account s0942
Change if you want to change the number of nodes, mil - to run on Mila
#SBATCH --ntasks=16 --constraint=mil
Uncomment and set according to your needs and privileges:
##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
```

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##SBATCH --mail-user=user@nasa.gov

# A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start\_date and end\_date
  - In namelist.input look for start\_ and end\_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end\_day - start\_day = run\_days.
- For **any** other changes please refer to the user's guide.

## **GEOGRID**

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For N domains (max\_dom in namelist.wps), N geo\_em files will be created.

Before running GEOGRID ensure your domain is in the right location. To do so run plotgrids\_new.ncl (or  $./view\_geo.reg)$ 

- > module load ncl
- > cd \$RUNDIR
- > ncl \$NUWRFDIR/WPS/util/plotgrids\_new.ncl

This is where you would edit namelist.wps to modify the domain information. Now run GEOGRID:

- > cd \$RUNDIR
- > sbatch geogrid.reg

When done, check for "Successful completion" string in the file geogrid.slurm.out. geogrid.log.nnnn (nnnn is the cpu number) files will also be created for tracking run failures or debugging.

# Use of GEOS-5 Meteorological Data

Another source of NU-WRF initial and lateral boundary conditions is NASA's GEOS-5 global model. A number of dataset options exist from GEOS-5, including archived MERRA and MERRA-2 reanalyses. However, there are some issues to keep in mind.

First of all the GEOS-5 land surface data cannot be used to initialize WRF, due to fundamental differences between the GEOS-5 Catchment LSM and those in WRF. Thus, the GEOS-5 data in the current workflow also includes WRF-LIS. Second, GEOS-5 writes output in netCDF (and historically HDF4 and HDFEOS2) instead of GRIB. And furthermore, GEOS-5 often does not output all the variables expected by WPS.

To address these issues, special preprocessing software has been developed: MERRA2WRF. MERRA2WRF is a program customized to process the 6-hourly reanalyses from MERRA and MERRA-2. For 3-hourly MERRA-2 processing users must fall back to GEOS2WRF, which is not discussed here.

## **MERRA2WRF**

Process MERRA2 reanalysis for WRF initial and lateral boundary conditions.

The merra2wrf.reg script does two things: retrieves the MERRA-2 data from the NASA GES DISC web servers; and processes the downloaded data into data readable by METGRID. Note this tutorial only deals with MERRA-2 data. For MERRA data retrieval/processing please see the NU-WRF user's guide.

- > cd \$RUNDIR
- > ./merra2wrf.reg # Not a batch script. It may take a
  minute or two to complete...

Note that the script downloads data with start date = 20150711 and end date = 20150712.

> cp \$RUNDIR/data/merra2wrf/MERRA\* \$RUNDIR

## SST2WRF

SST2WRF processes several sea surface temperature (SST) products produced by Remote Sensing Systems (RSS; see http://www.remss.com).

### To run:

- > cd \$RUNDIR
- > ./sst2wrf.reg # Not a batch script. It may take a few seconds to complete...
- Note that the script downloads data with start date = 20150711 and end date = 20150712.
- When done, SSTRSS\* files will be created in the \$RUNDIR/ data/mw/ directory. These files must be copied to \$RUNDIR before running the METGRID component.
- > cp \$RUNDIR/data/mw/SSTRSS\* \$RUNDIR

## **METGRID**

METGRID horizontally interpolates MERRA and SSTRSS data to the WRF domains, and combines them with the output from GEOGRID.

- Input: namelist.wps, MERRA\*, SSTRSS\* and geo\_em\* files.
- Output: Several met\_em\* files corresponding to the number of intervals (interval\_seconds) in simulation length (start/end dates).

#### To run:

- > cd \$RUNDIR
- > sbatch metgrid.reg

When done, check for "Successful completion" string in the file metgrid.slurm.out. metgrid.log.nnnn (nnnn is the cpu number) files also be created for tracking run failures or debugging.

# LISWRFDOMAIN (optional step)

LISWRFDOMAIN is used to customize (and check) LDT and LIS config files so their domain(s) (grid size, resolution, and map projection) match that of WRF. It uses the output from GEOGRID to determine the reference latitude and longitude. For this tutorial, we are using pre-defined lis.config.\* and ldt.config.\* files that do not need to be modified (or checked). However, if you do change your GEOGRID domain then you may need to run LISWRFDOMAIN.

- Input: lis.config, ldt.config and geo\_em\* files.
- Output: lis.config, ldt.config (will be identical to original config files if no changes are necessary).

### Example:

- cd \$RUNDIR
- ./liswrf\_domain.reg

Running the script will replace, if necessary, the original files with the "new" ones before running LDT, thus ensuring that the domain parameters between LIS and WRF are consistent.



# LDT (pre-LIS)

LDT processes data inputs for different surface models. In this use-case we are using the Noah-MP v3.6 land surface model.

- Input: Idt.config (Idt.config.prelis gets copied into Idt.config by Idt\_prelis.reg )
- Output: lis\_input\* files for each NU-WRF domain.

### To run:

- > cd \$RUNDIR
- > sbatch ldt\_prelis.reg

When done, check for "Finished LDT run" string in the file ldtlog\_pt.0000

## LIS

LIS can be run in various modes. Here we run in "retrospective" mode (a very short LIS spin-up) to produce restart and history files. LDT postlis use the history files and the restart files are used by WRF.

- Input: lis\_input\* files for each NU-WRF domain (this is the output from LDT pre-LIS), lis.config.coldstart, forcing\_variables\_merra2.txt,
   NOAHMP36 OUTPUT LIST SPINUP TBI
- Output: surface model output in the OUTPUT/SURFACEMODEL/2015 directory.

#### To run:

- > cd \$RUNDIR
- > sbatch lis.reg

When done, lis.reg copies the LIS restart/history files in OUTPUT to \$RUNDIR

Check this file for successful run completion: lis.slurm .out

lislog.nnnn files will also be created for tracking run failures or debugging.

# LDT (post-LIS)

After running LIS, it is necessary to rerun LDT in "NUWRF preprocessing for real" mode. This requires modifications to ldt.config to specify the static output file from LDT and the dynamic output file from LIS. Fields from both will be combined and written to a new netCDF output file for use by REAL

- Input: Idt.config (Idt.config.postlis gets copied into Idt.config by Idt\_postlis.reg ), LIS history files in OUTPUT directory.
- Output: lis4real\_input\* files for each NU-WRF domain.

#### To run:

> cd \$RUNDIR

```
> sbatch ldt_postlis.reg
When done, check for "Finished LDT run" string in the
    file ldt_log_postlis.0000
```

## REAL

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input.real, met\_em\* files, geo\_em\*, lis4real\_input\* files.
- Output: wrfinput\* files (one for each domain), wrfbdy\_d01.

#### To run:

- > cd \$RUNDIR
- > sbatch real.reg

Check real.slurm.out for run completion. If necessary check the real\_logs directory for real.rsl.out.nnnn and real.rsl.error.nnnn files.

## WRF

Running WRF, in this case, is similar to the basic case, except that WRF will also read some LIS files (config, model output table) and the restarts that were produced during the "retrospective" run.

- Input: namelist.input.wrf, lis.config.wrf, NOAHMP36\_OUTPUT\_LIST.TBL wrfinput\* files (one for each domain), wrfbdy\_d01.
- Output: wrfout\* files (one for each domain).

### To run:

- > cd \$RUNDIR
- > sbatch wrf.reg

Check wrf.slurm.out for run completion. If necessary check the wrf\_logs directory for wrf.rsl.out.nnnn and wrf.rsl.error.nnnn files.



# Post-processing on Discover

### Using NCVIEW:

- > module load ncview
- > ncview <filename>

# Post-processing on Discover

### Using RIP (NCAR graphics). Submit the rip job:

```
> cd $RUNDIR
> ./rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename
rip.bash will run ripdp_wrfarw and rip to generate NCAR
   Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin -
   where $NCARG ROOT is
$PROJECTDIR/lib/sles12/ekman/intel-intelmpi/ncarg
Sample RIP plot specification tables are in $NUWRFDIR/
   scripts/rip and are looped through by rip.bash
```

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm
 for info on customizing plots with RIP.
Minor changes to rip.bash may be necessary.

# **Chemistry Workflow**

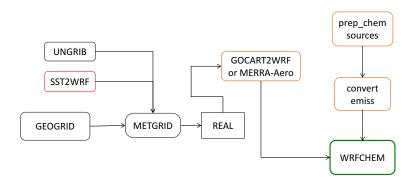
NU-WRF offers advanced aerosol modeling using the implementation of GOCART. This workflow incorporates steps from the basic and the default workflow. However, it excludes the LIS steps and instead adds the GOCART2WRF preprocessor for providing chemical boundary conditions from GEOS-5 as well as the community PREP\_CHEM\_SOURCES program for emissions.

GOCART2WRF supports four possible sources of GOCART data:

- offline GOCART
- on-line GOCART from GEOS5
- MERRAero reanalyses
- MERRA-2

We will describe the "offline GOCART" case only. LIS is not used.

### NU-WRF chemistry workflow.



This NU-WRF CHEM workflow uses atmospheric initial and lateral boundary conditions from GRIB files, RSS SST (Remote Sensing Systems SST product), chemical tracers using prep\_chem\_sources passing through the convert\_emiss utility, aerosol data from GOCART or MERRA-Aero and finally runs WRF-CHEM.

# Required files for chemistry workflow

### Copy the following files to **RUNDIR**:

```
> export RUNDIR=/discover/nobackup/<my_user_id>/scratch/
   chemistry_workflow
> cp -r $PROJECTDIR/tutorial/chemistry_workflow/*
   SRUNDIR
Where:
common.reg : shared script with settings used by other
   scripts.
*.reg : scripts to run pre-processors and model.
namelist*: namelist files required by executables.
data/ungrib : GRIB atmospheric data for initial
   conditions used by UNGRIB component.
data/gocart : data files used by GOCART
```

# Required script changes

> cd \$RUNDIR

Use your favorite editor to edit **common.reg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
```

# \*\*\* Please make sure these settings are correct \*\*\*

##SBATCH --mail-user=user@nasa.gov

RUNDIR = CHANGE THIS>

You may need to edit all the .reg files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code: #SBATCH --account s0942
Change if you want to change the number of nodes, mil - to run on Mila #SBATCH --ntasks=16 --constraint=mil
Uncomment and set according to your needs and privileges: ##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
```

# A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start\_date and end\_date
  - In namelist.input look for start\_ and end\_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - You may need to modify the namelists. For example in namelist.input, make sure end\_day - start\_day = run\_days.
- For any other changes please refer to the user's guide.

## **GEOGRID**

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For N domains (max\_dom in namelist.wps), N geo\_em files will be created.

Before running GEOGRID ensure your domain is in the right location. To do so run plotgrids\_new.ncl

- > module load ncl
- > ncl \$NUWRFDIR/WPS/util/plotgrids\_new.ncl

This is where you would edit namelist.wps to modify the domain information. Now run GEOGRID:

- > cd \$RUNDIR
- > sbatch geogrid.reg

When done, check for the "Successful completion" string in the file geogrid.slurm.out. geogrid.log.nnnn (nnnn is the cpu number) files will also be created for tracking run failures or debugging.

## **UNGRIB**

UNGRIB unpacks GRIB1 or GRIB2 files that contain meteorological data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and writes specific fields in a WPS intermediate format.

- Input: namelist.wps and GRIB input data.
- Output: Several GFS\* files corresponding to the number of intervals (interval\_seconds) in simulation length (start/end dates).

#### Notes:

- The GRIB input is referenced in the run script, ungrib.reg: ./link\_grib.csh data/ungrib/gfs\*
- The UNGRIB output (GFS) is determined by the settings in the WPS namelist (namelist.wps).
- makes use of Vtables that list the fields and their GRIB codes that must be unpacked from the GRIB files.

#### To run:

- > cd \$RUNDIR
- > ./ungrib.reg

When done, check for "Successful completion" string in file ungrib\_logs/ungrib.log.



## **METGRID**

METGRID horizontally interpolates UNGRIB and SSTRSS output to the WRF domains, and combines them with the output from GEOGRID.

- Input: namelist.wps, geo\_em\*, NAM\*, and SSTRSS\* files.
- Output: Several met\_em\* files corresponding to the number of intervals (interval\_seconds) in simulation length (start/end dates).

### To run:

- > cd \$RUNDIR
- > sbatch metgrid.reg

When done, check for the "Successful completion" string in the file metgrid.slurm.out. metgrid.log.nnnn (nnnn is the cpu number) files also be created for tracking run failures or debugging.

### **REAL**

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input, met\_em\* files, geo\_em\* files.
- Output: wrfinput\* files (one for each domain), wrfbdy\_d01.

### To run:

- > cd \$RUNDIR
- > sbatch real.reg

Check real.slurm.out for run completion. If necessary check the real\_logs directory for real.rsl.out.nnnn and real.rsl.error.nnnn files.

## **GOCART2WRF**

GOCART2WRF extracts aerosol data from GEOS-5 netCDF4 GOCART files (or MERRA reanalysis aerosol data files); horizontally and vertically interpolates the fields to the WRF grid; and appends them to the initial and lateral boundary condition files of WRF (wrfinput\_d\* and wrfbdy\_d01). Users can choose GOCART aerosol data or MERRA reanalysis Aerosol data.

- Input: namelist.gocart2wrf, grib\_input/\*, wrfinput\* files (one for each domain), wrfbdy\_d01.
- Output: wrfinput\* files (one for each domain), wrfbdy\_d01. Original wrfinput\* and wrfbdy\_d01 files will be backed up with .gocart2wrf extension.

#### To run:

```
> cd $RUNDIR
>./gocart2wrf.reg # runs in serial
```

Check this file for successful run completion: gc2wrf.log.



## PREP\_CHEM\_SOURCES

This community tool processes several biogenic, anthropogenic, volcanic, and wildfire emissions. The NU-WRF version has several modifications that are discussed in the user's guide. Running prep\_chem\_sources requires a prep\_chem\_sources.inp file and upon completion, it produces map projection data (that can be visualized by plot\_chem) as well as other files used by convert\_emiss.

Input: prep\_chem\_sources.inp

Output: nuwrf-T\* files

### To run:

```
> cd $RUNDIR
```

> ./prep\_chem\_sources.reg # runs in serial

Check this file for successful run completion: pcs.log.

### Convert\_Emiss

This is a community WRF-Chem preprocessor that takes the output from PREP CHEM SOURCES and rewrites the fields in new netCDF files for reading by WRF-Chem.

- Input: namelist.input.convert\_emiss files (one for each domain).
- Output: wrfchemi\_gocart\_bg\* and wrfchemi\* files (one for each domain).

#### To run:

- > cd \$RUNDIR
- > sbatch convert\_emiss.reg

Check ce.slurm.out for run completion.

## WRF

If we get to this point then we are ready to run WRF with chemistry.

- Input: namelist.input, wrfinput\* files (one for each domain), wrfbdy\_d01, wrfchemi\_gocart\_bg\* and wrfchemi\* files.
- Output: wrfout\* files (one for each domain).

#### To run:

- > cd \$RUNDIR
- > sbatch wrf.reg

Check wrf.slurm.out for run completion. If necessary check the wrf\_logs directory for wrf.rsl.out.nnnn and wrf.rsl.error.nnnn files.

# Post-processing on Discover

### Using NCVIEW:

- > module load ncview
- > ncview <filename>

## Post-processing on Discover

### Using RIP (NCAR graphics). Submit the **rip** job:

> cd \$RUNDIR

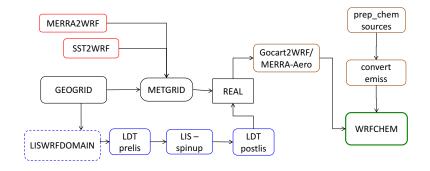
```
> ./rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename

rip.bash will run ripdp_wrfarw and rip to generate NCAR
    Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/
    scripts/rip and are looped through by rip.bash

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm
    for info on customizing plots with RIP.
Minor changes to rip.bash may be necessary.
```

The workflow just described can be modified to use MERRA/ MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS SST (Remote Sensing Sytems SST product) along with LIS land surface model initial conditions (see diagram on the next page). Just replace the UNGRIB step with the MERRA2WRF step and add the LDT-LIS-LDT steps before running REAL.

### Alternate NU-WRF chemistry workflow.



This NU-WRF-CHEM workflow uses MERRA/MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS SST (Remote Sensing Sytems SST product) along with LIS land surface model initial conditions, chemical tracers from prep\_chem\_sources and runs WRF-CHEM

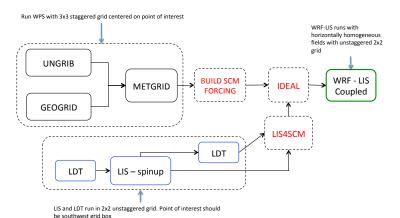
## **SCM Workflow**

The SCM workflow describes the steps necessary to setup and run WRF-LIS (like the default workflow) using a single point domain.

No chemistry is used.

### NU-WRF Single Column Model (SCM) workflow.

#### New WRF-LIS Single Column Model workflow



## Required files for SCM workflow

### Copy the following files to **RUNDIR**:

- > export RUNDIR=/discover/nobackup/<my\_user\_id>/scratch/
   scm\_workflow
- > cp -r \$PROJECTDIR/tutorial/scm\_workflow \$RUNDIR

#### Where:

 ${\tt common.reg}$  : shared script with settings used by other scripts.

# Required script changes

> cd \$RUNDIR

Use your favorite editor to edit **common.reg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

# \*\*\* Please make sure these settings are correct \*\*\*

##SBATCH --mail-user=user@nasa.gov

```
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
RUNDIR=<CHANGE THIS>
```

You may need to edit all the .reg files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:
#SBATCH --account s0942
Change if you want to change number of nodes, hasw - to run on haswell
#SBATCH --ntasks=16 --constraint=hasw
Uncomment and set according to your needs and privileges:
##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
```

# A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start\_date and end\_date
  - In namelist.input look for start\_ and end\_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end\_day - start\_day = run\_days.
- For any other changes please refer to the user's guide.

### **GEOGRID**

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For N domains (max\_dom in namelist.wps), N geo\_em files will be created.

#### To run GEOGRID:

- > cd \$RUNDIR
- > sbatch geogrid.reg

When done, check for "Successful completion" string in the file geogrid.slurm.out. geogrid.log file will also be created which can be used for tracking run failures or debugging.

## **UNGRIB**

UNGRIB reads GRIB or GRIB2 files with dynamic meteorological and dynamic terrestrial data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and writes specific fields in a WPS intermediate format.

- Input: namelist.wps, ungrib\_input/\* files.
- Output: NARR\* files.

**NOTE**: The GRIB input is referenced in the run script, run\_ungrib.bash:

 $./link\_grib.csh\ ungrib\_input/*$ 

The UNGRIB output (NARR) is determined by the settings in the WPS namelist (namelist.wps).

#### To run:

- > cd \$RUNDIR
- > ./ungrib.reg

When done, check for "Successful completion" string in the file ungrib.slurm.out. ungrib.log will also be created for tracking run failures or debugging.



## **METGRID**

METGRID horizontally interpolates the output from UNGRIB to the WRF domains, and combines it with the output from GEOGRID.

- Input: namelist.wps, NARR\* files, geo\_em\* files.
- Output: Several met\_em\* files corresponding to number of intervals (interval\_seconds) in simulation length (start/end dates).

### To run:

- > cd \$RUNDIR
- > sbatch metgrid.reg

When done, check for "Successful completion" string in the file metgrid.slurm.out. metgrid.log.nnnn (nnnn is the cpu number) files also be created for tracking run failures or debugging.

## BUILD\_SCM\_FORCING

BUILD\_SCM\_FORCING scripts use WPS output and generate column initial conditions profile\_init.txt and surface\_init.txt.

Note that this script depends on NCL and when on Discover one needs to load the *ncl* module.

- Input: WPS output, forcing\_file.cdl and several \*.ncl files.
- Output: profile\_init.txt, surface\_init.txt, and a directory, 2006-07-14\_00:00:00, containing forcing\_file.nc and input\_sounding data.

#### To run:

```
> cd $RUNDIR
```

Edit build\_scm\_forcing.bash: set metPath and forceArcRoot equal to RUNDIR value.

> ./build\_scm\_forcing.bash # runs in serial

After some other "messages" you should see "SUCCESS" printed on the terminal.



# LDT (pre-LIS)

LDT processes data inputs for different surface models. In this use-case we are using the Noah v3.6 land surface model.

- Input: Idt.config
- Output: lis\_input\* files for each NU-WRF domain.

#### To run:

```
> cd $RUNDIR
> sbatch ldt_prelis.reg
```

When done, check for "Finished LDT run" string in the file ldt\_log\_prelis.0000

### LIS

LIS can be run from a cold start or from a restart. A cold start run is usually a multi-year simulation, not appropriate for a tutorial - though one can concoct a short spin up run for demo purposes. In the restart case we have to provide restart files as input (LIS\_RST\* files) and the LIS run can be significantly shorter. Nevertheless, the restart (and history) files have already been generated for this tutorial and the user can **skip** this step. If you want to run a LIS spin up for this case you may look at the default workflow and use those scripts and config files as a template.

# LDT (post-LIS)

After running LIS, it is necessary to rerun LDT in "NUWRF preprocessing for real" mode. This requires modifications to ldt.config to specify the static output file from LDT and the dynamic output file from LIS. Fields from both will be combined and written to a new netCDF output file for use by REAL

- Input: Idt.config
- Output: lis4real\_input\* files for each NU-WRF domain.

### To run:

- > cd \$RUNDIR
- > sbatch ldt\_postlis.reg

When done, check for "Finished LDT run" string in the file ldt\_log\_postlis.0000

## LIS4SCM

LIS4SCM copies data from southwest grid point to remainder of LIS/LDT domain (becomes horizontally homogenous): LIS4SCM imposes identical lat/lon at each LIS point in the restart file.

- Input: namelist.lis4scm, LDT-LIS-LDT output
- Output: Horizontally homogeneous lis\_input file (lis\_input.d01.nc)

### To run:

- > cd \$RUNDIR
- > ./lis4scm.reg # Note this runs in serial

## **IDEAL**

IDEAL creates wrfinput file from text column data and homogeneous LIS/LDT file.

• Input: LIS4SCM output

Output: wrfinput file (wrfinput\_d01).

### To run:

- > cd \$RUNDIR
- > sbatch ideal.reg

## WRF-LIS

WRF-LIS reads wrfinput and the homogenous LIS restart file.

- Input: wrfinput file
- Output: wrfoutput file.

#### To run:

- > cd \$RUNDIR
- > sbatch wrf.reg

#### Notes:

- Tested case uses periodic LBCs (thus, no wrfbdy file).
- Tested case also used no forcing (no external advection, etc).
- Tested case used dx = 1 km, dt = 6 sec (runs very fast!)

# Post-processing on Discover

### Using NCVIEW:

- > module load ncview
- > ncview <filename>

## Post-processing on Discover

### Using RIP (NCAR graphics). Submit the **rip** job:

```
> cd $RUNDIR
> ./rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename
rip.bash will run ripdp_wrfarw and rip to generate NCAR
   Graphics cqm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/
   scripts/rip and are looped through by rip.bash
See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm
   for info on customizing plots with RIP.
Minor changes to rip.bash may be necessary.
```

Regression testing

### **Definition**

### From Wikipedia:

Regression testing is a type of software testing that verifies software previously developed and tested still performs correct even after it was changed or interfaced with other software. Changes may include software enhancements, patches, configuration changes, etc. During regression testing, new software bugs or regressions may be uncovered.

# Testing types

Software testing can be roughly divided into three categories:

- Automated regression tests. These tests compile and run a very large number of model configurations and may perform various checks.
- Manual/user testing. These tests are intended to be performed by users that wish to verify their changes prior to pushing to a central repository. In detail, these tests are similar to automated tests but are more easily executed from the command line.
- Unit tests. These tests execute extremely quickly and provide a finer-grained verification than the other regression tests, albeit with far less coverage of the source code. Unit tests do not form part of the NU-WRF code base at this time.

In this section, we discuss the available NU-WRF regression testing infrastructure and how it can be used to perform automated and manual tests.

# NU-WRF regression testing scripts

The NU-WRF regression scripts are a set of python scripts and configuration files designed to run tests on the NU-WRF code base. The scripts' functionality is all driven by the settings specified in a single configuration file.

The configuration file is a text file with a particular structure readable by the python scripts and easily understood by humans too! The files are organized into sections, and each section contains name-value pairs for configuration data.

# NU-WRF regression testing scripts

There is one configuration file required by the scripts - specified as a command line argument. The file can have any name but must have the '.cfg' extension. A sample configuration file (sample.cfg) is included \$NUWRFDIR/scripts/python/regression that can be modified and used for "personalized" testing.

### Note:

There are three additional files that are used specifically for NU-WRF testing: master.cfg, develop.cfg and comp.cfg. These files should not be modified or used for anything other than as a reference to build your own customized configuration.

### Workflows revisited

In this document, we have discussed 4 workflows: basic, default, chemistry and scm. For the purposes of regression testing workflows are categorized as follows:

```
wrf: default WRF-ARW runs (without LIS) (basic)
wrflis: like wrf but with LIS-coupling (default and scm)
chem: like wrf with chemistry (chemistry)
kpp: like wrf with chemistry - uses KPP
```

This distinction is necessary to specify test cases in the configuration file. For a list of all supported NU-WRF configurations see:

\$NUWRFDIR/scripts/python/regression/master.cfg

# Python scripts

The python scripts are the following:

- reg : Main driver.
- RegPool.py: A class with functionality to parallelize tasks.
- regression.py: A driver script to execute the NU-WRF component tasks.
- RegRuns.py: A class that defines regression test run instances.
- RegTest.py: A class that defines regression test instances.
- reg\_tools.py: Various tools used by the main drivers.
- shared/utils.py : Various utilities used by all the scripts.

The scripts can be used to perform both automated regression tests as well as "manual testing".

# Manual testing

Before running the regression testing scripts make sure you duplicate the sample.cfg file and customize it to your needs. When ready to run the scripts, specify the configuration file name as an argument to reg and wait for the results:

```
$ cd $NUWRFDIR/scripts/python/regression
```

```
$ reg <cfg_file> &
```

Note that the configuration file name extension should not be specified.

## Manual testing

Upon execution, you will see some messages echoed to STDOUT but all the output will be logged to a file named <cfq\_file>.LOG.

There will be other "log" files, one for each <workflow> and one for each <experiment>, that will be generated for each 'reg' run.

Workflow builds, a maximum of four, will be generated in <scratch\_dir>/builds

Each build will have its own make.log as well as <workflow>.ou and <workflow>.err files that will be useful to diagnose build /run errors.

# Manual testing

Run logs will be generated in each run directory under <scratch dir>/results.

These will have the name <experiment>-regression.log and should also be very useful to diagnose test-case-specific run-time issues.

At the end of a "reg" an email test report will be emailed to the recipient specified in the mail\_to field in USERCONFIG.

Note that all 'reg' runs are tagged with a unique time stamp corresponding to the date/time the run was executed.

# Manual testing within interactive queue

One can run NU-WRF test cases interactively. To do so make sure you set use\_batch=no in your configuration file. Also, if running interactively, one can only use one compiler option; i.e. in the 'compilers' setting you can only use intel-sgimpt or gnu-openmpi. With those caveats in mind: Request an interactive queue on DISCOVER, for example:

```
> salloc --ntasks=84 --time=1:00:00 --account=s0492 --
constraint=cas
```

### Once you get the prompt

```
$ cd $NUWRFDIR/scripts/python/regression
$ reg <cfg_file> &
```

Note that the extension should not be specified.



As you may have figured out, all the workflows described earlier in this tutorial can be recreated with the appropriate configuration file and the testing scripts.

For more information about regression testing or any workflow described in this tutorial please feel free to contact the NU-WRF software integration group.