NU-WRF
NASA Unified Weather Research and Forecasting Model
Tutorial

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For NUWRF Version 7 Patch 4

NU-WRF userguide: https://nuwrf.gsfc.nasa.gov/sites/default/files/users/nuwrf_userguide.pdf
NU-WRF website: https://nuwrf.gsfc.nasa.gov

Purpose

- Walks through the process of downloading, compiling, and running NUWRF for three different workflows:
  - Simple: Based on WRF ARW
  - Default: The recommended non-chemistry NUWRF workflow
  - Chemistry: The recommended chemistry (non-LIS) NUWRF workflow
- Assumes users are running on Discover or Pleiades
  - Examples focus on Discover, changes for Pleiades summarized in handful of slides

Useful Links

- Community ARW User Guide:
  - http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3.5/contents.html
  - Includes detailed information on input file settings and data
- Community WRF ARW Online Tutorial:
  - http://www2.mmm.ucar.edu/wrf/OnLineTutorial/index.htm
  - More detailed information on configuring for different domains
- NOTE: The details for building the software on Discover and Pleiades are automatically handled by NUWRF's build scripts!

- Documentation for using Discover and other NCCS systems: http://www.nccs.nasa.gov/primer/
- Documentation for using Pleiades and other NAS systems: http://www.nas.nasa.gov/hecc/support/kb/161/

Special Notes About Discover

On Discover, you must choose between nodes running SLES11 SP3 and SLES11 SP1 operating systems

- SP3 will eventually become standard, but normal “discover” login nodes still run SP1 (as of late August 2015)
- The same operating system should be used to compile and to run your programs!
- In this tutorial, we assume you will run on SP3 since this lets you use the fastest computer nodes (with Haswell chips)

These issues don’t exist on Pleiades!

Download the code

Tar files are available to NCCS and NAS s0942 group members.

On Discover:

- /discover/nobackup/projects/nu-wrf/releases/stable/nu-wrf_v7lis7-3.5.1-p4.tar.bz2
- /discover/nobackup/projects/nu-wrf/releases/stable/nu-wrf_v7lis7-3.5.1-p4.tgz

On Pleiades:

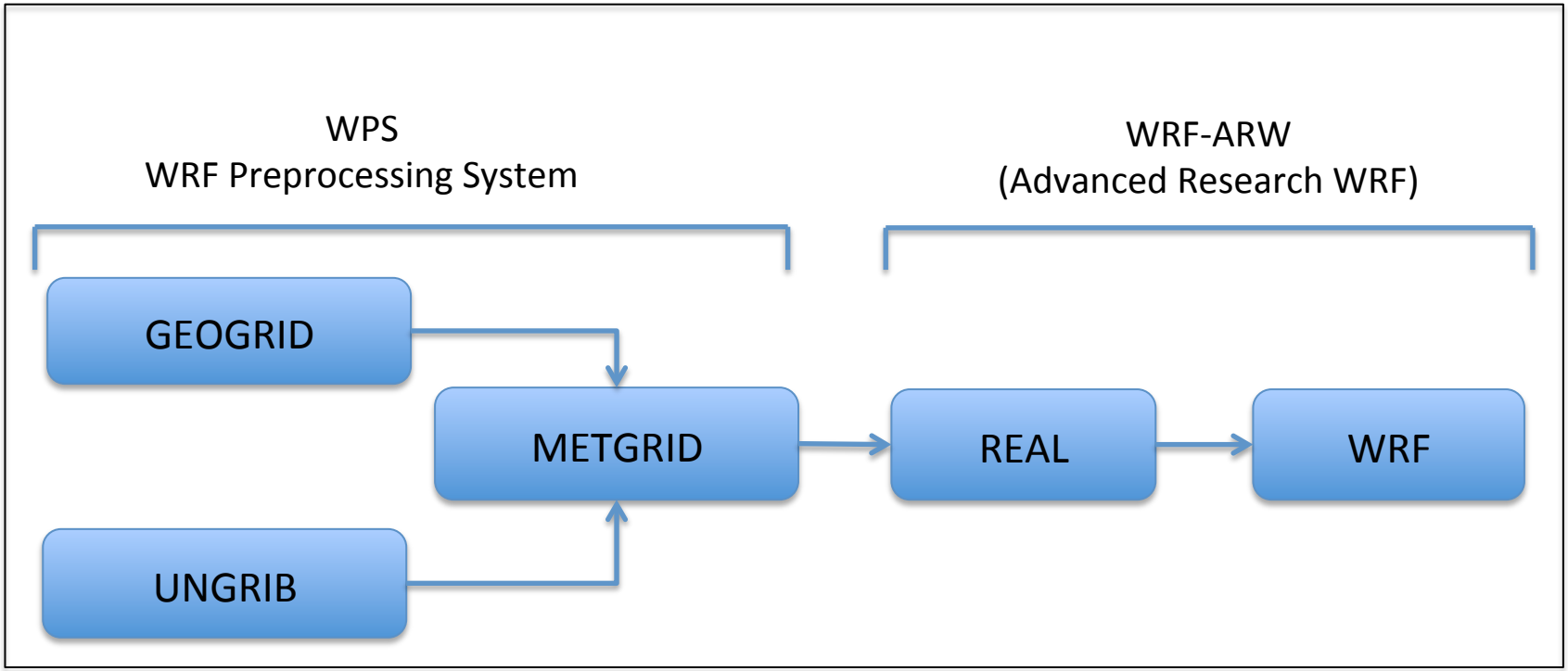
- /nobackupp8/nuwrf/releases/stable/nu-wrf_v7lis7-3.5.1-p4.tar.bz2
- /nobackupp8/nuwrf/releases/stable/nu-wrf_v7lis7-3.5.1-p4.tgz
- To untar the tar ball: >tar –xvz nu-wrf_v7lis7-3.5.1-p4.tgz

Developers can also check out code from SVN:

- svn co svn+ssh://progressdirect/svn/nu-wrf/code/tags/stable/v7lis7-3.5.1-p4
- svn co svn+ssh://progress.nccs.nasa.gov/svn/nu-wrf/code/tags/stable/v7lis7-3.5.1-p4
- See https://modelingguru.nasa.gov/docs/DOC-1834#Using_the_Source_Repository for instructions on setting up SVN access

TUTORIAL 1: SIMPLE WORKFLOW

NU-WRF simple workflow (Similar to WRF ARW)



How to run NU-WRF simple workflow

- Compile
- Model setup on Discover
- Run components on Discover
- Post processing on Discover
- Adjustments for Pleiades

Compile NU-WRF

Discover: Login to "discover", and then ssh –YC discover-sp3 (for nodes running SP3)

Pleiades: Login to a Pleiades front end node

cd /path/to/your/v7lis7-3.5.1-p4 (we'll call this NUWRFDIR)

./build.sh wps wrf rip >& log.out & (Compiles WPS, WRF and RIP with default config file, runs in background, saves output in log.out; other cfg files exist for SP1 and other MPI implementations; specify --config filename.cfg to use)

Or

./build.sh all >& log.out & (Compiles WRF and all pre and post processors with default config file, runs in background, save output in log.out)

When '--config' flag is not used, build.sh will load discover.cfg or pleiades.cfg by default.

Default MPI implementation on Discover is Intel MPI; on Pleiades it is SGI MPT

Compile NU-WRF

Where are the executables?

Key WPS executables

$NUWRFDIR/WPS/geogrid.exe
$NUWRFDIR/WPS/metgrid.exe
$NUWRFDIR/WPS/ungrib.exe

Key WRF executables

$NUWRFDIR/WRFV3/main/real.exe
$NUWRFDIR/WRFV3/main/wrf.exe

Key RIP4 executables

$NUWRFDIR/RIP4/ripdp_wrfarw
$NUWRFDIR/RIP4/rip

Model setup on Discover

NUWRFDIR: /path/to/your/v7lis7-3.5.1-p4/

Select a directory for running the model. Call this $RUNDIR.

Note: It is preferable to create the RUNDIR outside of NUWRFDIR. This is useful when switching between NU-WRF versions or for updating to new changes.

In CSH shell, you can define environment variable using:

```
>setenv NUWRFDIR /path/to/your/v7lis7-3.5.1-p4/
>setenv RUNDIR /path/to/your/RUNDIR
```

In BASH environment, you can define environment variable using:

```
>export NUWRFDIR = /path/to/your/v7lis7-3.5.1-p4/
>export RUNDIR = /path/to/your/RUNDIR
```

Model setup on Discover

Configuration files, run scripts, input files needed to run the basic WRF case with NU-WRF is also provided in the directory:

/discover/nobackup/projects/nu-wrf/tutorial/7p4/WRF-basic/

```
>set WRF_basic = /discover/nobackup/projects/nu-wrf/tutorial/7p4/WRF-basic/ # Assumes csh
```

Copy the following shell scripts to your $RUNDIR:

```
>cp $NUWRFDIR/scripts/discover/config.discover.sh $RUNDIR/.
>cp $NUWRFDIR/scripts/discover/run*.sh $RUNDIR/.
>cp $NUWRFDIR/defaults/namelist.wps $RUNDIR/.
>cp $NUWRFDIR/defaults/namelist.input $RUNDIR/.
```

Or user can copy all the files from the $WRF_basic directory.

Copy the GRIB atmospheric data for initial conditions from $WRF_basic/grib_input/ to $RUNDIR

```
cp $WRF_basic/grib_data/fnl* $RUNDIR/.
```

Model setup on Discover

The batch job scripts use a common config file to store paths and other information.

Edit config.discover.sh to set the following:

module load compiler_mod mpi_mod # Set to match modules in build cfg file.
NUWRFDIR=/path/to/your/NUWRFDIR
WORKDIR=/path/to/your/RUNDIR
NCAR_ROOT=/path/to/NCAR/Graphics/used/in/build/config/file

Batch script general changes:

Edit all the runscripts (run* files) for account information changes:
#SBATCH --account s0942
(Change s0942 to appropriate SBU charge code)
#SBATCH --ntasks=16 --constraint=hasw
(Change if you want to change number of nodes, hasw – to run on haswell nodes)
##SBATCH --qos=high (Uncomment, set according to your needs and privileges)
#Substitute your e-mail here
##SBATCH --mail-user=user@nasa.gov (User must partially uncomment lines involving e-mails, remove first #, provide valid e-mail address)

Run components on Discover -- GEOGRID

>cd $RUNDIR

- User should edit run script run_geogrid.discover.sh to change the links to GEOGRID.TBL depend on the run. Note: There are multiple GEOGRID.TBL files to support different dynamical cores and options in WRF. GEOGRID.TBL.ARW is used for non-chemistry NUWRF runs.
- A sample namelist.wps file is available in the directory: $NUWRFDIR/defaults/namelist.wps. Copy this file to your $RUNDIR and make changes in namelist.wps if you need domain changes. User can refer to ARW online tutorial / web for more details on namelist.wps options: http://www2.mmm.ucar.edu/wrf/users/tutorial/201501/WPS_RUN.pdf
- Make sure that you have access to the directory: '/discover/nobackup/projects/nu-wrf/cases/geog'

Submit the job with this command:

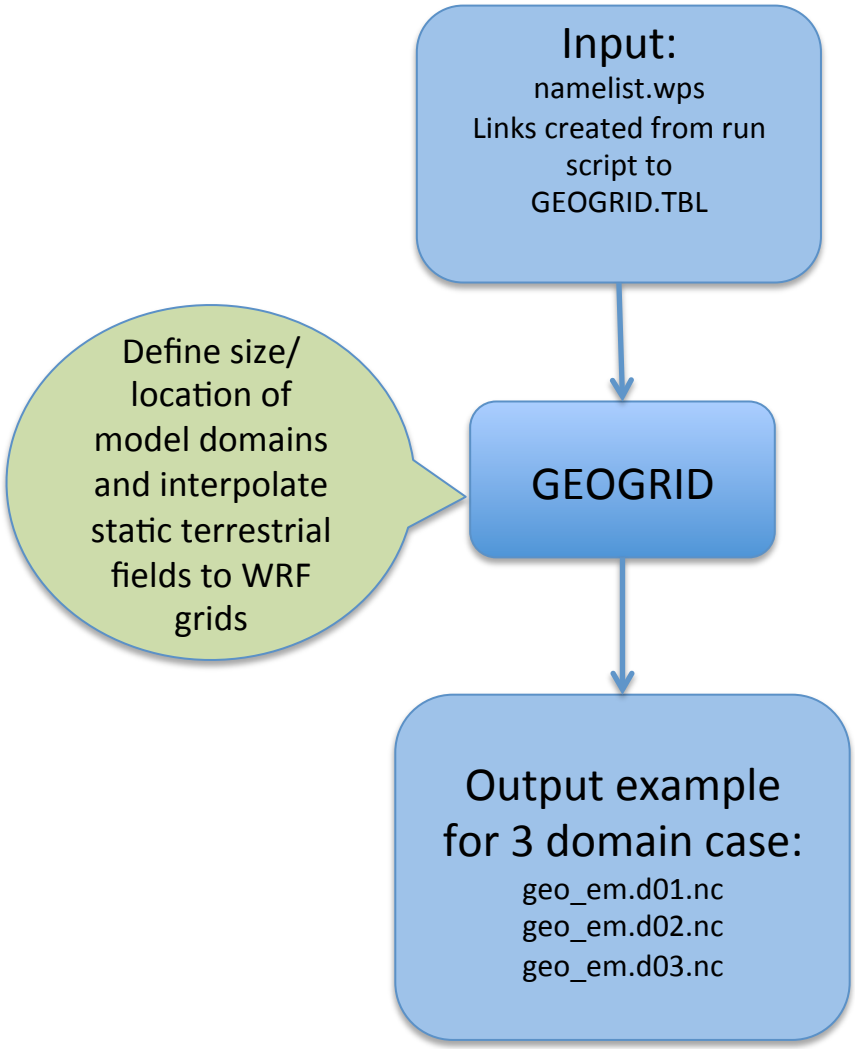
>qsub run_geogrid.discover.sh

Or

>sbatch run_geogrid.discover.sh

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

geogrid.log.<node> will also be created for tracking run failures/ debugging.



Run components on Discover -- UNGRIB

>cd RUNDIR

Copy the ungrib files to your RUNDIR, example:

>cp $WRF_basic/fnl* $RUNDIR/.

Make sure you have namelist.wps file in your $RUNDIR.

Edit run script run_ungrib.discover.sh

- User should change the link to **Vtable** to the correct Vtable files for a specific run depend on what input files are used. Some Vtables are provided with WPS in the $NUWRFDIR/**WPS/ungrib/Variable_Tables** directory- E.g., Vtable.GFS, Vtable.SST, Vtable.ECMWF

ln -fs $NUWRFDIR/WPS/ungrib/Variable_Tables/Vtable.GFS Vtable

- User should edit the GRIB file prefix . Example:

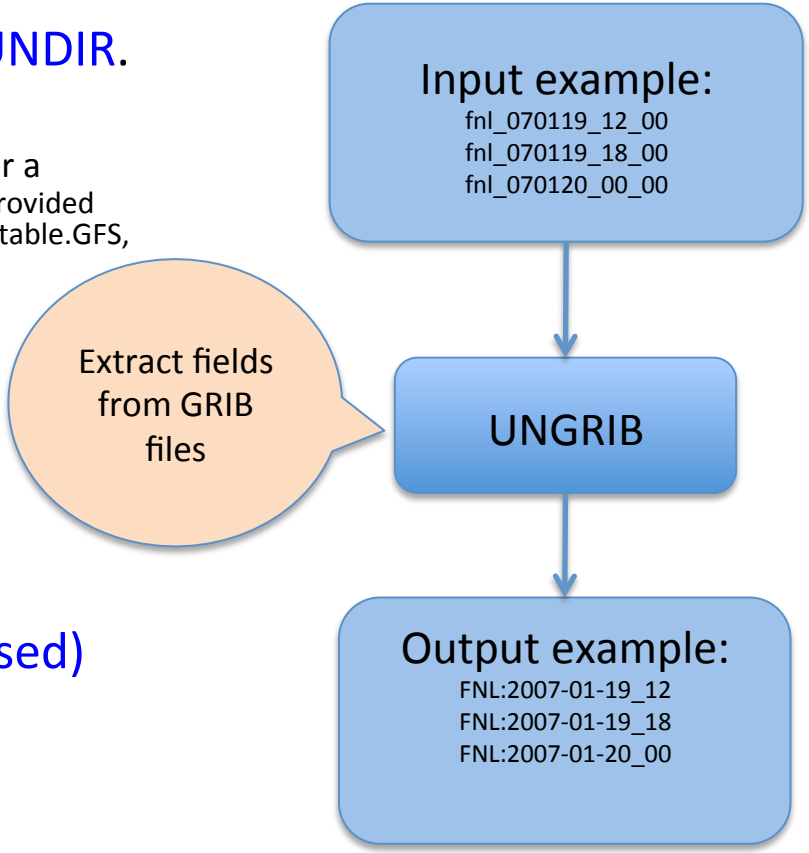
./link_grib.csh fnl.* || exit 1

Submit the job with this command:

>qsub run_ungrib.discover.sh (or sbatch can be used)

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

ungrib.log will also be created for tracking run failures/ debugging.



Run components on Discover -- METGRID

>cd RUNDIR

Edit run script run_metgrid.discover.sh

- User should change the link to METGRID.TBL. There are multiple METGRID.TBL files to support multiple dynamical cores in WRF. For NUWRF, use METGRID.TBL.ARW

```
ln -fs $NUWRFDIR/WPS/metgrid/METGRID.TBL.ARW metgrid/METGRID.TBL
```

Make sure you have namelist.wps file in your $RUNDIR.

- Metgrid block in the namelist.wps file will look like this.

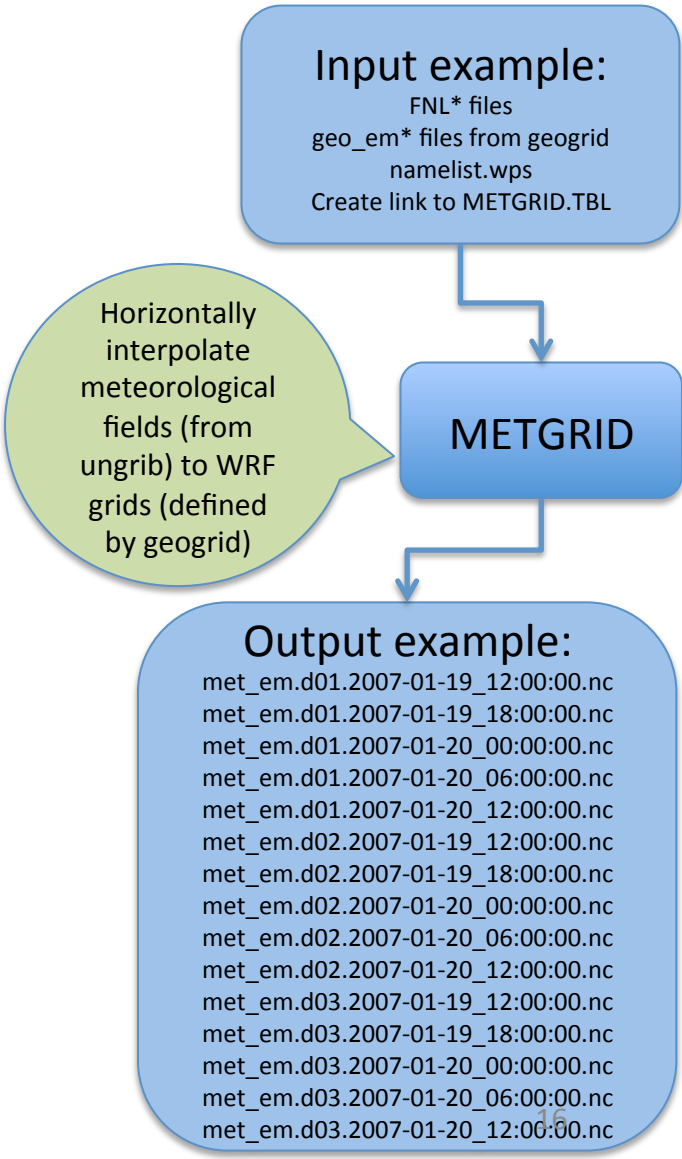
```
&metgrid
 fg_name = 'FNL',
 io_form_metgrid = 2,
/
```

Submit the job with this command:

>qsub run_metgrid.discover.sh (or sbatch can be used)

Check this file for run completion: metgrid.slurm.out

metgrid.log.<node> also will also be created for debugging purposes.



Run components on Discover -- REAL

>cd $RUNDIR

Edit run script run_real.discover.sh

Make sure you have namelist.input file in your $RUNDIR. A sample namelist.input file is available in

$NUWRFDIR/defaults/namelist.input.

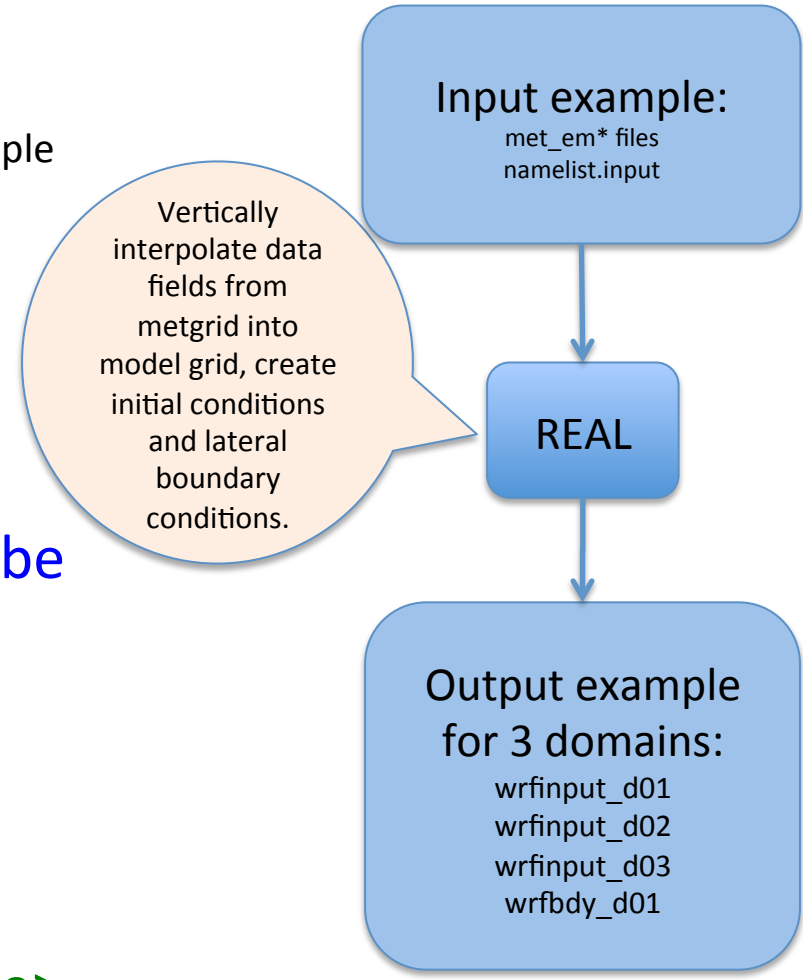
Or in $WRF_basic/namelist.input

Submit the job with this command:

>qsub run_real.discover.sh (or sbatch can be used)

Check this file for run completion:
real.slurm.out

real.rsl.out.<node> and real.rsl.error.<node> also will also be created.



Run components on Discover -- WRF

>cd RUNDIR

Edit run script run_wrf.discover.sh

The runscripts will create links for

LS_PARAMETERS

MET_FORCING and many other input files.

Edit namelist.input file if the user need any option changes.

Refer userguide for namelist.input options for different workflows.

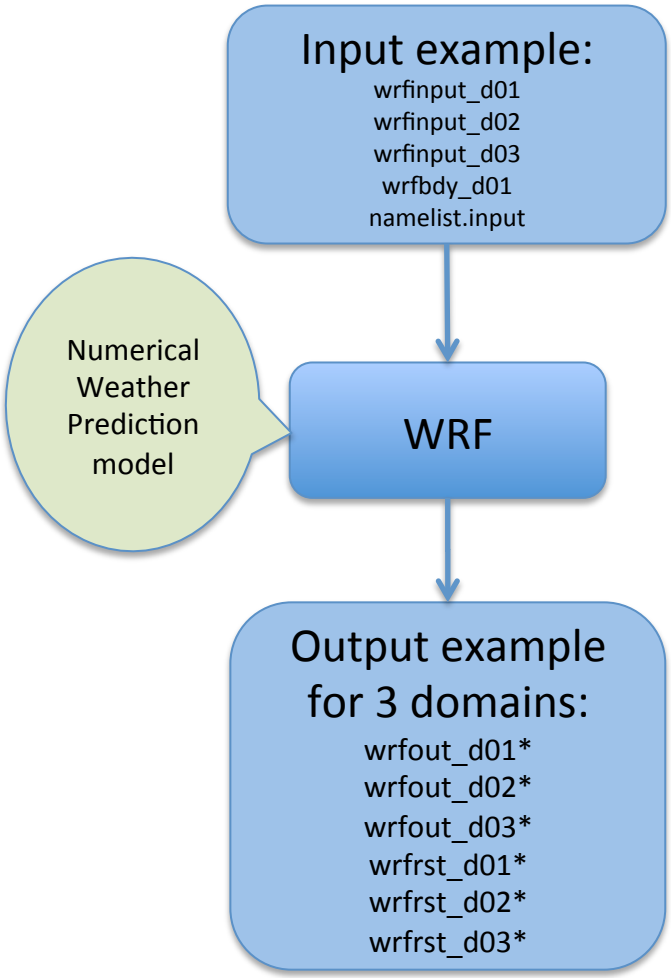
Sample namelist.input is available in NUWRFDIR/defaults/ directory.

Submit the job with this command:

>qsub run_wrf.discover.sh (or sbatch can be used)

Check this file for run completion: wrf.slurm.out

wrf.rsl.out.<node> and wrf.rsl.error.<node> also will also be created.



Post Processing on Discover

- NCVIEW

WRF output files (NETCDF4) can be viewed using a special version of ncview.

On discover:

```
>/usr/local/other/SLES11/ncview/2.1.1/bin/ncview filename
```

- RIP (NCAR Graphics)

```
>qsub run_rip.discover.sh # (or use sbatch)
>idt filename.cgm # Substitute actual filename
```

run_rip.discover.sh 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 run_rip.discover.sh

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on customizing plots with RIP. Minor changes to run_rip.discover.sh 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, see http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3.5/users_guide_chap9.htm

And ARW User homepage: http://www2.mmm.ucar.edu/wrf/users/

Can also use GSDSU (simulates satellite data)

Adjustments for Pleiades

- Use alternative batch scripts:

>cp $NUWRFDIR/scripts/pleiades/config.pleiades.sh $RUNDIR/.

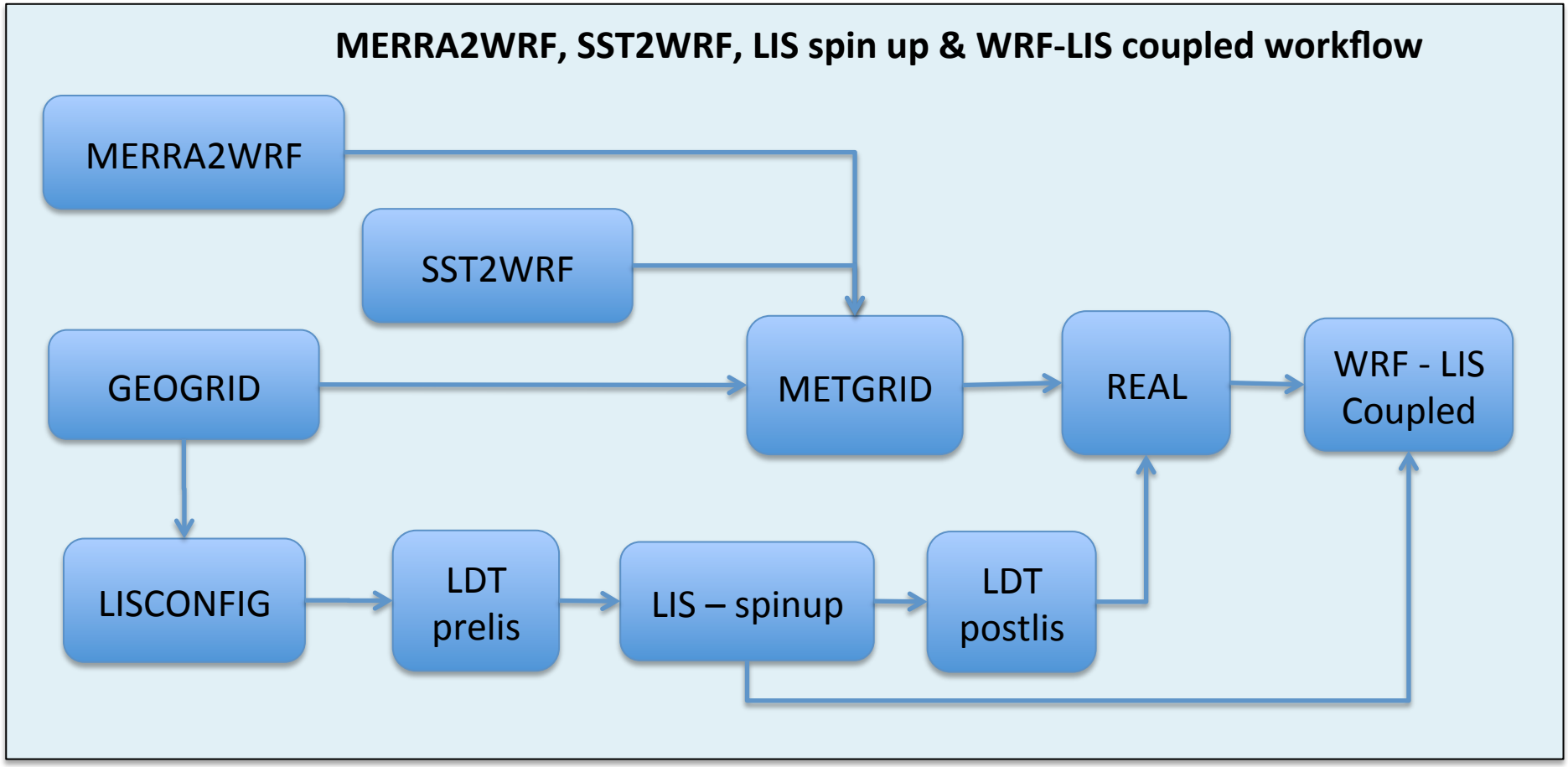
>cp $NUWRFDIR/scripts/pleiades/run*.sh $RUNDIR/.

Edit all the runscripts (run* files) for account information changes:
#PBS -W group_list=s0942
(Change s0942 to appropriate SBU charge code)
#PBS -l select=6:ncpus=16:mpiprocs=16:model=san
(Change if you want to change number of nodes, processes per node. san – To run on Sandy Bridge nodes, has for Haswell nodes)
##PBS -q devel (Uncomment, set according to your needs and privileges)
#Substitute your e-mail here
##PBS -M=user@nasa.gov (User must partially uncomment lines involving e-mails, remove first #, provide valid e-mail address)

- Check names of batch scripts when running components (e.g., use run_wrf.pleiades.sh instead of run_wrf.discover.sh)
- On Pleiades, must use qsub to submit jobs (sbatch not installed)

TUTORIAL 2: NUWRF DEFAULT WORKFLOW

NU-WRF Default Workflow



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

How to run NU-WRF Default workflow

- Compile
- Model setup on Discover
- Run components on Discover
- Post processing on Discover
- Adjustments for Pleiades

Compile NU-WRF

Similar to compile steps for simple workflow, but we need to compile more components

./build.sh wps lisconfig ldt lis merra2wrf sst2wrf wrf rip >& log.out &
(Add LISCONFIG, LDT, LIS, MERRA2WRF, SST2WRF to compilation list)

Or

./build.sh all >& log.out & (Compiles WRF and all pre and post processors with default config file, runs in background, save output in log.out)

Compile NU-WRF

Where are the executables?

Key WPS executables

$NUWRFDIR/WPS/geogrid.exe
$NUWRFDIR/WPS/metgrid.exe
$NUWRFDIR/WPS/ungrib.exe

Key MERRA2WRF executables

$NUWRFDIR/utils/geos2wrf_2/bin/merra2wrf

Key WRF executables

$NUWRFDIR/WRFV3/main/real.exe
$NUWRFDIR/WRFV3/main/wrf.exe
$NUWRFDIR/WRFV3/lis/make/LIS

Key LISCONFIG executables

$NUWRFDIR/utils/lisconfig/bin/lisWrfDomain

Key LDT executables

$NUWRFDIR/LDT/make/LDT

Key SST2WRF executables

$NUWRFDIR/utils/sst2wrf/bin/sst2wrf

Key RIP4 executables

$NUWRFDIR/RIP4/ripdp_wrfarw
$NUWRFDIR/RIP4/rip

Model setup on Discover

Similar to simple workflow, but additional input files needed.

Run scripts, configuration files and input files specific for this tutorial are available in the directory:

```
>set WRF_LIS_DIR = /discover/nobackup/projects/nu-wrf/tutorial/7p4/WRF-LIS/
```

Sample files are also in the directory: $NUWRFDIR/defaults/

Copy the following files from $WRF_LIS_DIR to your $RUNDIR:

```
>cp $WRF_LIS_DIR/namelist.wps $RUNDIR/.
>cp $WRF_LIS_DIR/namelist.input* $RUNDIR/.
>cp $WRF_LIS_DIR/lis.config* $RUNDIR/.
>cp $WRF_LIS_DIR/ldt.config* $RUNDIR/.
>cp $WRF_LIS_DIR/forcing_variables*.txt $RUNDIR/.
>cp $WRF_LIS_DIR/NOAH33_OUTPUT_LIST*.TBL $RUNDIR/.
```

Model setup on Discover

- When editing config.discover.sh, make sure to also set LISDIR:

LISDIR=/discover/nobackup/projects/lis

And make sure your user account has read access to this directory!

Run components on Discover -- GEOGRID

>cd $RUNDIR

- User should edit run script run_geogrid.discover.sh to change the links to GEOGRID.TBL depend on the run. Note: There are multiple GEOGRID.TBL files to support different dynamical cores and options in WRF. GEOGRID.TBL.ARW is used for non-chemistry NUWRF runs.
- A sample namelist.wps file is available in the directory: $NUWRFDIR/defaults/namelist.wps. Copy this file to your $RUNDIR and make changes in namelist.wps if you need domain changes. User can refer to ARW online tutorial / web for more details on namelist.wps options: http://www2.mmm.ucar.edu/wrf/users/tutorial/201501/WPS_RUN.pdf
- Make sure that you have access to the directory: '/discover/nobackup/projects/nu-wrf/cases/geog'

Submit the job with this command:

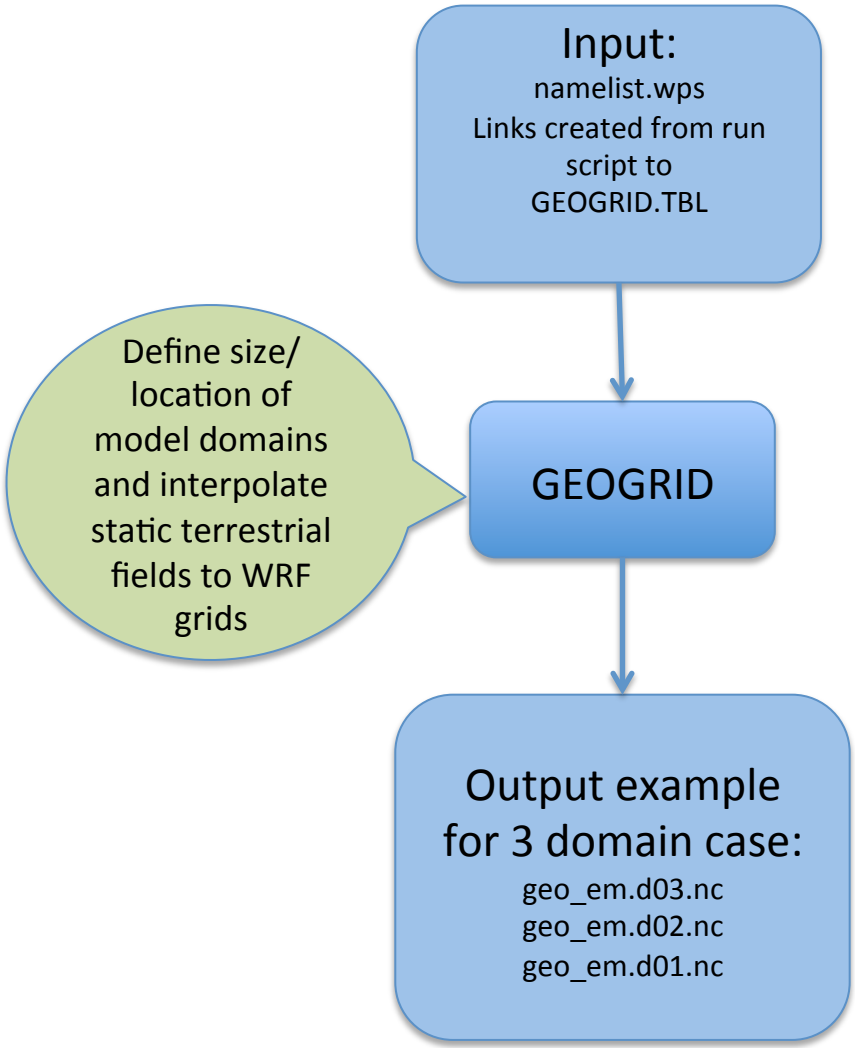
>qsub run_geogrid.discover.sh

Or

>sbatch run_geogrid.discover.sh

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

geogrid.log.<node> will also be created for tracking run failures/ debugging.



SAME AS FOR SIMPLE WORKFLOW

Run components on Discover -- MERRA2WRF

>cd $RUNDIR

Case 1 - MERRA reanalysis for WRF initial and lateral boundary conditions:

>cp $NUWRFDIR/utils/geos2wrf_2/RUN_MERRA/Run_MERRA.csh $RUNDIR/.

For example for start date = 20070119 and end date = 20070120

>./Run_MERRA.csh 20070119 20070120 . $NUWRFDIR

(This program will ftp MERRA data from the website ftp://goldsmr2.sci.gsfc.nasa.gov/data/s4pa//MERRA_MONTHLY/)

Sample input and output files are given in $WRF_LIS_DIR/MERRA/

cp $RUNDIR/data/merra2wrf/MERRA* .

Case 2 - MERRA2 reanalysis for WRF initial and lateral boundary conditions:

>cp $NUWRFDIR/utils/geos2wrf-2/RUN_MERRA2/Run_MERRA2.csh $RUNDIR/.

For example for start date = 20070119 and end date = 20070120

>./Run_MERRA2.csh 20070119 20070120 . $NUWRFDIR

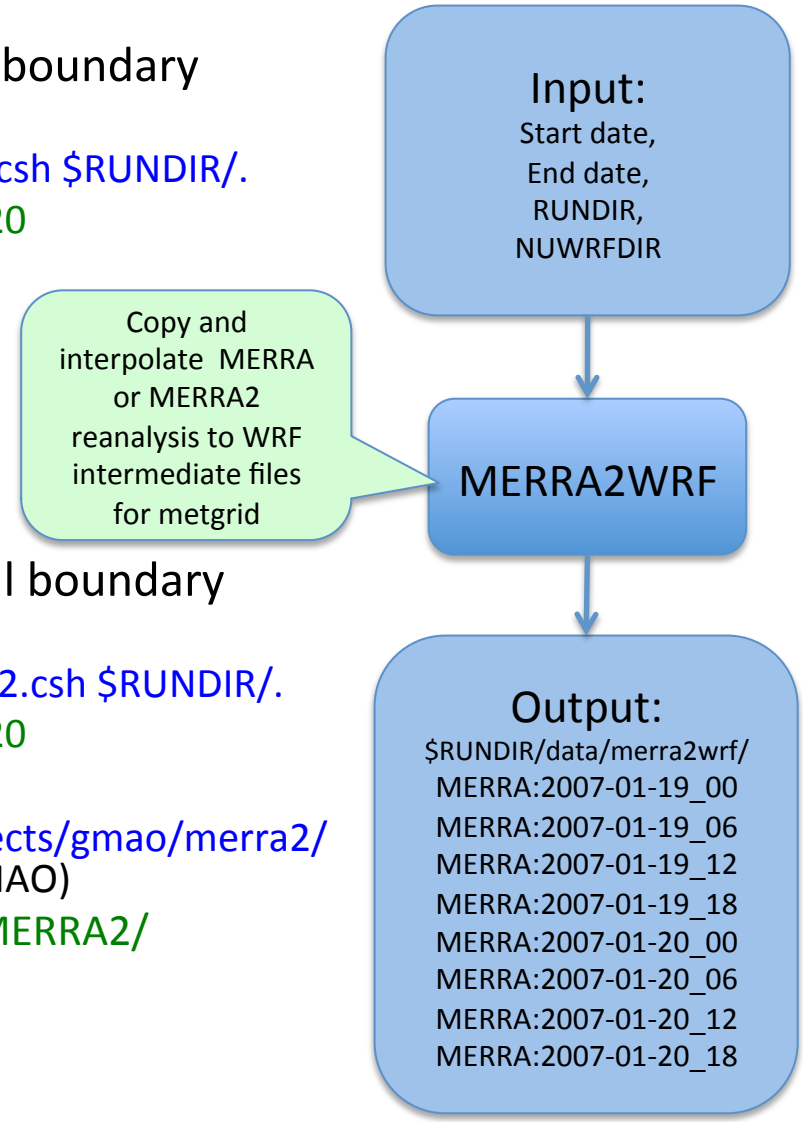
(MERRA2 data is staged on discover: /discover/nobackup/projects/gmao/merra2/merra2/scratch/ and requires special read permission from GMAO)

Sample input and output files are given in $WRF_LIS_DIR/MERRA2/

Copy the MERRA2WRF output to the $RUNDIR

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

NEW WORKFLOW STEP



Run components on Discover -- SST2WRF

```
>cd $RUNDIR
>mkdir $RUNDIR/RUN_SST2WRF
>cd $RUNDIR/RUN_SST2WRF
>cp $NUWRFDIR/utils/sst2wrf/scripts/Run_SST.csh $RUNDIR/RUN_SST2WRF/.
```

For a start date = 20070119 and end date of 20070120:

```
>./Run_SST.csh 20070119 20070120 mw_ir . $NUWRFDIR
```

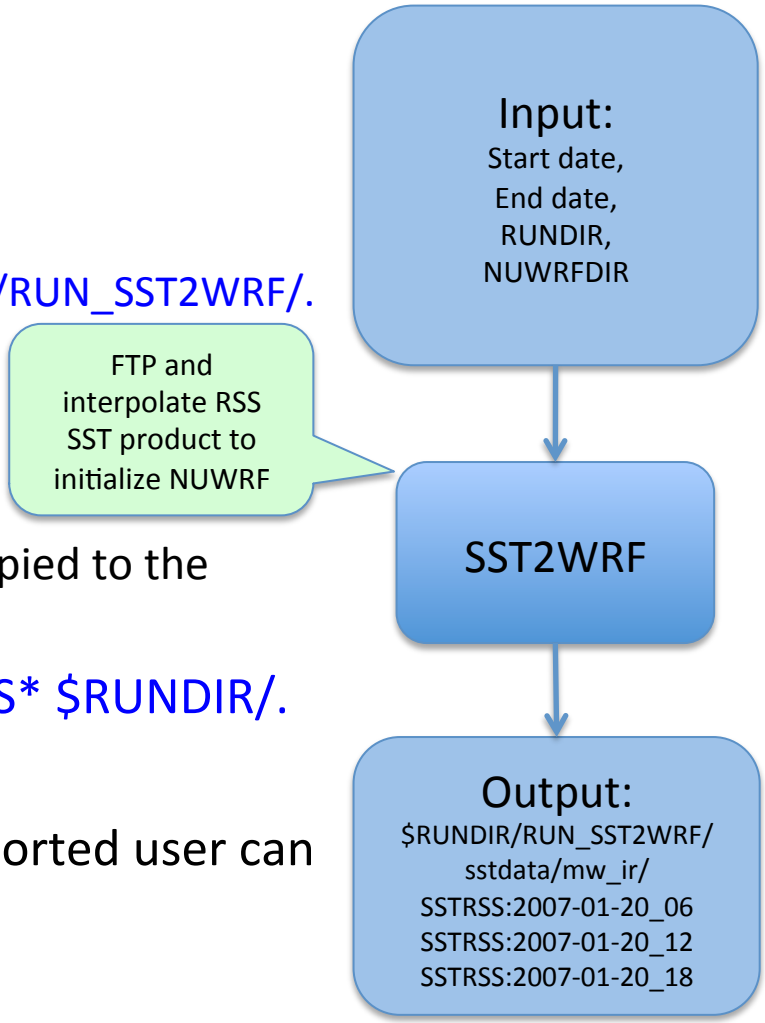
SSTRSS:* files will be created, and these files should be copied to the RUNDIR before running METGRID component.

```
>cp $RUNDIR/RUN_SST2WRF/sstdata/mw_ir/SSTRSS* $RUNDIR/.
```

For more details on the options and data types supported user can refer to NU-WRF userguide section 5.8

Sample input and output files are given in $WRF_LIS_DIR/sst2wrf/

NEW WORKFLOW STEP



Run components on Discover -- METGRID

>cd RUNDIR

Edit run script run_metgrid.discover.sh

- User should change the link to METGRID.TBL. There are multiple METGRID.TBL files to support multiple dynamical cores in WRF. For NUWRF, use METGRID.TBL.ARW

ln -fs $NUWRFDIR/WPS/metgrid/METGRID.TBL.ARW metgrid/METGRID.TBL

Make sure you have namelist.wps file in your $RUNDIR.

- Metgrid block in the namelist.wps would look like this to utilize MERRA and SSTRSS data.

```
&metgrid
 fg_name = 'MERRA', 'SSTRSS',
 io_form_metgrid = 2,
/
```

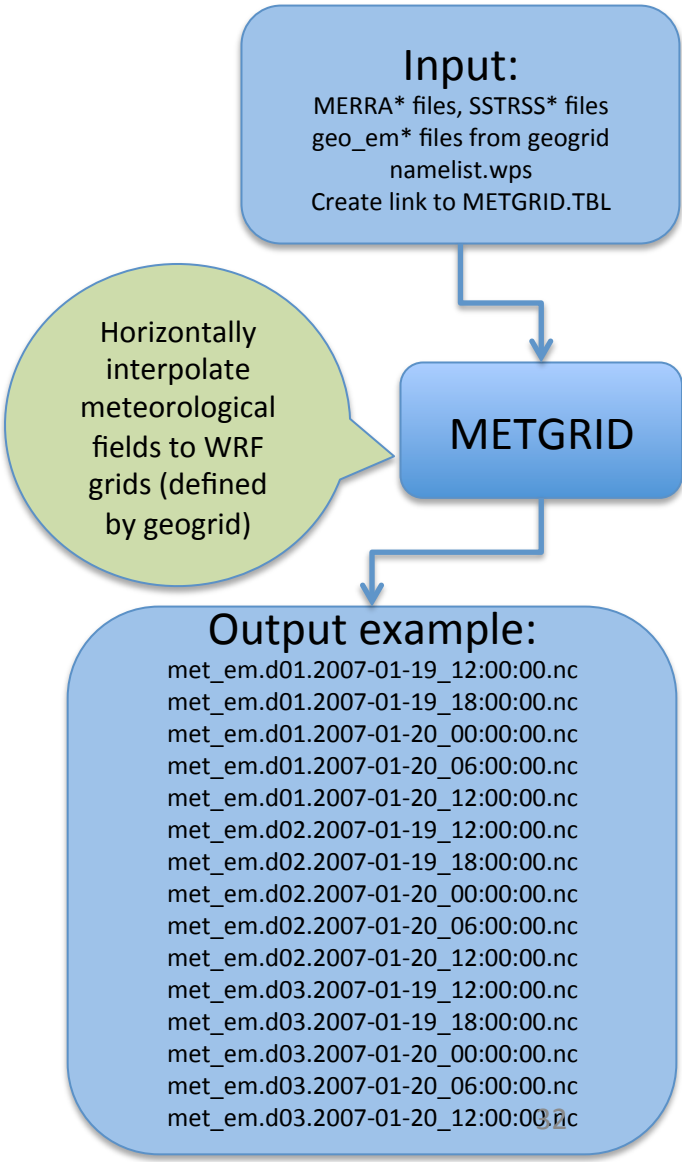
Differs from Simple Workflow!

Submit the job with this command:

>qsub run_metgrid.discover.sh (or sbatch can be used)

Check this file for run completion: metgrid.slurm.out

metgrid.log.<node> also will also be created for debugging purposes.

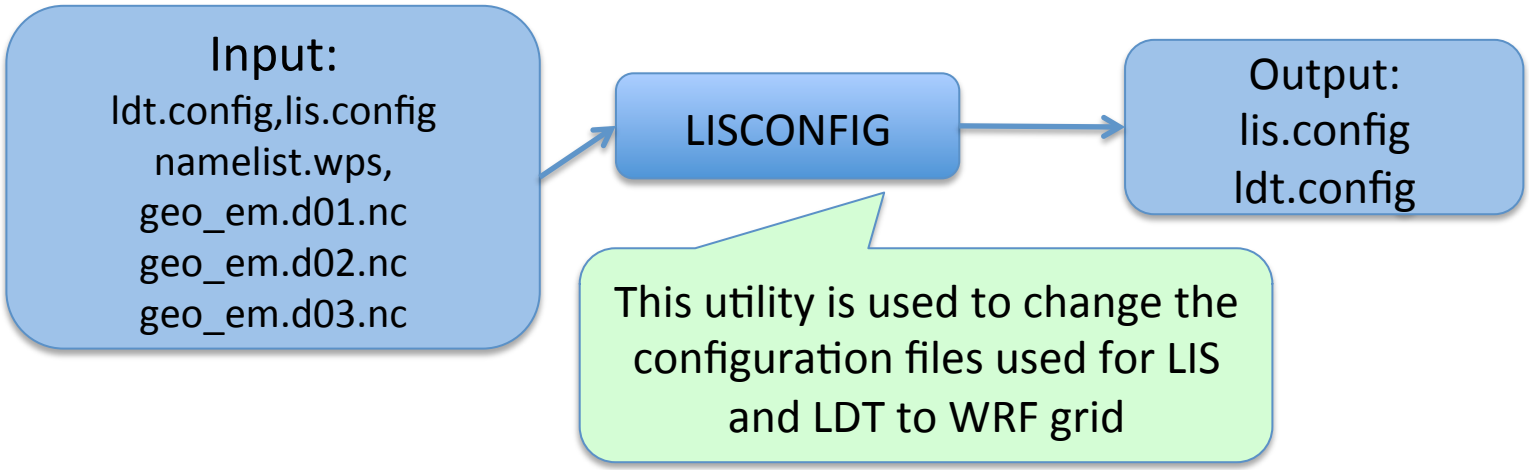


Run components on Discover -- LISCONFIG

LISCONFIG is an optional utility to change the LIS and LDT config files to match the WRF domain. If you use the lis.config and ldt.config files from the $WRF_LIS_DIR directory you don't need to run this utility.

```
>cd $RUNDIR
>cp $NUWRFDIR/utils/lisconfig/scripts/lisWrfDomain.py $RUNDIR/.
>ln –sf lis.config LISCONFIG
>ln –sf ldt.config LDTCONFIG
>ln –sf $RUNDIR WPSDIR
>ln –sf  $NUWRFDIR/utils/lisconfig/src/lisWrfDomain DOMAINPROG
>lisWrfDomain.py DOMAINPROG LISCONFIG LDTCONFIG WPSDIR
```

NEW WORKFLOW STEP



Run components on Discover -- LDT prelis

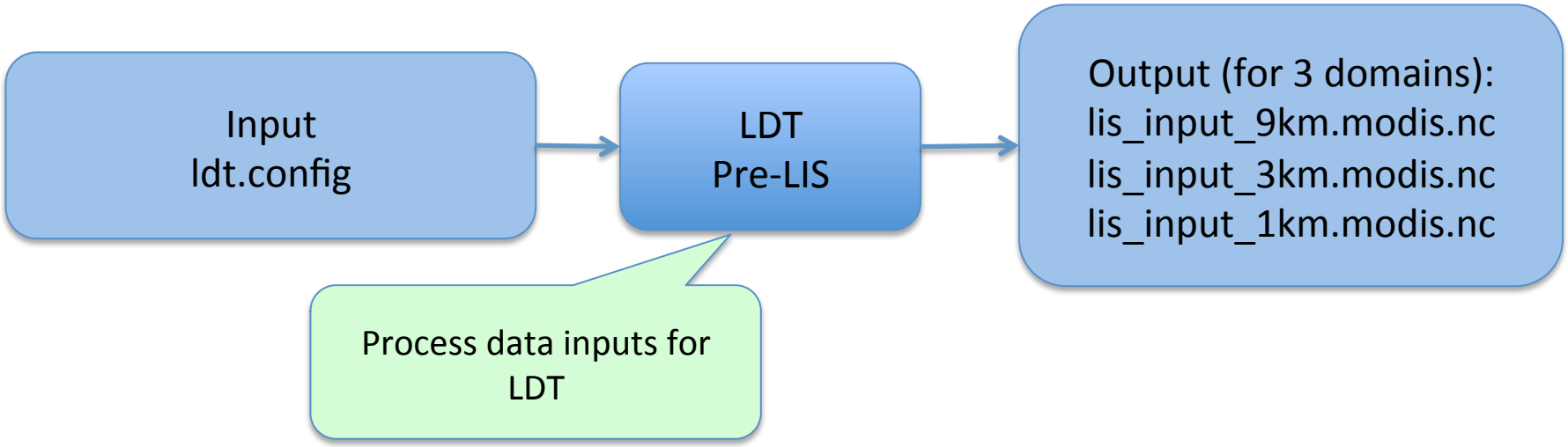
LDT – prelis step

NEW WORKFLOW STEP

```
>cd $RUNDIR
>cp ldt.config.modis.prelis ldt.config
>qsub run_ldt_prelis.discover.sh
```

(make sure to have config.discover.sh file in $RUNDIR)

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



For more information, user should refer to documentation http://lis.gsfc.nasa.gov/LDT/

Run components on Discover -- LIS spinup

>cd $RUNDIR

LIS spin up can be run from cold start or from a restart.

Starting from coldstart: Use lis.config.coldstart

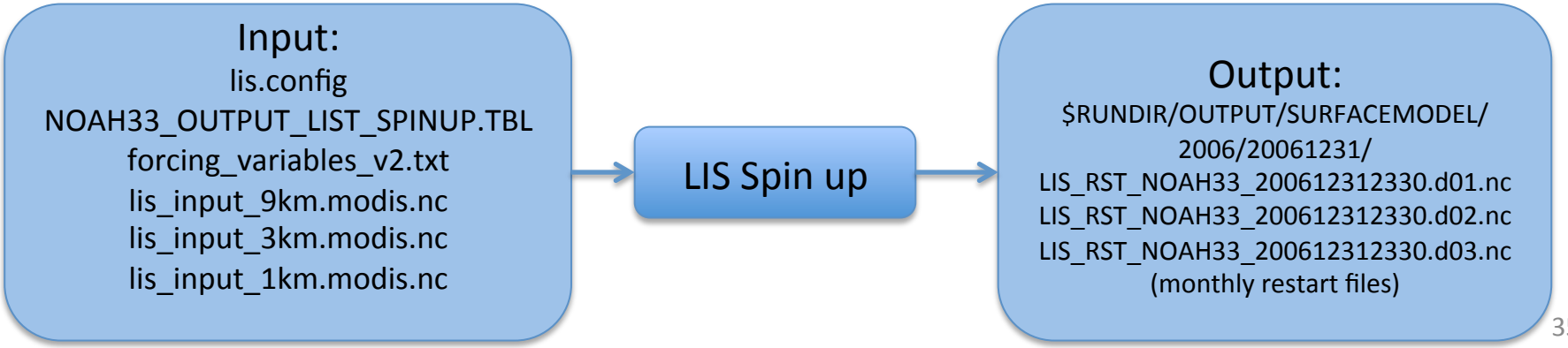
>cp lis.config.coldstart lis.config

NEW WORKFLOW STEP

(Make sure that you have the following files in your $RUNDIR:
forcing_variables_v2.txt ,
NOAH33_OUTPUT_LIST_SPINUP.TBL or the user specified files in lis.config)

>qsub run_lis.discover.sh

Check this file for successful run completion: lis.slurm.out
lislog.<node> will also be created for tracking run failures/ debugging.



Run components on Discover -- LIS spinup

>cd $RUNDIR

LIS spin up from a restart (Sample restart files provided in $WRF_LIS_DIR)

>cp lis.config.restart lis.config

NEW WORKFLOW STEP

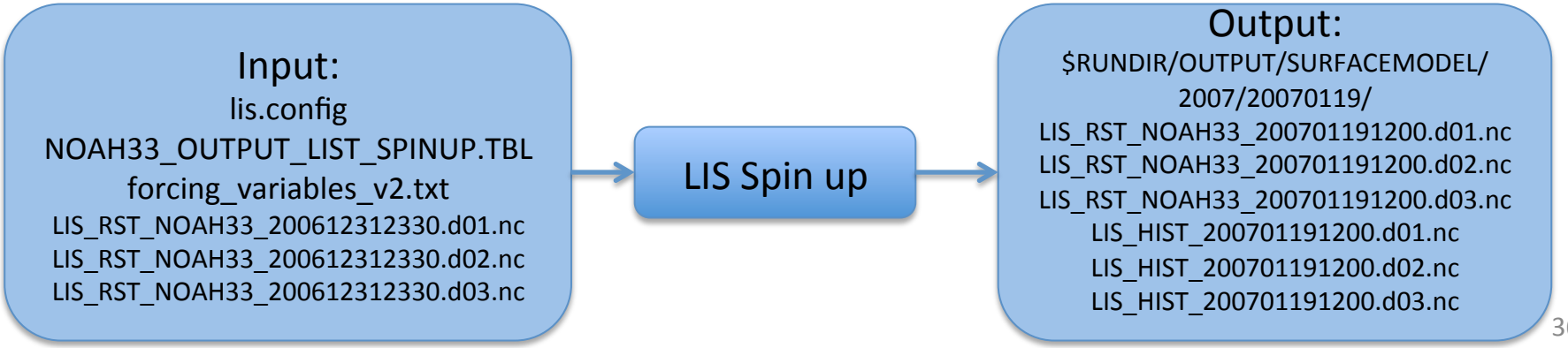
>cp $WRF_LIS_DIR/LIS_restarts/LIS* $RUNDIR/.

(or user defined restart files. Restart files should match the NOAH33_OUTPUT_LIST_SPINUP.TBL for variables)

>qsub run_lis.discover.sh

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

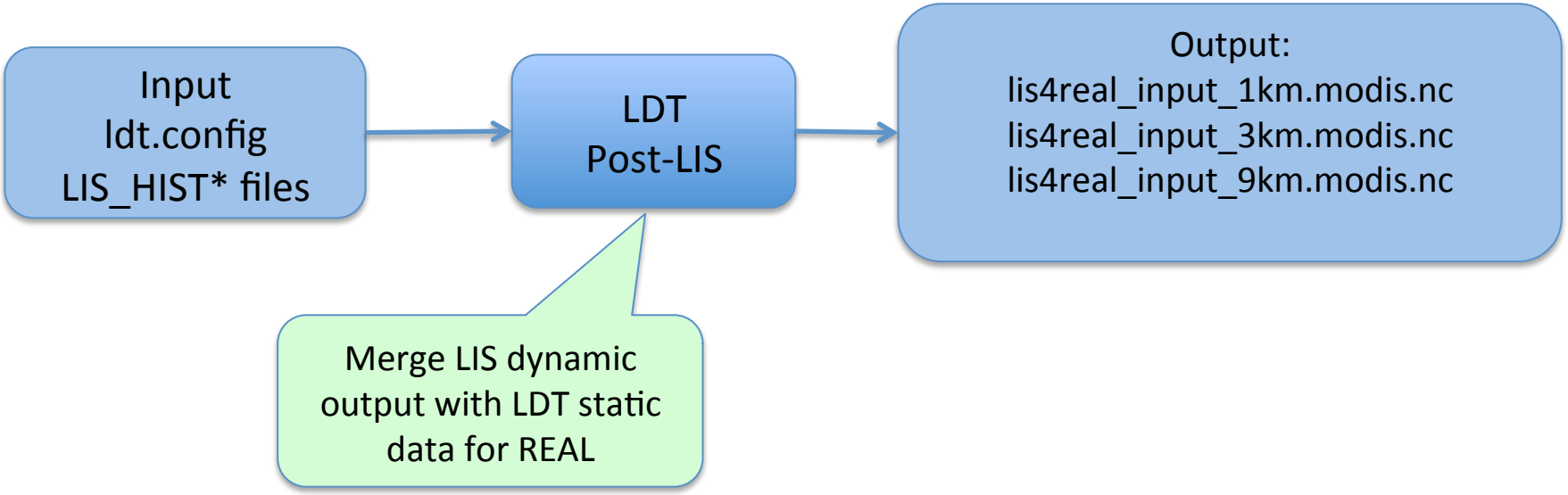
lislog.<node> will also be created for tracking run failures/ debugging.



Run components on Discover -- LDT postlis

```
>cd $RUNDIR
>cp ldt.config.modis.postlis ldt.config
>cp $RUNDIR/OUTPUT/SURFACEMODEL/2007/20070119/LIS_HIST* $RUNDIR/.
>qsub run_ldt_postlis.discover.sh
```

NEW WORKFLOW STEP



For more information, user should refer to documentation http://lis.gsfc.nasa.gov/LDT/

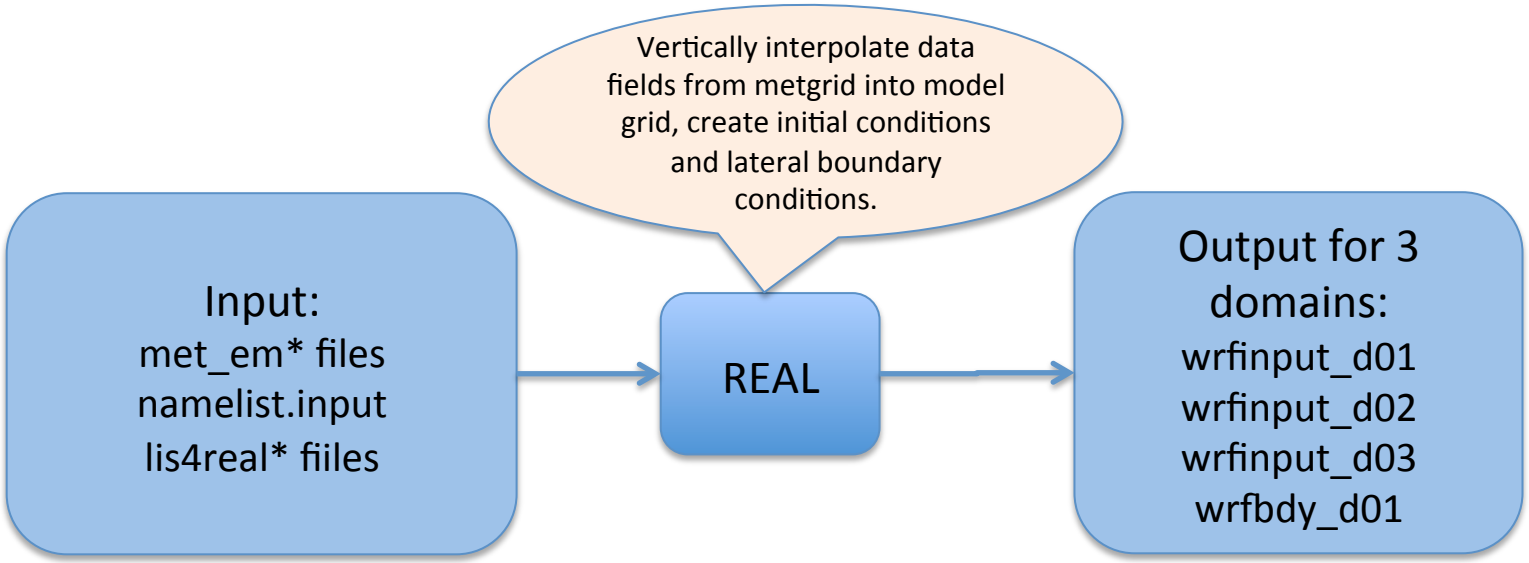
Run components on Discover -- REAL

>cd RUNDIR
The option in the number of land cover
>cp namelist.input.real namelist.input

Include &lis namelist block to process lis4real files

Copy the LIS Restart files created in LIS Spinup.
>cp $RUNDIR/OUTPUT/SURFACEMODEL/2007/20070119/LIS_RST* $RUNDIR/.
Submit the job with this command:
>qsub run_real.discover.sh (or sbatch can be used)

Check this file for run completion: real.slurm.out
real.rsl.out.<node> and real.rsl.error.<node> also will also be created.



Run components on Discover -- WRF-LIS coupled

>cd RUNDIR

Copy the LIS Restart files created in LIS Spinup.

>cp $RUNDIR/OUTPUT/SURFACEMODEL/2007/20070119/LIS_RST* $RUNDIR/.

Edit namelist.input file if the user need any option changes.

Refer to userguide for namelist.input options for different workflows.

Sample namelist.input is available in NUWRFDIR/defaults/ directory and in $WRF_LIS_DIR/ for this tutorial.

>cp namelist.input.wrf namelist.input

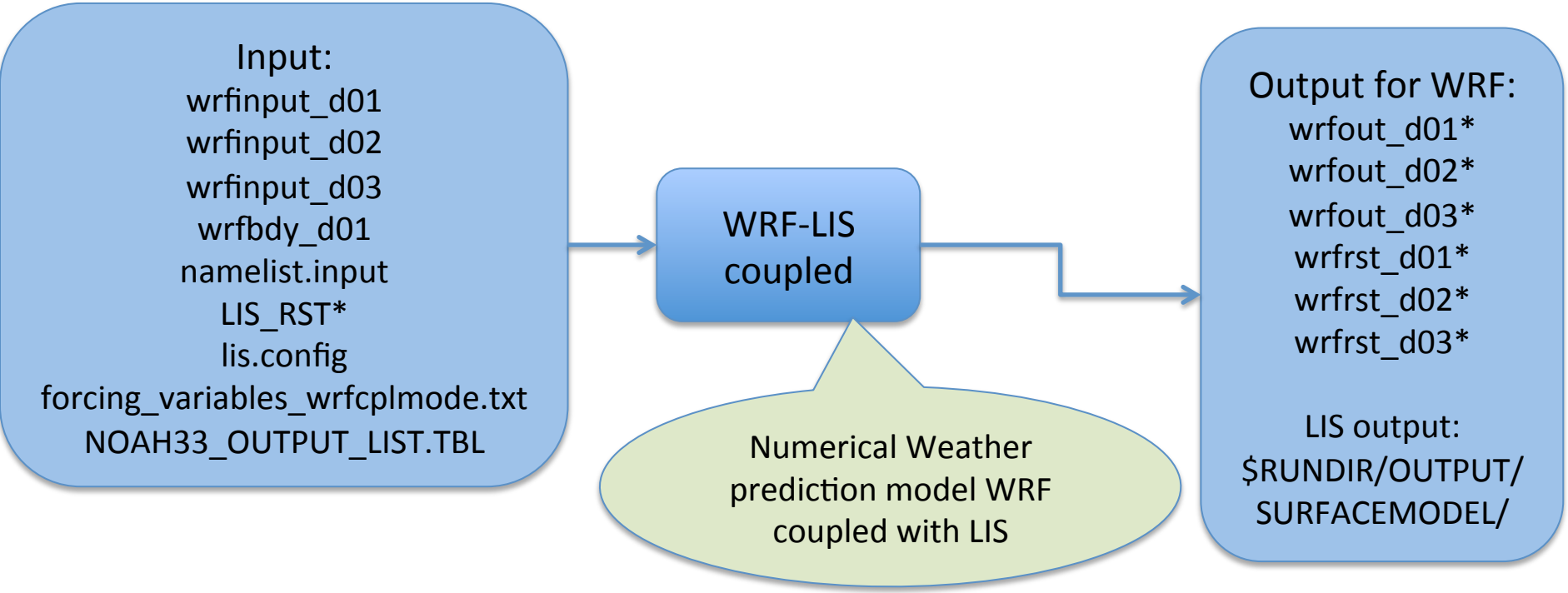
>cp lis.config.modis.coupled lis.config

(Make sure that you have the following files in your $RUNDIR:
forcing_variables_wrfcplmode.txt ,
NOAH33_OUTPUT_LIST_SPINUP.TBL or the user specified files in lis.config)

Submit the job with this command:

>qsub run_wrf.discover.sh (or sbatch can be used instead of qsub)

Run components on Discover -- WRF-LIS coupled



Check this file for run completion: wrf.slurm.out

wrf.rsl.out.<node>, wrf.rsl.error.<node>, and lislog.<node> will also be created for debugging/tracking of failures.

Post Processing on Discover

- All options from Simple Workflow can be used
- In addition, can use LVT (land surface verification toolkit)

- See http://lis.gsfc.nasa.gov/LVT/ for information

Adjustments for Pleiades

- Same as for Simple Workflow, except for path for LISDIR:

/nobackup8/nuwrf

  - This directory has subset of LS_PARAMETER and MET_FORCING data staged on Discover

TUTORIAL 3: NUWRF CHEM WORKFLOW

NU-WRF CHEM Workflows

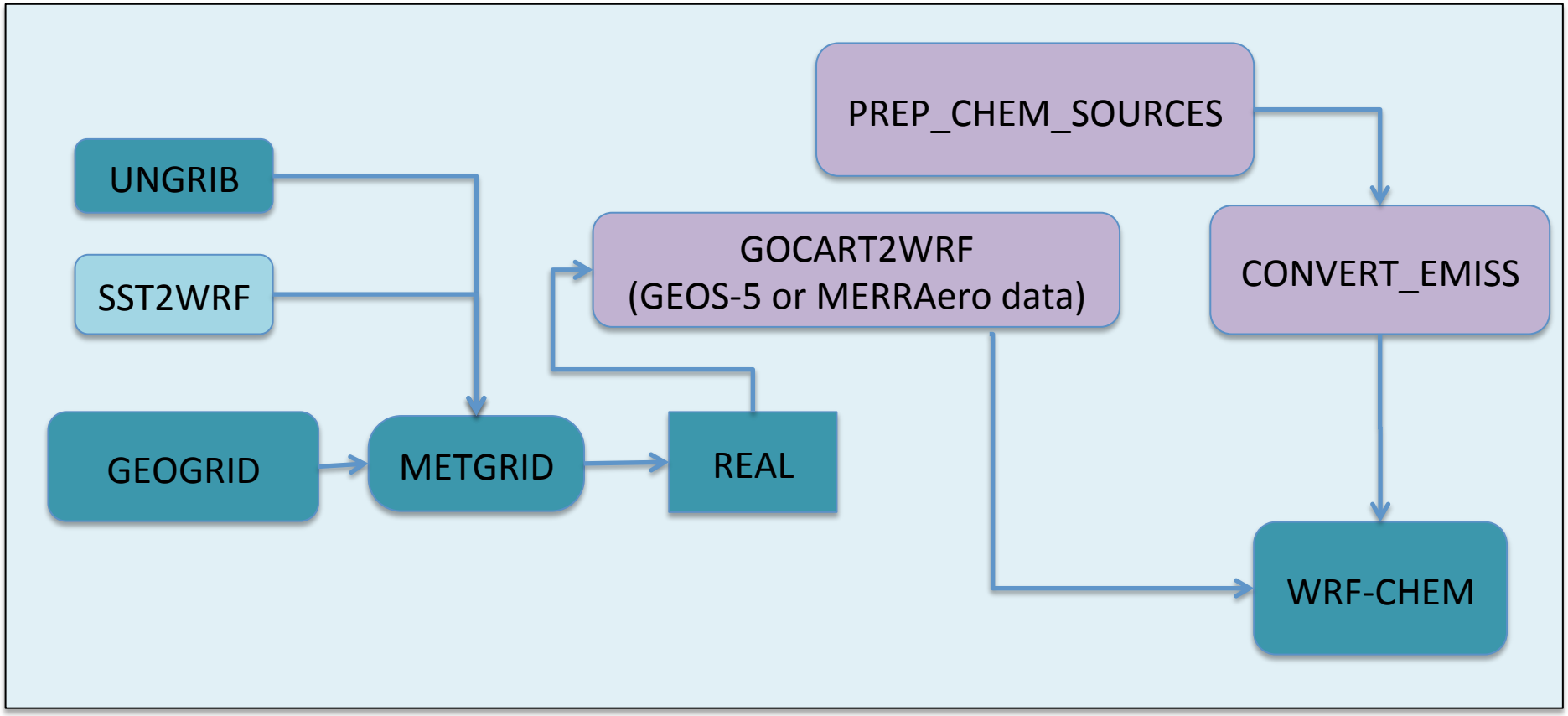
Initial and Lateral boundary conditions can be selected from different sources.

Case 1: GRIB files from Numerical Weather Prediction Models – NAM (North American Mesoscale model) or GFS (Global Forecasting Systems)

Case 2: MERRA or MERRA2 reanalysis combined with land initial conditions from LIS or other sources.

In this tutorial, a description of Case1, using GRIB files initial / boundary conditions is given.

NU-WRF CHEM Workflow : Case 1



This NU-WRF CHEM workflow uses atmospheric initial and lateral boundary conditions from GRIB files and RSS SST (Remote Sensing Systems SST product), chemical emissions using PREP_CHEM_SOURCES, CONVERT_EMISS, aerosol data compatible with GOCART, and runs WRF-CHEM.

Compile NU-WRF

Similar to compile steps for simple workflow, but we need to compile more components <u>including</u> chemistry library

./build.sh allchem >& log.out & (Compile WRF-Chem and all pre- and post-processors)

Or

./build.sh allkpp >& log.out & (Compiles WRF-Chem with Kinetic Preprocessor for advanced gas chemistry, plus all pre- and post-processors)

Or

./build.sh wps sst2wrf gocart2wrf prep_chem_sources chem rip >& log.out & (Compiles WPS, SST2WRF, GOCART2WRF, PREP_CHEM_SOURCES, WRF-Chem, and RIP. WPS includes GEOGRID, UNGRIB, and METGRID. CHEM target includes REAL and CONVERT_EMISS)

Compile NU-WRF

Where are the executables?

Key WPS executables

$NUWRFDIR/WPS/geogrid.exe
$NUWRFDIR/WPS/metgrid.exe
$NUWRFDIR/WPS/ungrib.exe

Key PREP_CHEM_SOURCE executables

$NUWRFDIR/utils/prep_chem_sources/bin/prep_chem_sources_RADM_WRF_FIM.exe

Key WRF executables

$NUWRFDIR/WRFV3/main/real.exe
$NUWRFDIR/WRFV3/main/wrf.exe
$NUWRFDIR/WRFV3/chem/convert_emiss.exe

Key SST2WRF executables

$NUWRFDIR/utils/sst2wrf/bin/sst2wrf

Key GOCART2WRF executables

$NUWRFDIR/utils/gocart2wrf/src/gocart2wrf

Key RIP4 executables

$NUWRFDIR/RIP4/ripdp_wrfarw
$NUWRFDIR/RIP4/rip

Model setup on Discover

Similar settings as for Simple Workflow.

Run scripts, configuration files and input files specific for this tutorial are available in the directory:

>set WRF_CHEM_DIR = /discover/nobackup/projects/nu-wrf/tutorial/7p4/WRF-CHEM/

Sample files are also in the directory: $NUWRFDIR/defaults/

Copy the following files from $WRF_CHEM_DIR to your $RUNDIR:

>cp $WRF_CHEM_DIR/namelist.wps $RUNDIR/.

>cp $WRF_CHEM_DIR/namelist.input* $RUNDIR/.

Run components on Discover -- GEOGRID

>cd $RUNDIR

- User should edit run script run_geogrid.discover.sh to change the links to GEOGRID.TBL depending on the run. Note: There are multiple GEOGRID.TBL files to support multiple dynamical cores in WRF. Use GEOGRID.TBL.ARW_CHEM_NUWRF for chemistry cases.

New file!!!

- User will need a namelist.wps file. For this tutorial to run on discover, it can be copied from $WRF_CHEM_DIR. Another sample namelist.wps file is avaiable in the directory: $NUWRFDIR/defaults/namelist.wps. User can refer to ARW online tutorial / web for more details on namelist.wps "&geogrid" block options: http://www2.mmm.ucar.edu/wrf/users/tutorial/201501/WPS_RUN.pdf

- Make sure that you have access to the directory: '/discover/nobackup/projects/nu-wrf/cases/geog'

Submit the job with this command:

>qsub run_geogrid.discover.sh

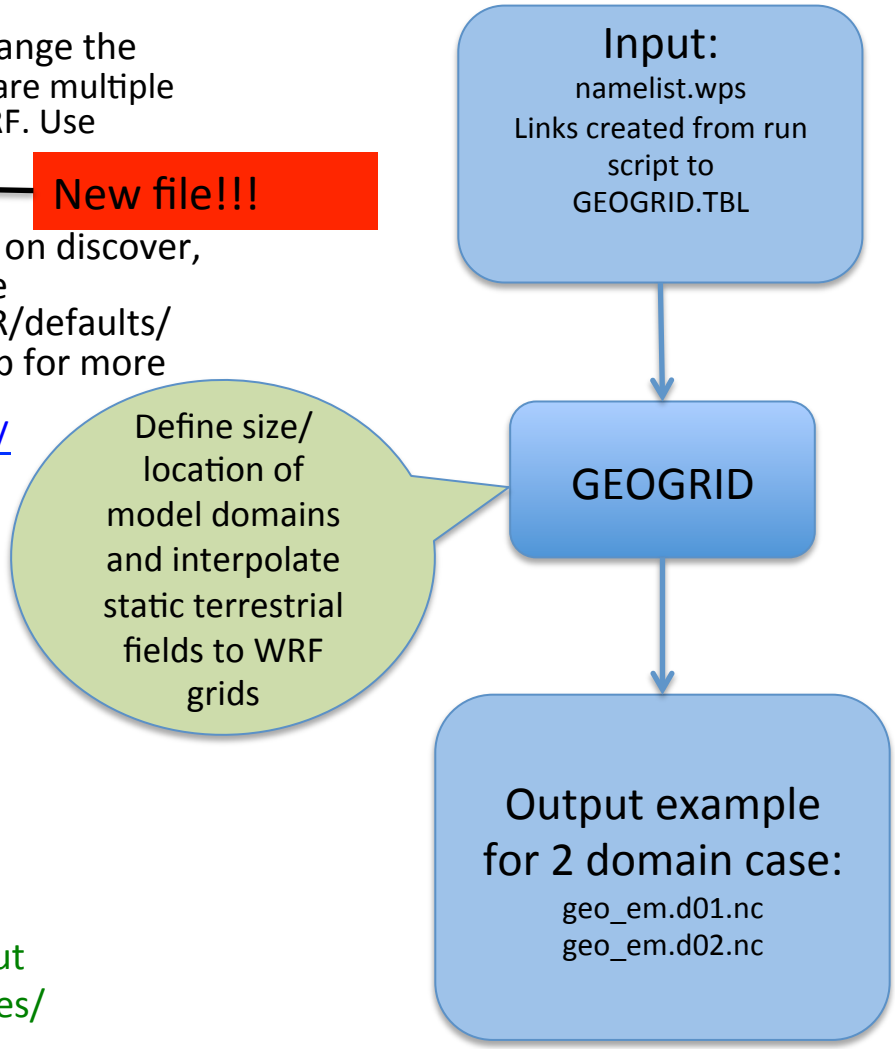
Or

>sbatch run_geogrid.discover.sh

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

geogrid.log.<node> will also be created for tracking run failures/debugging.

GEOGRID output file samples are given in $WRF_CHEM_DIR/geogrid/geogrid_output/



Run components on Discover -- UNGRIB

>cd RUNDIR

Copy the ungrib files to your RUNDIR, example:

>cp $WRF_CHEM_DIR/ungrib/grib_data/nam* $RUNDIR/.

Make sure you have namelist.wps file in your $RUNDIR.

Edit run script run_ungrib.discover.sh

- User should change the link to **Vtable** to the correct Vtable files for a specific run depend on what input files are used. Some Vtables are provided with WPS in the $NUWRFDIR/**WPS/ungrib/Variable_Tables** directory- E.g., Vtable.GFS, Vtable.SST, Vtable.ECMWF

```
ln -fs $NUWRFDIR/WPS/ungrib/Variable_Tables/Vtable.NAM Vtable
```

- User may need to change the grib file prefix depending on their data source. Example:

```
./link_grib.csh nam.* || exit 1
```

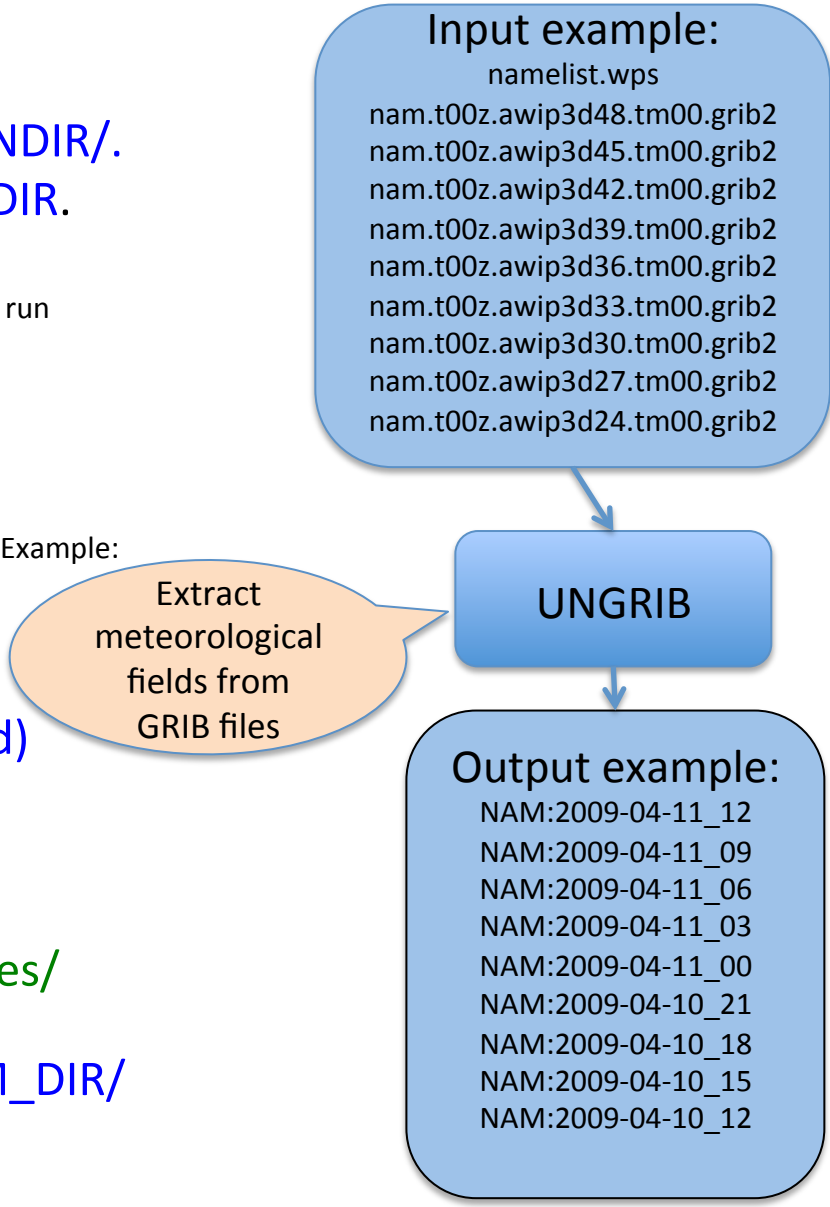
Submit the job with this command:

>qsub run_ungrib.discover.sh (or sbatch can be used)

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

ungrib.log will also be created for tracking run failures/ debugging.

Ungrib output file samples are given in $WRF_CHEM_DIR/ ungrib/ungrib_output/



Run components on Discover -- SST2WRF

```
>cd $RUNDIR
>mkdir $RUNDIR/RUN_SST2WRF
>cd $RUNDIR/RUN_SST2WRF
>cp $NUWRFDIR/utils/sst2wrf/scripts/Run_SST.csh $RUNDIR/.
```

For a start date = 20090410 and end date of 20090411:

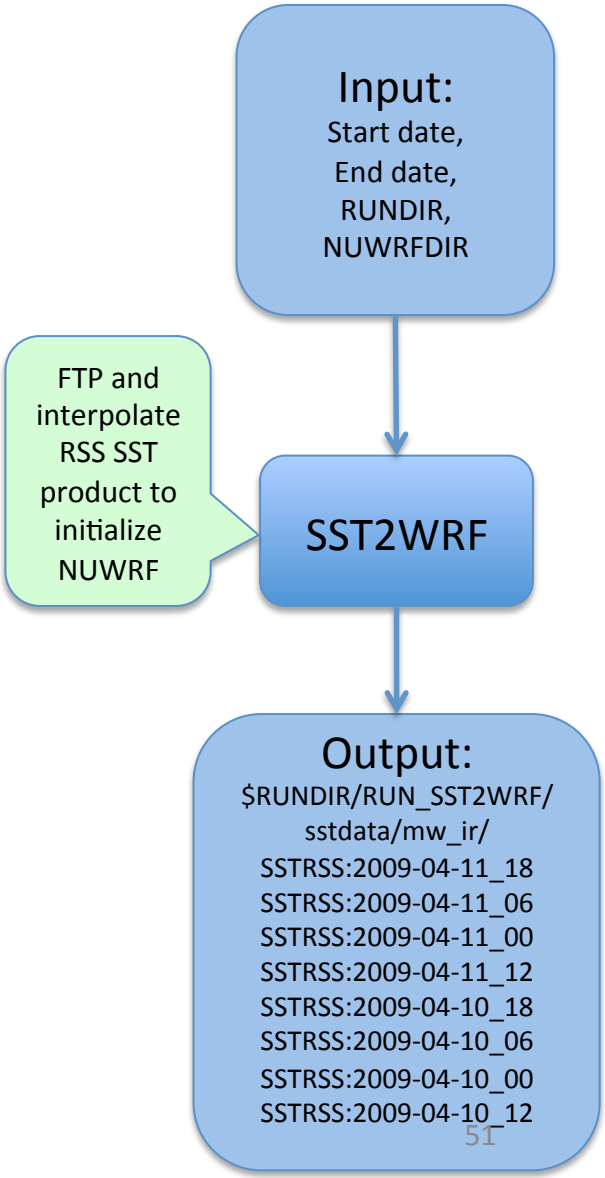
```
>./Run_SST.csh  20090410 20090410 mw_ir . $NUWRFDIR
```

SSTRSS:* files will be created, and these files should be copied to the RUNDIR before running METGRID component.

```
>cp sstdata/mw_ir/SSTRSS* $RUNDIR/.
```

For more details on the options and data types supported user can refer to NU-WRF userguide section 5.8.

Sample input and output files are given in $WRF_CHEM_DIR/sst2wrf/



Run components on Discover -- METGRID

>cd RUNDIR

Edit run script run_metgrid.discover.sh

- User should change the link to METGRID.TBL. There are multiple METGRID.TBL files to support multiple dynamical cores in WRF. Use METGRID.TBL.ARW for NUWRF.

```
ln -fs $NUWRFDIR/WPS/metgrid/METGRID.TBL.ARW metgrid/METGRID.TBL
```

Make sure you have namelist.wps file in your $RUNDIR.

- Metgrid block in the namelist.wps would look like this to utilize MERRA and SSTRSS data.

```
&metgrid
 fg_name = 'NAM', 'SSTRSS'
 io_form_metgrid = 2,
/
```

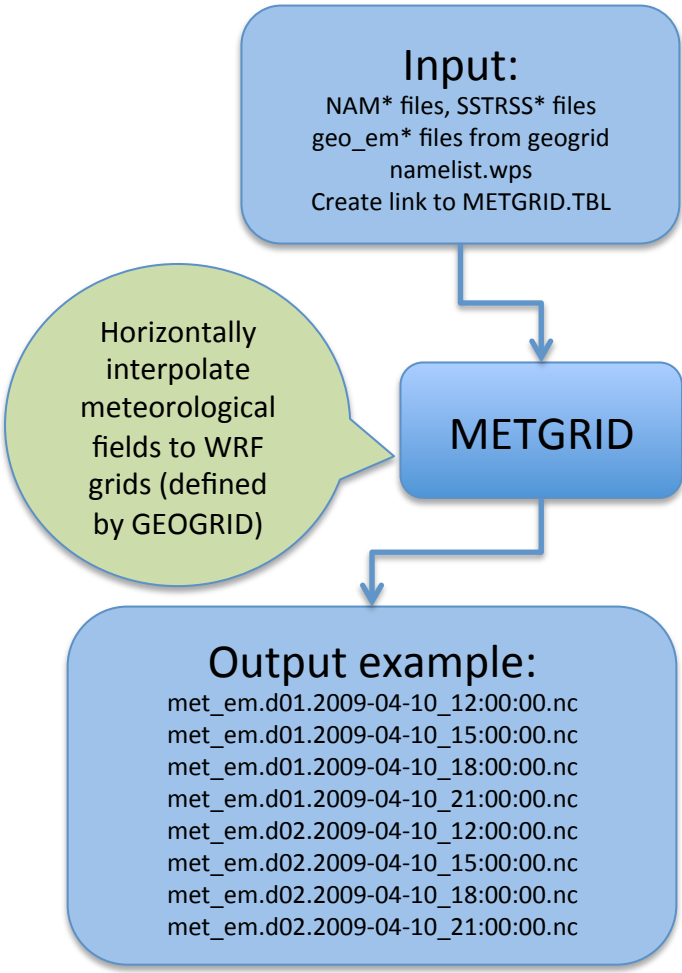
Submit the job with this command:

>qsub run_metgrid.discover.sh (or sbatch can be used)

Check this file for run completion: metgrid.slurm.out

metgrid.log.<node> also will also be created for debugging purposes.

Sample Metgrid input and output files are in $WRF_CHEM_DIR/metgrid/.



Run components on Discover -- REAL

>cd RUNDIR

>cp namelist.input.real namelist.input

Note that the namelist.input file with *&chem* block will give an error for "REAL".

Submit the job with this command:

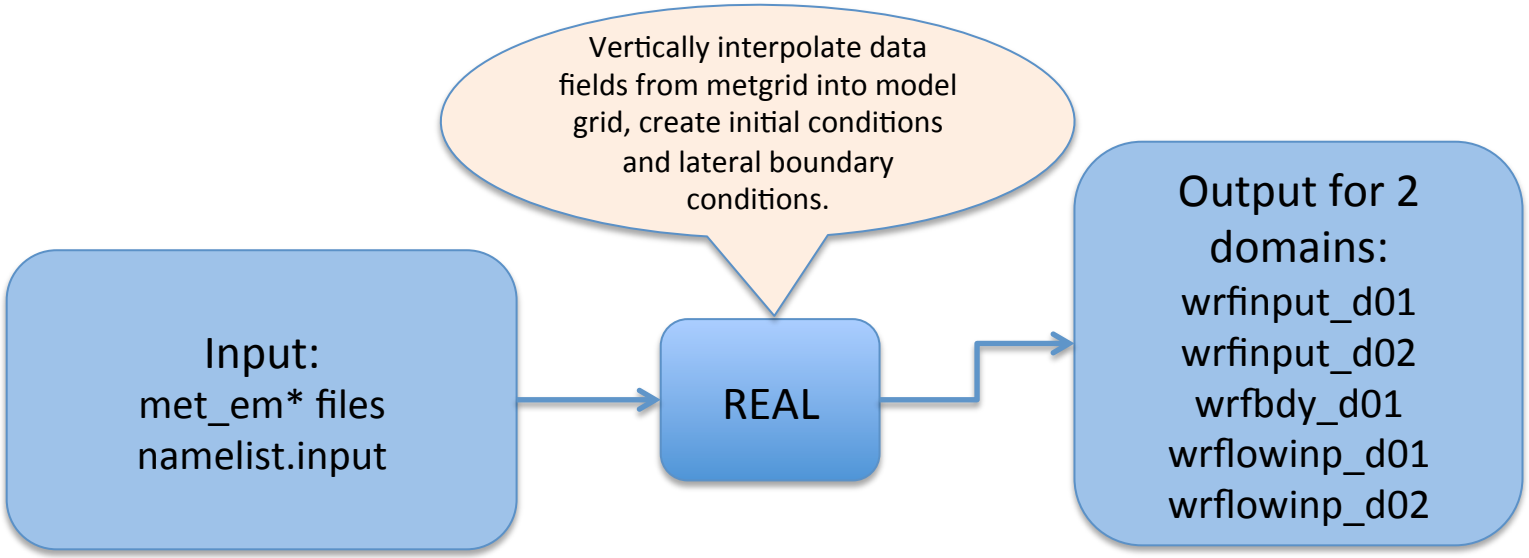
>qsub run_real.discover.sh (or sbatch can be used)

Check this file for run completion: real.slurm.out

real.rsl.out.<node> and real.rsl.error.<node> also will also be created for debugging purposes.

Sample input and output files are given in $WRF_CHEM_DIR/real/.

Note that for namelist option: io_form_auxinput4=2, output file wrflowinp_d01 and wrflowinp_d01 are also created in addition to the regular wrfinput and wrfbdy output files.



Run components on Discover -- GOCART2WRF

User can choose GOCART aerosol data from GEOS-5 or MERRAero reanalysis.

MERRA2 not supported yet!

>cd $RUNDIR

User need a file namelist.gocart2wrf, for running this component. A sample file is given in the $NUWRFDIR/utils/gocart2wrf_2/input/namelist.gocart2wrf. User need to modify this file for 'wrf_dir', 'max_dom', 'gocart_dir', 'gocart_prefix'. For this tutorial, user can use the namelist.gocart2wrf file from $WRF_CHEM_DIR/. GOCART data files to test run this tutorial are also given in $WRF_CHEM_DIR.

>cp –r $WRF_CHEM_DIR/gocart/gocart_input $RUNDIR/.

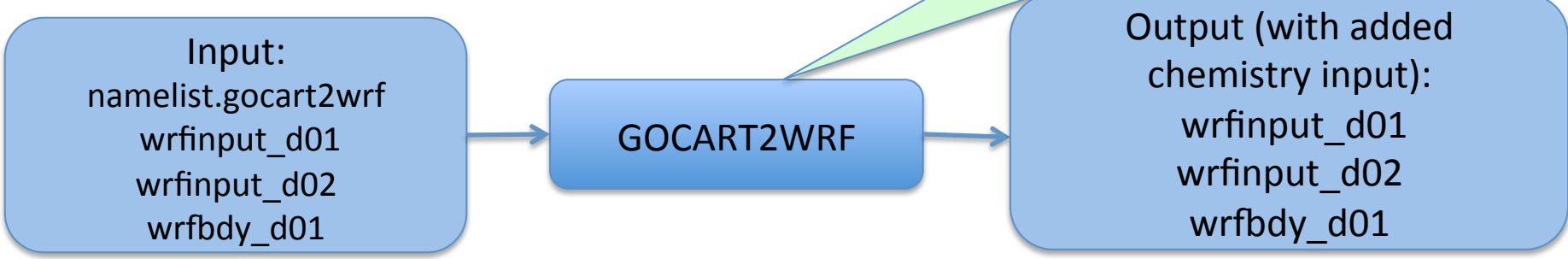
>qsub run_gocart2wrf.discover.sh

Check this file for successful run completion: go2w.slurm.out

Sample input and output files for using GOCART aerosol data are given in $WRF_CHEM_DIR/gocart/.

NEW WORKFLOW STEP

A preprocessor to extract aerosol data from GEOS-5 netCDF4 GOCART files (or MERRAero data files); horizontally and vertically interpolate the fields to the WRF grid; and append them to the initial and lateral boundary condition files of WRF (wrfinput_d* and wrfbdy_d01).



Run components on Discover -- GOCART2WRF

MERRA Aerosol data:

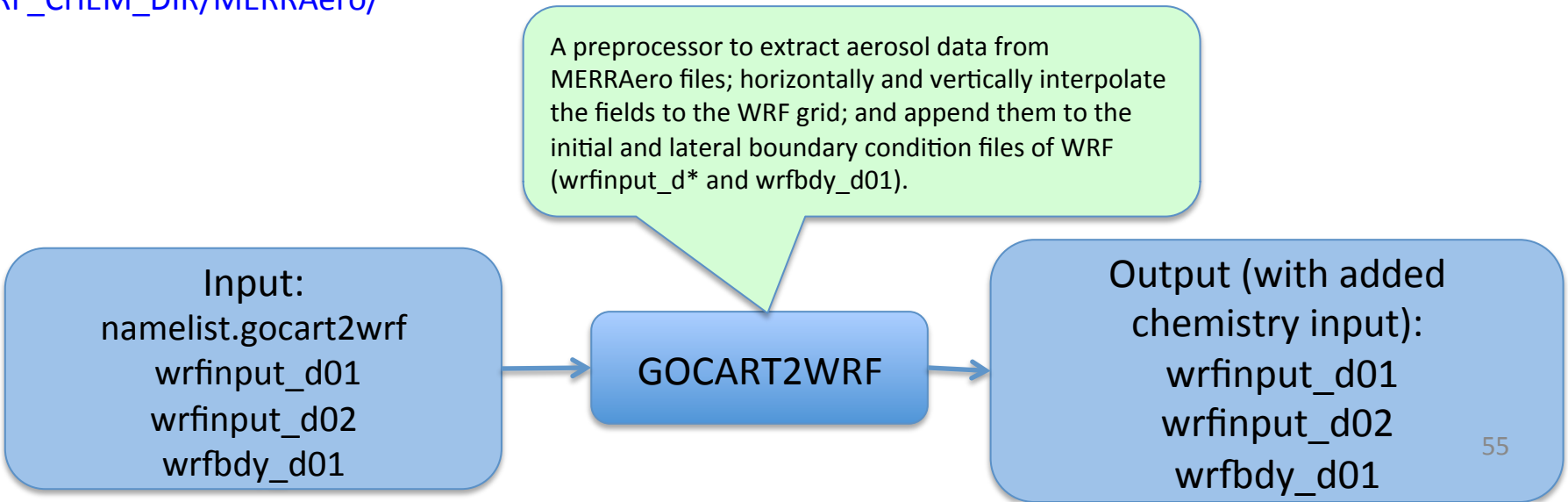
If the user wants to use MERRAero data the GOCART2WRF utility can be used. The namelist.gocartwrf file should be modified for 'wrf_dir', 'max_dom', 'gocart_dir', 'gocart_prefix'. A sample file is given in $NUWRFDIR/utils/gocart2wrf_2/input/namelist.gocart2wrf_MERRAero. For this tutorial, a sample file is also given in $WRF_CHEM_DIR/MERRAero/namelist.gocart2wrf_MERRAero. Note that this file need to be renamed as namelist.gocart2wrf before running gocart2wrf. For testing this tutorial, user can use the MERRAero data provided in the $WRF_CHEM_DIR/MERRAero/Merraero_input.

```
>cp –r $WRF_CHEM_DIR/MERRAero/Merraero_input $RUNDIR/.
>cp $WRF_CHEM_DIR/MERRAero/namelist.gocart2wrf_MERRAero $RUNDIR/namelist.gocart2wrf
>qsub run_gocart2wrf.discover.sh
```

Check this file for successful run completion: go2w.slurm.out

NEW WORKFLOW STEP

Sample input and output files for using MERRA Aerosol data are given in $WRF_CHEM_DIR/MERRAero/



Run components on Discover -- PREP_CHEM_SOURCES

>cd $RUNDIR

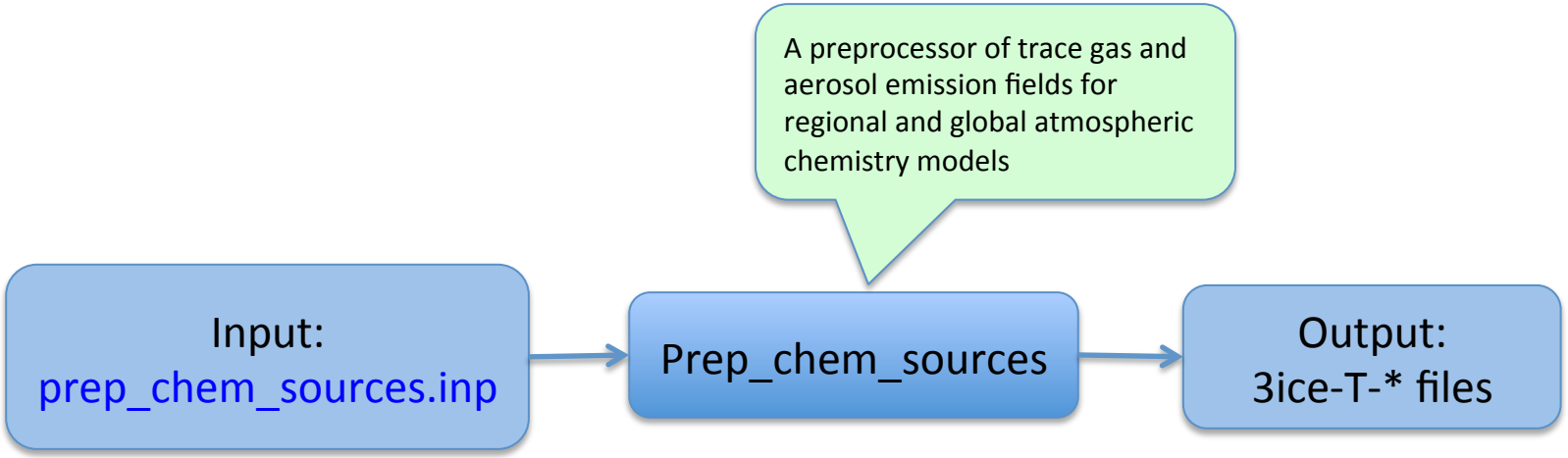
User need a file prep_chem_sources.inp for running this component. A sample file is given in the $NUWRFDIR/utils/prep_chem_sources/bin/prep_chem_sources.inp. For this tutorial, user can run using the prep_chem_sources.inp file from the $WRF_CHEM_DIR.

>cp $WRF_CHEM_DIR/prep_chem_sources.inp $RUNDIR/.

>qsub run_prep_chem_sources.discover.sh

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

Sample input and output files are given in $WRF_CHEM_DIR/prep_chem_sources/.



Run components on Discover -- CONVERT_EMISS

>cd $RUNDIR

User should edit this runscript: run_convert_emiss_discover.sh and change 'numDomains'. CONVERT_EMISS does not work for nested domains, so the runscript is designed such that each domain need to be run separately.

User should edit the namelist.input file to create a namelist.input file for both domains to run as single domain.

Sample files are given in $WRF_CHEM_DIR/convert_emiss/namelist.input.convert_emiss.d01 and namelist.input.convert_emiss.d02.

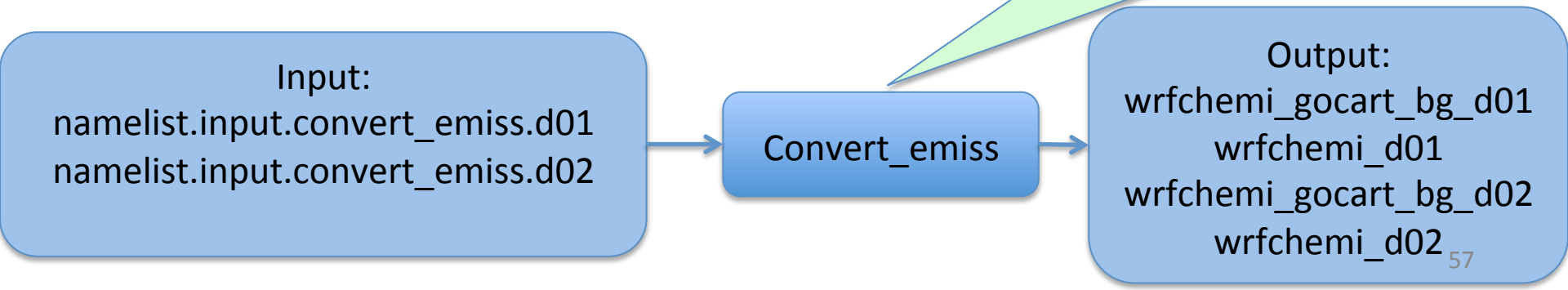
```
>cp $WRF_CHEM_DIR/convert_emiss/namelist.input.convert_emiss.d01 $RUNDIR/.
>cp $WRF_CHEM_DIR/convert_emiss/namelist.input.convert_emiss.d02 $RUNDIR/.
>qsub run_convert_emiss.discover.sh
```

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

Sample input and output files are given in $WRF_CHEM_DIR/convert_emiss/.

User can refer to NU-WRF userguide section 5.6 and WRF-CHEM userguide (http://ruc.noaa.gov/wrf/WG11/Users_guide.pdf) for more details.

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.



Run components on Discover -- WRF-CHEM

>cd RUNDIR

Sample namelist.input is available in $NUWRFDIR/defaults/ directory. Edit namelist.input file if the user need any namelist option changes. User can refer to NU-WRF userguide section 5.6 and WRF-CHEM userguide (http://ruc.noaa.gov/wrf/WG11/Users_guide.pdf) for more details on available namelist.input options.

For this tutorial, user can use the namelist.input.wrf file from $WRF_CHEM_DIR.

>cp $WRF_CHEM_DIR/namelist.input.wrf $RUNDIR/namelist.input

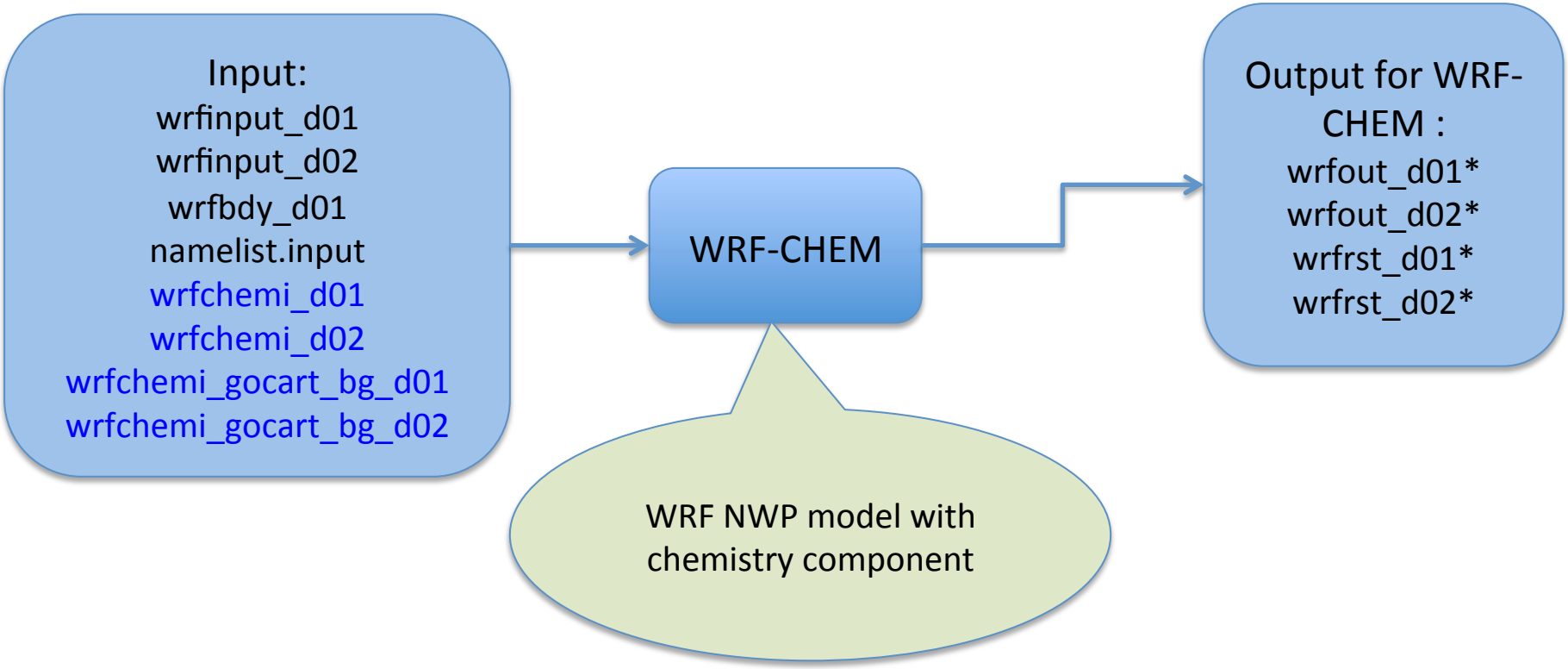
User need to rename the convert emission files to the naming convention expected by WRF CHEM.

```
>set start_date = '2009-04-10_12:00:00'
>cp wrfchemi_d01 wrfchemi_d01_$start_date
>cp wrfchemi_d02 wrfchemi_d02_$start_date
>set start_date = '2009-04-10'
>cp wrfchemi_gocart_bg_d01 wrfchemi_gocart_bg_d01_$start_date
>cp wrfchemi_gocart_bg_d02 wrfchemi_gocart_bg_d02_$start_date
```

Submit the job with this command:

>qsub run_wrf.discover.sh (or sbatch can be used instead of qsub)

Run components on Discover -- WRF-CHEM



Check this file for run completion: wrf.slurm.out

wrf.rsl.out.<node> and wrf.rsl.error.<node> also will also be created for debugging/ track failures.

Post Processing On Discover

Same options as for Simple Workflow!

Adjustments for Pleiades

- Same as for Simple Workflow