**WRF-chem doc**

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The installation of WRF chem on NASA HPC now utilizes version 4.4, as the previously employed 4.1.2 version is no longer in use. This transition is necessitated by the presence of various data sets with differing units in the current version, leading to variations in the resulting Aerosol Optical Depth (AOD) values when compared to the older version. Additionally, the installation of the Weather Research and Forecasting (WRF) Preprocessing System (WPS) on the server is imperative for data preprocessing. This is because NASA HPC lacks essential compression libraries such as ZLIB, libpng, and jasper, which are vital for compiling WPS, especially for ungrib with GRIB2 capability. Detailed instructions, including the required commands and namelists for both WRF and WPS, are provided as part of the WRF installation and execution procedures.

WRF and WPS installation

The line marked with "#" is the comment line, while the other line represents the command line. Please begin by reviewing the comment line before executing the command line step by step. I am using an open-source model, and I have adhered to the official instructions provided on their website. Certain technical instructions and commands are derived from and aligned with the official guidelines. To install WPS on the server, you can obtain the necessary libraries from: <https://www2.mmm.ucar.edu/wrf/OnLineTutorial/compilation_tutorial.php#STEP1>

## #Make directory for wps

mkdir Build\_WRF

# #Building Libraries

# cd Build\_WRF

# making a directory called "LIBRARIES"

mkdir LIBRARIES

#Required libraries can be downloaded form:

#<https://www2.mmm.ucar.edu/wrf/OnLineTutorial/compilation_tutorial.php#STEP1>

#Hint: The version of the library may be different, remember to change the version #name in the code if it is different, The sample libraries are old (installed last year #and the original package was uploaded in 2018) may not work with the #current version. I suggest trying the new packages to facilitate consistency with #WRF.

cd LIBRARIES

pwd

# get your path

## 1.NetCDF:

# Before installing the libraries, these paths need to be set:

# netcdf set envir (envir = environment)

export DIR=your path0

export CC=gcc

export CXX=g++

export FC=gfortran

export FCFLAGS=-m64

export F77=gfortran

export FFLAGS=-m64

tar xzvf netcdf-4.1.3.tar.gz

cd netcdf-4.1.3

./configure --prefix=$DIR/netcdf --disable-dap \--disable-netcdf-4 --disable-shared

make

make install

#netcdf set envir

export PATH=$DIR/netcdf/bin:$PATH

export NETCDF=$DIR/netcdf

cd ..

## 2.mpich

### This library is necessary if you are planning to build WRF in parallel.

tar xzvf mpich-3.0.4.tar.gz

cd mpich-3.0.4

./configure --prefix=$DIR/mpich

make

make install

mpich set envir

export PATH=$DIR/mpich/bin:$PATH

cd ..

## 3. zlib:

## This is a compression library necessary for compiling WPS (specifically ungrib) ##with GRIB2 capability

#zlib set envir

export LDFLAGS=-L$DIR/grib2/lib

export CPPFLAGS=-I$DIR/grib2/include

cd zlib-1.2.7

./configure --prefix=$DIR/grib2

make

make install

cd ..

## 4. libpng:

#This is a compression library necessary for compiling WPS #(specifically ungrib) with GRIB2 #capability

tar xzvf libpng-1.2.50.tar.gz

cd libpng-1.2.50

./configure --prefix=$DIR/grib2

make

make install

cd ..

## 5. JasPer:

#This is a compression library necessary for compiling WPS #(specifically ungrib) with GRIB2 #capability

tar xzvf jasper-1.900.1.tar.gz

cd jasper-1.900.1

./configure --prefix=$DIR/grib2

make

make install

cd ..

this area

Library Compatibility Tests (same as the official instruction since it is the test running of installed libraries)

#Check in the official website for detail. #https://www2.mmm.ucar.edu/wrf/OnLineTutorial/compilation\_tutorial.php#STEP1.

#Download the tar file that contains tests from: #https://www2.mmm.ucar.edu/wrf/OnLineTutorial/compilation\_tutorial.php#STEP1.

#Download the tar file named as: Fortran\_C\_NETCDF\_MPI\_tests.tar and place it #in the TESTS directory, and then "cd" into the TESTS directory:

##To unpack the tar file, type:

tar -xf Fortran\_C\_NETCDF\_MPI\_tests.tar

* There are 2 tests:
  1. **Test #1**: Fortran + C + NetCDF  
       
     The NetCDF-only test requires the include file from the NETCDF package be in this directory. Copy the file here:

cp ${NETCDF}/include/netcdf.inc .

Compile the Fortran and C codes for the purpose of this test (the -c option says to not try to build an executable). Type the following commands:

gfortran -c 01\_fortran+c+netcdf\_f.f  
gcc -c 01\_fortran+c+netcdf\_c.c  
gfortran 01\_fortran+c+netcdf\_f.o 01\_fortran+c+netcdf\_c.o \  
     -L${NETCDF}/lib -lnetcdff -lnetcdf  
./a.out

The following should be displayed on your screen:

C function called by Fortran  
Values are xx = 2.00 and ii = 1  
SUCCESS test 1 fortran + c + netcdf

* 1. **Test #2**: Fortran + C + NetCDF + MPI  
       
     The NetCDF+MPI test requires include files from both of these packages be in this directory, but the MPI scripts automatically make the mpif.h file available without assistance, so no need to copy that one. Copy the NetCDF include file here:

cp ${NETCDF}/include/netcdf.inc .

Note that the MPI executables mpif90 and mpicc are used below when compiling. Issue the following commands:

mpif90 -c 02\_fortran+c+netcdf+mpi\_f.f  
mpicc -c 02\_fortran+c+netcdf+mpi\_c.c  
mpif90 02\_fortran+c+netcdf+mpi\_f.o \  
02\_fortran+c+netcdf+mpi\_c.o \  
     -L${NETCDF}/lib -lnetcdff -lnetcdf  
mpirun ./a.out

The following should be displayed on your screen:

C function called by Fortran  
Values are xx = 2.00 and ii = 1  
status = 2  
SUCCESS test 2 fortran + c + netcdf + mpi

Building WPS

#Dowload the WPS from official website: #https://www2.mmm.ucar.edu/wrf/users/download/get\_source.html, I used the #version 4.1, if using a different version, remember to change the version name.

## go to the WPS directory

cd WPS

./clean

#WPS set envir

export JASPERLIB=$DIR/grib2/lib

export JASPERINC=$DIR/grib2/include

./configure

1

./compile >& log.compile

#If the compilation is successful, there should be 3 executables in the WPS top-#level directory, that are linked to their corresponding src/ directories:

#geogrid.exe -> geogrid/src/geogrid.exe

#ungrib.exe -> ungrib/src/ungrib.exe

#metgrid.exe -> metgrid/src/metgrid.exe

#Verify that they are not zero-sized (inside the \*/src/ directory).

#Done！

WRF install on NASA server

#remember to run line by line

# Download WRF v4.4.1 from the official website and download or upload to the #NASA HPC

# wrf download website: #https://www2.mmm.ucar.edu/wrf/users/download/get\_source.html

## Go to the WRF directory

cd WRF

# Load the necessary NAS modules in the NASA HPC

module purge

module load comp-intel

module load mpi-hpe

module load hdf4/4.2.12 hdf5/1.8.18\_serial netcdf/4.4.1.1\_serial

# Set NETCDF environment variable before running configure in your directory

setenv NETCDF /nasa/netcdf/4.4.1.1\_serial

# choose option 24 and 1

./configure << END

24

1

END

# Add mpi compile wrappers to DM\_FC and DM\_CC

sed -i "s/DM\_FC = \$(SFC)/DM\_FC = mpif90 -f90=\$(SFC)/g" configure.wrf

sed -i "s/DM\_CC = \$(SCC)/DM\_CC = mpicc -cc=\$(SCC)/g" configure.wrf

# Remove extras from LDFLAGS for now...

sed -i "s/\-ip \-lmpi//g" configure.wrf

# Remove ignore switch from the make command (otherwise it'll fail and keep #compiling)

sed -i "s/make \-i/make/g" configure.wrf

# Run the compile for the WRF, a install description can be generate by typing >& #log.compile after the compile commmand(option)

./compile em\_real

### the compiling takes hours

#Once the compilation completes, to check whether it was successful, you need to #look for executables in the WRF/main directory:

#ls -ls main/\*.exe

#If you compiled a real case, you should see:

#wrf.exe (model executable)

#real.exe (real data initialization)

#ndown.exe (one-way nesting)

#tc.exe (for tc bogusing--serial only)

#These executables are linked to 2 different directories:

#WRF/run

#WRF/test/em\_real

#You can choose to run WRF from either directory.

Running WRF

#Details can be found under: #[https://www2.mmm.ucar.edu/wrf/OnLineTutorial/#](https://www2.mmm.ucar.edu/wrf/OnLineTutorial/)

#3Please check the official website and the steps before running

### wps namelist

wrf\_core = 'ARW',

max\_dom = 2,

start\_date = '2020-05-26\_12:00:00','2018-05-25\_12:00:00',

end\_date = '2020-05-29\_00:00:00','2018-05-25\_12:00:00',

interval\_seconds = 21600,

io\_form\_geogrid = 2,

/

&geogrid

parent\_id = 1,1,

parent\_grid\_ratio = 1,3,

i\_parent\_start = 1,220,

j\_parent\_start = 1,37,

e\_we = 642,222

e\_sn = 521,520,

!

!!!!!!!!!!!!!!!!!!!!!!!!!!!! IMPORTANT NOTE !!!!!!!!!!!!!!!!!!!!!!!!!!!!

! The default datasets used to produce the MAXSNOALB and ALBEDO12M

! fields have changed in WPS v4.0. These fields are now interpolated

! from MODIS-based datasets.

!

! To match the output given by the default namelist.wps in WPS v3.9.1,

! the following setting for geog\_data\_res may be used:

!

! geog\_data\_res = 'maxsnowalb\_ncep+albedo\_ncep+default', 'maxsnowalb\_ncep+albedo\_ncep+default',

!

!!!!!!!!!!!!!!!!!!!!!!!!!!!! IMPORTANT NOTE !!!!!!!!!!!!!!!!!!!!!!!!!!!!

!

geog\_data\_res = 'default',' default ',

dx = 4000,

dy = 4000,

map\_proj = 'lambert',

ref\_lat = 50.893,

ref\_lon = 47.177,

truelat1 = 50.893,

truelat2 = 50.893,

stand\_lon = 47.177,

geog\_data\_path = 'your path to the WPS geog data'

/

&ungrib

out\_format = 'WPS',

prefix = 'FILE',

/

&metgrid

fg\_name = 'FILE'

io\_form\_metgrid = 2,

/

# WPS processing, before running remember to download your met data

# go to your WPS directory ../WPS/

# edit wps namelist then run comman:

###. Link-in the Vtable:

ln -sf ungrib/Variable\_Tables/Vtable.GFS Vtable

###Link in the GRIB data by making use of the script link\_grib.csh

./link\_grib.csh /your data location

./ungrib.exe

#Setup the Model domain (geogrid.exe)

./geogrid.exe

#The following should be displayed on your screen:

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! Successful completion of geogrid. !

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

#Interpolate the input data onto our model domain (metgrid.exe)

#. Run metgrid.exe to interpolate the input data on our model domain:

./metgrid.exe

#The following should be displayed on your screen:

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! Successful completion of metgrid. !

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

# Remember to check the generated nc files, download and check them with panoply.

### Run WRF on NASA HPC

## upload the met nc files from the previous steps to the NASA HPC

# edit your namelist for wrf run

###Run the model (real.exe & wrf.exe)

## Ensure you are in the WRF/ directory. For this case we are going to run in the test/em\_real/ directory.

cd test/em\_real

###### wrf namelist

&time\_control

run\_days = 3,

run\_hours = 0,

run\_minutes = 0,

run\_seconds = 0,

start\_year = 2018, 2018, 2000,

start\_month = 05, 05, 01,

start\_day = 26, 25, 24,

start\_hour = 00, 12, 12,

end\_year = 2018, 2018, 2000,

end\_month = 05, 05, 01,

end\_day = 29, 30, 25,

end\_hour = 00, 00, 12,

interval\_seconds = 21600,

input\_from\_file = .true.,.true.,.true.,

history\_interval = 60, 60, 60,

frames\_per\_outfile = 1000, 1000, 1000,

restart = .false.,

restart\_interval = 180,

io\_form\_history = 2,

io\_form\_restart = 2,

io\_form\_input = 2,

io\_form\_boundary = 2,

debug\_level = 0,

/

&domains

time\_step = 1,

time\_step\_fract\_num = 0,

time\_step\_fract\_den = 1,

max\_dom = 1,

e\_we = 642,

e\_sn = 521,

e\_vert = 33, 33, 33,

p\_top\_requested = 5000,

num\_metgrid\_levels = 32,

num\_metgrid\_soil\_levels = 4,

dx = 4000, 4000, 3333.33,

dy = 4000, 4000, 3333.33,

grid\_id = 1, 2, 3,

parent\_id = 1, 1, 2,

i\_parent\_start = 1, 220,

j\_parent\_start = 1, 37,

parent\_grid\_ratio = 1, 3,

parent\_time\_step\_ratio = 1, 3,

feedback = 1,

smooth\_option = 0,

/

&physics

mp\_physics = 3, 3, 3,

ra\_lw\_physics = 1, 1, 1,

ra\_sw\_physics = 1, 1, 1,

radt = 30, 30, 30,

sf\_sfclay\_physics = 1, 1, 1,

sf\_surface\_physics = 2, 2, 2,

num\_soil\_layers = 4,

bl\_pbl\_physics = 1, 1, 1,

bldt = 0, 0, 0,

cu\_physics = 1, 1, 0,

cudt = 5, 5, 5,

isfflx = 1,

ifsnow = 1,

icloud = 1,

surface\_input\_source = 3,

num\_land\_cat = 21,

sf\_urban\_physics = 0, 0, 0,

sf\_ocean\_physics = 0,

/

&fdda

/

&dynamics

hybrid\_opt = 2,

w\_damping = 0,

epssm = 0.2, 0.2, 0.2

diff\_opt = 1, 1, 1,

km\_opt = 4, 4, 4,

diff\_6th\_opt = 0, 0, 0,

diff\_6th\_factor = 0.12, 0.12, 0.12,

base\_temp = 290.

damp\_opt = 3,

zdamp = 5000., 5000., 5000.,

dampcoef = 0.2, 0.2, 0.2

khdif = 0, 0, 0,

kvdif = 0, 0, 0,

non\_hydrostatic = .true., .true., .true.,

moist\_adv\_opt = 1, 1, 1,

scalar\_adv\_opt = 1, 1, 1,

gwd\_opt = 1,

/

&bdy\_control

spec\_bdy\_width = 5,

spec\_zone = 1,

relax\_zone = 4,

specified = .true., .false., .false.,

nested = .false., .true., .true.,

/

&grib2

/

&namelist\_quilt

nio\_tasks\_per\_group = 0,

nio\_groups = 1,

/

&chem

kemit = 1,

chem\_opt = 300,300,

bioemdt = 0,0,

photdt = 0,0,

chemdt = 10,10,

io\_style\_emissions = 0,

emiss\_opt = 0,0,

emiss\_opt\_vol = 0,0,

emiss\_ash\_hgt = 20000.,

chem\_in\_opt = 0,0,

phot\_opt = 0,0,

gas\_drydep\_opt = 0,0,

aer\_drydep\_opt = 1,1,

bio\_emiss\_opt = 0,0,

dust\_opt = 3,

dust\_veg =1,

dust\_alpha = 10,

dmsemis\_opt = 0,

seas\_opt = 0,

gas\_bc\_opt = 0,0,

gas\_ic\_opt = 0,0,

aer\_bc\_opt = 1,1,

aer\_ic\_opt = 1,1,

gaschem\_onoff = 0,0,

aerchem\_onoff = 1,1,

wetscav\_onoff = 0,0,

cldchem\_onoff = 0,0,

vertmix\_onoff = 1,1,

chem\_conv\_tr = 0,0,

conv\_tr\_wetscav = 0,0,

conv\_tr\_aqchem = 0,0,

biomass\_burn\_opt = 0,0,

plumerisefire\_frq = 30,30,

have\_bcs\_chem = .false.,.true.,

aer\_ra\_feedback = 1,1,

aer\_op\_opt = 0,1,

opt\_pars\_out = 1,

###. Link in the met\_em files uploaded from server

ln -sf <your path to ncfiles>

# Check the created soft links to met\_em\* files

./real.exe

## Wait for the real running to finish, and this will overwrite wrfinput\_d01 and #wrfbdy\_d01 files you may have from previous runs, so save your old files #somewhere else if you would like to keep them.

# Check that the following two files have been created

wrfinput\_d01

wrfbdy\_d01

#If yes, go on

# Run wrf.exe with a script (verify that the program ran correctly)

# create a job script as follow:

#!/bin/csh

#PBS -l walltime=3:00:00

#PBS -lselect=30:ncpus=24:mpiprocs=24:model=has

#PBS -W umask=037

#PBS -j oe

#PBS -r n

#PBS -e myscript.err

module purge

module load comp-intel

module load mpi-hpe/mpt

module load hdf4/4.2.12 hdf5/1.8.18\_serial netcdf/4.4.1.1\_serial

setenv MPI\_PROCS number of processors.

mpiexec -np $MPI\_PROCS ./wrf.exe >& wrf.out

#####run the following command now the model is running

qsub your name for the script

#### you should see the following files have been created after the wrf running for ###a few hours with the error log files named as: rsl.\* …………

wrfout\_d01\_2018-05-26\_12:00:00

wrfout\_d01\_2018-05-26\_13:00:00

wrfout\_d01\_2018-05-26\_14:00:00

wrfout\_d01\_2018-05-26\_15:00:00

wrfout\_d01\_2018-05-26\_16:00:00

wrfout\_d01\_2018-05-26\_17:00:00

wrfout\_d01\_2018-05-26\_18:00:00

wrfout\_d01\_2018-05-26\_19:00:00

wrfout\_d01\_2018-05-26\_20:00:00

wrfout\_d01\_2018-05-26\_21:00:00

wrfout\_d01\_2018-05-26\_22:00:00

……..

Reference：

WRF users page：<http://www2.mmm.ucar.edu/wrf/users/>

WRF installation: https://www2.mmm.ucar.edu/wrf/OnLineTutorial/compilation\_tutorial.php#STEP1