

Practice Instruction for Online-Coupled WRF-Chem Version 4.6.0

Training Manual for the Hands-on Training Session on WRF-Chem

**The World Meteorological Organization's
Training course on Seamless Prediction of Air Pollution in Africa,
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1 WRF-Chem introduction

Many countries set their own standards for air pollutants criteria. The United States, the Environmental Protection Agency (US EPA) has established the National Ambient Air Quality Standards (NAAQS), while the World Health Organization (WHO) has set air quality guidelines (AQG) as global targets for national governments to improve air quality (US EPA, 2024; WHO, 2024). Reducing air pollution levels is a complex process, as the formation of ozone (O_3) and fine particulate matter ($PM_{2.5}$) involves many physical and chemical processes in the atmosphere. To effectively regulate the levels of O_3 and $PM_{2.5}$, it is essential not only to reduce emission sources but also to understand their formation pathways.

Three-dimensional (3-D) air quality models have been developed to resemble the various atmospheric processes that affect the fate and transport of air pollutants. They are powerful tools for a wide range of applications to understand air pollution and support the development of relevant emission reduction strategies in many countries of the world. These models estimate air pollutant concentrations based on emissions and meteorology (in case of offline models). The outputs help in understanding interactions between emissions and meteorology and their impacts on air quality, which can support not only short-term air pollution alerts and actions but also long-term emission control strategies for local governments.

The Weather Research and Forecasting (WRF) model coupled with Chemistry (WRF-Chem) is a 3-D online-coupled meteorology and chemistry model. It is a collaborative effort among scientists from NCAR, NOAA, and PNNL in the US, and many community users worldwide. Unlike offline models, WRF-Chem model accounts for two-way feedback between meteorology and chemistry (in particular, the aerosol-cloud-radiation-climate interactions), which can more realistically replicate the real atmosphere and thus improve the overall accuracy of air quality predictions and forecasts (Zhang, 2008; Grell and Baklanov, 2011; Baklanov et al., 2014).

2 Objectives of the Practice

We will set up two sets of simulations with the latest release of WRF-Chem 4.6.0. The objectives of this practice are to

1. Become familiar with WRF-Chem by reading WRF-Chem users' guide, this training manual, and relevant literatures on WRF-Chem
2. Learn how to compile, set up, and run WRF-Chem
3. Apply WRF-Chem over North Africa with 36-km resolution for two distinct weeks: January and April 2023, during which anthropogenic emissions in conjunction with temperature inversion and dust storms, respectively, were mainly responsible for observed high PM concentrations in Northern Africa.

4. Study the impacts of different PBL schemes, land surface modules, cumulus parameterizations, and dust emission schemes on air quality predictions.
5. Learn how to post-process the outputs, visualize the results, and evaluate the model with observational datasets and MERRA-2 reanalysis datasets.

3 Basic Linux commands

1. *ls* list the contents of a directory
2. *pwd* print out the full path of the current working directory
3. *cd* navigate between directories
4. *cd..* go up one directory
5. *mkdir* make directories/folders
6. *rm* delete files and folders
7. *mv* move files / directories from one to another; change name of files or directories
8. *cp* copy files / directories
9. *vim* open to edit files using VIM as a text editor
10. *tar* archive files with or without compression
11. *grep* search for specific files / keywords
12. *find* search for a file within a directory
13. *tail* print the last few lines from files
14. *diff* compare 2 files and print the differences
15. *wget* download files from the internet
16. *history* show previous command from terminal
17. *export* export the environment variables

https://docs.lxp.lu/first-steps/basic_linux/

4 Required Libraries and Environments

4.1 Required Libraries

- *zlib* (<https://www.zlib.net/>)
- *HDF5* (<https://www.hdfgroup.org/>)
- *NetCDF* (<https://downloads.unidata.ucar.edu/netcdf/>)
- *JasPer* (<https://www.linuxfromscratch.org/blfs/view/git/general/jasper.html>)
- *libpng* (<http://www.libpng.org/pub/png/libpng.html>)

4.2 Load available modules and export NETCDF/YACC/FLEX environments

HPCs have compiled libraries and software. Loading modules from HPCs allow us to use the required libraries without compiling the packages.

- `module load intel/compilers-2021.2.0`
- `module load intel/mpi-2021.2.0`
- `export NETCDF=/work/zhanglab/kdo/sharedDrive/wrf_libs_intel`
- `export NETCDF_classic=1`
- `export HDF5=/work/zhanglab/kdo/sharedDrive/wrf_libs_intel`
- `export FLEX_LIB_DIR='/work/zhanglab/kdo/sharedDrive/LIBRARIES/flex-2.5.3/lib'`
- `export YACC='/work/zhanglab/kdo/sharedDrive/LIBRARIES/yacc/byacc-20121003/yacc -d'`
- `export JASPERLIB=/work/zhanglab/kdo/sharedDrive/wrf_libs_intel/lib/`
- `export JASPERINC=/work/zhanglab/kdo/sharedDrive/wrf_libs_intel/include/`
- `export LD_LIBRARY_PATH=/work/zhanglab/kdo/sharedDrive/wrf_libs_intel/lib:${LD_LIBRARY_PATH}`

4.3 Set up environments for compiler (Intel)

- `export CC=icx`
- `export CXX=icx`
- `export F77=ifort`
- `export F90=ifort`
- `export FC=ifort`

4.4 Flags for WRF-Chem compilation

- `export WRFIO_NCD_LARGE_FILE_SUPPORT=1`
- `export WRF_EM_CORE=1`
- `export WRF_CHEM=1`
- `export WRF_KPP=1`

- `export WRF_NMM_CORE=0`
- `export WRF_DA_CORE=0`

5 WRF-Chem Compilation

5.1 Compile NCL and NCVIEW (Optional)

1. NCL language package for visualizing WRF Domain from namelist.wps

- `mkdir ~/ncl`
- `cd ~/ncl`
- `wget https://www.earthsystemgrid.org/dataset/ncl.640.nodap/file/ncl_ncarg-6.4.0-RHEL6.4_64bit_nodap_gnu447.tar.gz`
- `tar -xvzf ncl_ncarg-6.4.0-RHEL6.4_64bit_nodap_gnu447.tar.gz`
- `export NCARG_ROOT=$HOME/ncl`
- `export PATH=$NCARG_ROOT/bin:$PATH`

2. NCVIEW for visualizing WRF-Chem outputs

a. Move to a compute node by running the following command

```
srun --pty /bin/bash
```

Or

```
srun --time=6:00:00 --job-name=testWRF --ntasks=2 --partition=zhang --pty /bin/bash
```

b. Load anaconda module

```
module load anaconda3/2022.05
```

c. Set up a conda environment

i. First create a conda environment

```
conda create -n <your-env-name> python=3.11
```

ii. Activate your environment

```
source activate <your-env-name>
```

d. Install NCVIEW

```
conda install conda-forge::ncview
```

5.2 Compile WRF

Clone from GitHub

- `git clone --recurse-submodules https://github.com/wrf-model/WRF`

- cd WRF
- ./configure
- **Choose option: 16**
- ./compile em_real 2>&1 | tee compile.log

5.3 Compile WPS

- cd ..
- git clone <https://github.com/wrf-model/WPS>
- cd WPS
- export WRF_DIR=../WRF-4.2.1/
- export JASPERLIB=/home/kh.do/wrf/wrf_libs_intel/lib/
- export JASPERINC=/home/kh.do/wrf/wrf_libs_intel/include/
- export LD_LIBRARY_PATH=/home/kh.do/wrf/wrf_libs_intel/lib:\${LD_LIBRARY_PATH}
- ./configure
- **Choose option: 16**
- **Edit *configure.wps* by adding `-qopenmp` at the end of the lines that set WRF_LIB (after `-lnetcdf -lnetcdf`)**
- ./compile 2>&1 | tee compile.log

Note: in case that you are not able to compile, you can use NETCDF from module

- export NETCDF=/shared/centos7/netcdf/4.7.4-intel2020

6 Simulation Design and Model Configurations

Table 1 summarizes the simulation design and purposes. Two sets of simulations will be carried out in January and April 2023. Each set will have 5 simulations including 1 baseline, and 4 sensitivity simulations. The baseline WRF-Chem configurations for the two simulation periods are identical (simulations 1 and 6), simulations 2-5 for January and 7-10 for April will change one scheme at one time and the results can be compared with respective baseline simulations to study the impacts of different schemes on meteorology and air quality predictions.

Table 1. Simulation design and purposes

Time period	Model configuration	Simulation & Group#
-------------	---------------------	---------------------

January 1-7, 2023	Baseline	January baseline case, Group 1
	YSU PBL scheme+ Monin-Obukhov surface layer scheme (change bl_pbl_physics from 7 to 1 and sf_sfclay_physics_ from 7 to 1)	PBL scheme coupled with the Monin-Obukhov surface layer scheme, Group 2
	Lin scheme (change mp_physics from 10 to 2)	Cloud macrophysics, Group 3
	Tiedtke cumulus scheme (change cu_physics from 11 to 6)	Cumulus parametrization, Group 4
	Dust (Shao et al., 2011) (change the dust_opt 3 to 4 and set dust_scheme to 3)	Dust emissions
April 1-7, 2023	Baseline	April baseline case, Group 5
	YSU PBL scheme (change bl_pbl_physics from 7 to 1 and sf_sfclay_physics_ from 7 to 1)	PBL scheme coupled with the Monin-Obukhov surface layer scheme, Group 6
	Lin scheme (change mp_physics from 10 to 2)	Cloud macrophysics, Group 7
	Tiedtke cumulus scheme (change cu_physics from 11 to 6)	Cumulus parametrization, Group 8
	Dust (Shao et al., 2011) (change the dust_opt 3 to 4 and set dust_scheme to 3)	Dust emissions, Group 9

Table 2. Sources of the WRF-Chem inputs

Inputs	Sources	Links to datasets
Meteorology IC/BC	NCEP Final analysis	https://rda.ucar.edu/datasets/d083003/

	0.25 degree (NCEP-FNL, 2020)	
Fire emissions	FINNv2.5	https://rda.ucar.edu/datasets/ds312.9/dataaccess/
Biogenic emissions	MEGAN2	https://www.acom.ucar.edu/wrf-chem/download.shtml
Anthropogenic emis	EDGARv8.1	https://edgar.jrc.ec.europa.eu/dataset_ap81
Chem IC/BC	WACCM	https://rda.ucar.edu/datasets/d313006/dataaccess
Geographic data	WPS V4 Geographical Static Data	https://www2.mmm.ucar.edu/wrf/users/download/get_sources_wps_geog.html
Land use data	MODIS	https://modis.gsfc.nasa.gov/data/dataproduct/mod12.php

6.1 WRF-Chem model setup

Table 3 summarizes the physics and chemistry options used in WRF-Chem simulations.

Table 3. WRF-chem 4.6.0 model options.

Parameter	Options
Shortwave radiation	RRTMG shortwave (Iacono et al., 2008)
Longwave radiation	Updated RRTMG scheme (Iacono et al., 2008)
Cloud microphysics	Morrison 2-moment scheme (Morrison et al., 2009)
Surface layer	Pleim-Xiu (Pleim, 2006)
Land surface	Pleim-Xiu Land Surface Model (Pleim & Xiu, 1995, 2003; Xiu & Pleim, 2001)
Boundary layer	ACM2 PBL (Pleim, 2007)
Cumulus clouds	Multi-scale Kain-Fritsch Scheme (Zheng et al., 2016) 2005 Carbon Bond chemistry mechanism (CB05)
Gas-phase chemistry	(Wang et al., 2015)
Photolysis	Fast-J photolysis (Barnard, 2004; Wild et al., 2000) Modal aerosol dynamics model for Europe (MADE)
Aerosol chemistry	(Ackermann et al., 1998)
Secondary organic aerosol	Volatility Basis Set (VBS) (Ahmadov et al., 2012)
Biogenic emissions	Model of Emissions of Gases and Aerosols from Nature (MEGAN 2) (Guenther et al., 2006) GOCART ^a dust emissions with AFWA ^b modifications
Dust emissions	(LeGrand et al., 2019)
Sea salt emissions	GOCART ^a sea salt emission scheme (Gong, 2003)
Fire emissions	Fire Inventory from NCAR (FINN) (Wiedinmyer et al., 2011)
Surface roughness correction	Jiménez & Dudhia (2012)
Urban canopy model	Urban Canopy Model (Chen et al., 2011)

^a Global Ozone Chemistry Aerosol Radiation and Transport; ^b US Air Force Weather Agency

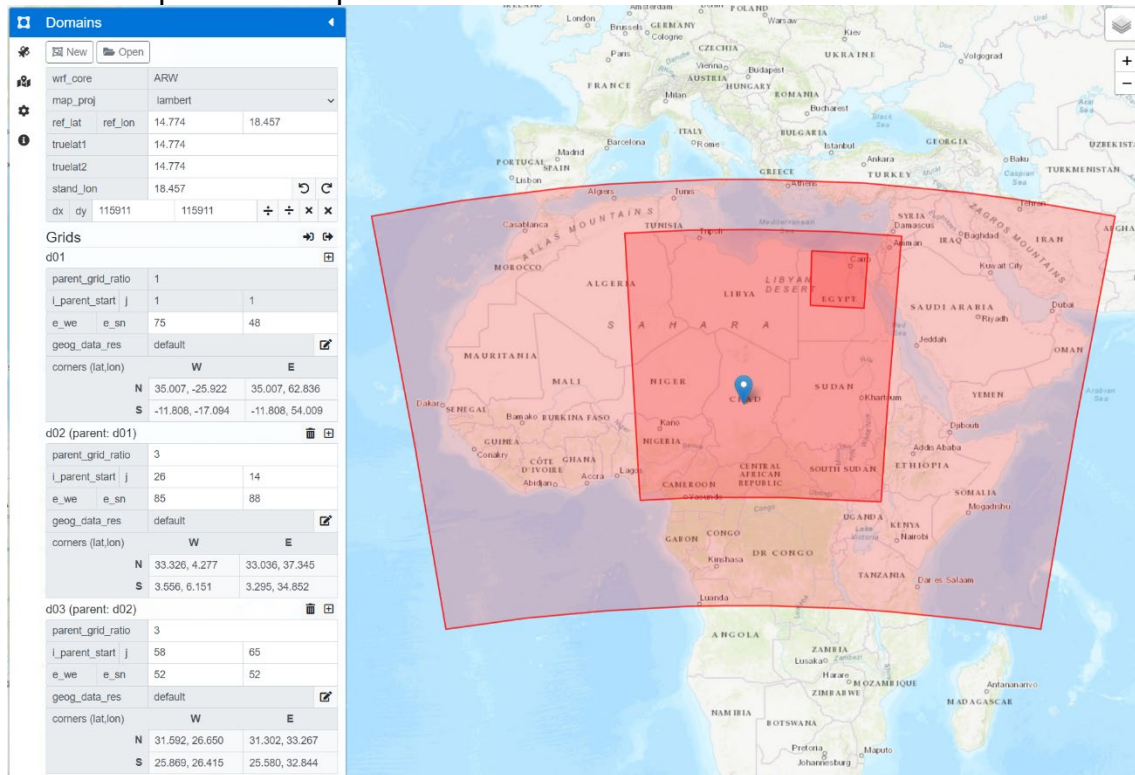
7 Schedule for the Exercise

Schedule for the training (excluding coffee break and lunch time)

Date	Time	Duration	Materials to be Covered	Comments
Day 1	9:00-9:30	30-min	Welcome and introduction of the hands-on by Zeinab Salah (EMA) and Sara Basart (WMO)	All groups together
	9:30-10:30	1-hr	Overview of the training by Yang Zhang, input processing by Daniel Schuch, and model setup, job submission and post-processing by Khanh Do	All groups together
	11:00-12:30	1.5-hr	Hands-on WRF-Chem practice based on the training manual (model setup, compilation, job submission)	Split into 9 working groups in two rooms
	13:30-15:00	1.5-hr	Continue to practice WRF-Chem and submit the jobs	Split into 9 working groups in two rooms
	15:30-17:00	1.5-hr	Continue to practice WRF-Chem and submit the jobs	Each group working with a goal to submit the job successfully on Day 1
Day 2	9:00-9:15	15-min	Welcome and follow-up of the previous day by Zeinab Salah (EMA) and Sara Basart (WMO)	All groups together
	9:15-10:30	1-hr and 15-min	African emission data processing by Sekou Keita	All groups together
	10:45-12:00	1-hr and 15-min	Hands-on WRF-Chem practice based on the training manual (output post-processing and evaluation, and analysis)	Split into 9 working groups in two rooms
	14:00-15:45	1-hr and 45-min	Continue to postprocess results, and generate presentation slides for January (by Groups 1-4) and April (Groups 5-9) simulations	Groups 1-4 and 5-9 work together to compare results and make slides for each group
	16:00-17:00	1-hr	Group presentations: 20 min presentation + 10 min discussion for each presentation group	Each working group sends a representative to form a 4- or 5-person presentation group for Jan and April, and give group presentations
	17:00-17:30	30-min	Reflections and feedback	All groups together

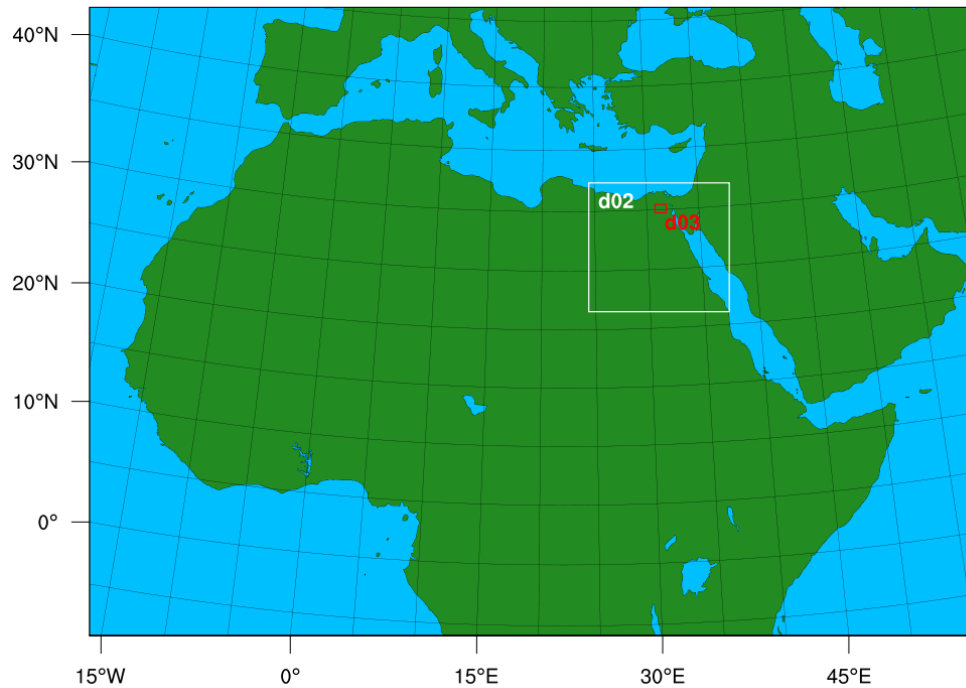
8 Design a WRF domain

- Preliminarily design and visualize the WRF domain using WRF Domain Wizard, <https://jirichter.github.io/WRFDomainWizard/>, which provides a friendly graphical user interface. Fine tune the domain should be verified by plotting the namelist.wps or the output from WPS.



- Copy the namelist.wps to ~/WPS/util folder and run ncl plotgrids_new.ncl to visualize the domain design.

WPS Domain Configuration



- For more information
 - https://www2.mmm.ucar.edu/wrf/users/namelist_best_prac_wps.html

9 Exercises

9.1 Use Discovery

- Linux and MAC systems
 - Open terminal and log in Discovery with `ssh username.login.discovery.neu.edu`
- On Windows computers
 - Option 1
 - Use PowerShell from Windows and log in with `username.login.discovery.neu.edu`
 - Option 2
 - Download PuTTY from <https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html>
 - Open PuTTY and enter `login.discovery.neu.edu` in Host Name
 - Login as: your username and password

- Shared folder on Discovery located at /work/zhanglab/kdo/sharedDrive where the required inputs can be found (i.e., anthropogenic, fire, biogenic emissions, GFS, and run scripts).

9.2 Run WRF-Chem

9.2.1 Run WPS

- Make a new WPS directory and symbolic soft link the files from original WPS directory to the newly created WPS directory.

- Load the require environments and libraries

```
module load intel/compilers-2021.2.0
module load intel/mpi-2021.2.0
module load netcdf/4.7.4-intel2020
module load hdf5/1.12.0-intel2021.2
module load anaconda3/2020.02
export
LD_LIBRARY_PATH=/home/kh.do/wrf/wrf_libs_intel/lib:${LD_LIBRARY_PATH}
```

- Modify the namelist.wps according to:

```
&share
wrf_core = 'ARW',
max_dom = 3,
start_date = '2023-01-01_00:00:00','2023-01-01_00:00:00','2023-01-01_00:00:00',
end_date   = '2023-02-01_00:00:00','2023-02-01_00:00:00','2023-02-01_00:00:00',
interval_seconds = 21600,
/
```

```
&geogrid
parent_id           = 1, 1, 2,
parent_grid_ratio  = 1, 6, 6,
i_parent_start     = 1, 129, 103,
j_parent_start     = 1, 84, 153,
e_we               = 229, 217, 103,
e_sn               = 162, 199, 79,
geog_data_res      = '30s','30s','30s',
dx                 = 36000,
dy                 = 36000,
```

```

map_proj          = 'lambert',
ref_lat           = 20.715,
ref_lon           = 19.336,
truelat1          = 0.0,
truelat2          = 30.0,
stand_lon         = 22.0,
geog_data_path    = '/scratch/schuch/DATA/WPS_GEOG/'
/

&ungrib
out_format = 'WPS',
prefix = 'FILE',
/

&metgrid
fg_name = 'FILE'
/

```

- Run `./link_grib.csh`
`/work/zhanglab/kdo/sharedDrive/aprilData/GFS/*` . to create soft link the gfs data files to WPS folder.
- Run `./geogrid.exe`. This task takes a lot of time for this large domain. We recommend using our pre-processed geogrid files located in the shared folder.
- Run `./ungrib.exe`. Note that `geogrid.exe` is independent of `ungrib.exe`. However, `metgrid.exe` requires both outputs from `geogrid` and `ungrib`.
- Finally, run `metgrid.exe` to complete the WPS.

9.2.2 Run WRF-Chem

- Go to your scratch folder
- Make a new WRF directory and copy the files from original WRF directory to the newly created WRF directory.
 - `mkdir WRF_Chem && cd WRF_Chem`
 - `cp -r /work/zhanglab/kdo/sharedDrive/WRFv4_6/WRF/` .
- Remove the `namelist.input` and copy the `namelist.input` from the sharedDrive
 - `rm namelist.input`
 - `cp`
`/work/zhanglab/kdo/sharedDrive/namelists/namelist_base`
`/*` .
- Copy emissions from the sharedDrive to the working WRF folder

- o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/emissions/* .
- Copy fire emissions to the working directory
 - o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/fire/* .
- Copy preprocessed met_em* from WPS
 - o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/met_em/* .
- Copy biogenic emissions
 - o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/megan/* .
- Copy the run script to the working directory
 - o cp /work/zhanglab/kdo/sharedDrive/aprilData/runWRF.sh .
- Copy met ICON/BCONS
 - o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/ICBC/* .
- Copy chem ICON/BCONS for warm start
 - o cp /work/zhanglab/kdo/sharedDrive/**aprilData**/output/* .
- Copy the run script to the working folder
 - o cp /work/zhanglab/kdo/sharedDrive/namelist/**run_WRF-Chem_apr_node4000.sh** .
- Submit the jobs: sbatch **run_WRF-Chem_apr_node4000.sh**
- Monitor the jobs: squeue -u **yourAccount**

9.3 Evaluation

Create and load **conda** environment. If you have created conda environment from the previous steps, start from step 3b (source activate <your-env-name>).

1. Move to compute node


```
srun --pty /bin/bash
```
2. Load anaconda module


```
module load anaconda3/2022.05
```
3. Set up a conda enviroment
 - a. First create a conda environment


```
conda create -n <your-env-name> python=3.11
```
 - b. Activate your environment:


```
source activate <your-env-name>
```
4. Install packages using pip or conda
 - a. pip install netCDF4
 - b. pip install geopandas
 - c. pip install xarray

d. other libraries

For all evaluation, change the file input path in python evaluation scripts

9.4 Meteorology evaluation

Dataset descriptions: For meteorology, we use the NOAA Global Hourly Integrated Surface Database (ISD), including wind speed (WS), wind direction (WD), temperature (T), dew point (DT), precipitation, and other parameters over 35,000 stations around the world from 1901 – present (<https://www.ncei.noaa.gov/products/land-based-station/integrated-surface-database>). The ISD dataset can be downloaded at <https://www.ncei.noaa.gov/data/global-hourly/>. Note that all evaluation results in terms of tables and figures were based on initial configurations used during the preliminary testing, they may not be the same as the results based on the final model configurations used in this training.

Scripts for evaluation: We provided the downloaded ISD data for 2023 in the Discovery shared folder. Copy scripts from the `sharedDrive/evaluation/met_evaluation` folder in the shared folder to your scratch directory.

1. Request interactive compute node and load conda environment
 - a. `srun --pty /bin/bash`
 - b. `module load anaconda3/2022.05`
 - c. `source activate /scratch/kh.do/WRFChemWorkshop/`
2. Copy evaluation scripts from sharedDrive to your local folder `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/met_evaluation/* /your/folder/path/`
3. Run `extract_met_based_on_WRF_domain.py` to extract the meteorological data from 13,400 locations, filtering it to only locations within the simulation domain for the specified timeframe.

Table 4. Extracted meteorological observations from ISD based on WRF domain.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	
1	STATION	DATE	SOURCE	LATITUDE	LONGITUDE	ELEVATION	NAME	REPORT_TYPE	CALL	SIGN	QUALITY_CONTROL	WIND	CIG	VIS	TMP	DEW	SLP
2	7502099999	2023-01-01T00:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	100.1.N.0015.1	99999.9.9.N	060000.1.9.9	+0147.1	+0029.1	10191.1
3	7502099999	2023-01-01T00:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	999.9.V.0015.1	99999.9.9.Y	009900.5.9.9	+0150.1	+0030.1	99999.9
4	7502099999	2023-01-01T00:30:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	070.1.V.0015.1	99999.9.9.Y	009900.5.9.9	+0150.1	+0030.1	99999.9
5	7502099999	2023-01-01T01:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	180.1.N.0051.1	99999.9.9.N	060000.1.9.9	+0152.1	+0030.1	10189.1
6	7502099999	2023-01-01T01:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	180.1.N.0051.1	99999.9.9.Y	009900.5.9.9	+0150.1	+0030.1	99999.9
7	7502099999	2023-01-01T01:30:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	180.1.N.0057.1	99999.9.9.Y	009900.5.9.9	+0160.1	+0030.1	99999.9
8	7502099999	2023-01-01T02:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	190.1.N.0057.1	99999.9.9.N	060000.1.9.9	+0156.1	+0031.1	10191.1
9	7502099999	2023-01-01T02:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	190.1.N.0057.1	99999.9.9.Y	009900.5.9.9	+0160.1	+0030.1	99999.9
10	7502099999	2023-01-01T02:30:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	250.1.V.0041.1	99999.9.9.Y	009900.5.9.9	+0160.1	+0070.1	99999.9
11	7502099999	2023-01-01T03:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	260.1.N.0046.1	99999.9.9.N	050000.1.9.9	+0161.1	+0076.1	10198.1
12	7502099999	2023-01-01T03:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	260.1.V.0046.1	99999.9.9.Y	009900.5.9.9	+0160.1	+0080.1	99999.9
13	7502099999	2023-01-01T03:30:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	260.1.V.0046.1	99999.9.9.Y	009900.5.9.9	+0160.1	+0080.1	99999.9
14	7502099999	2023-01-01T04:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	310.1.N.0015.1	99999.9.9.N	017000.1.9.9	+0144.1	+0092.1	10195.1
15	7502099999	2023-01-01T04:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	310.1.N.0015.1	99999.9.9.Y	009900.5.9.9	+0140.1	+0090.1	99999.9
16	7502099999	2023-01-01T04:30:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	090.1.N.0026.1	99999.9.9.Y	009900.5.9.9	+0120.1	+0080.1	99999.9
17	7502099999	2023-01-01T05:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-12			99999 V020	999.9.C.0000.1	99999.9.9.N	019000.1.9.9	+0108.1	+0075.1	10192.1
18	7502099999	2023-01-01T05:00:00	4	44.533333	-1.125	25.6	CAZAUX, FR	FM-15			99999 V020	999.9.C.0000.1	99999.9.9.Y	009900.5.9.9	+0110.1	+0080.1	99999.9

- Run `extract_model_and_ISD_data_points.py` to extract model meteorology data along with the corresponding ISD data and write the results to CSV files. This script also calculates domain-wide statistics.

Table 5. Model and observational meteorological data based on temporal and spatial information.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Site Number	Latitude	Longitude	Date_Time	Temperature_Obs	Temperature_Model	Wind_Speed_Obs	Wind_Speed_Model	Wind_Direction_Obs	Wind_Direction_Model	RH_Obs	RH_Model
2	7502099999	44.533333	-1.125	2023-01-01 00:00:00	288.15	289.16	1.50	7.54	999.00	220.28	83.00	53.56
3	7502099999	44.533333	-1.125	2023-01-01 01:00:00	288.35	288.01	5.10	4.47	180.00	206.36	82.74	56.18
4	7502099999	44.533333	-1.125	2023-01-01 02:00:00	288.75	287.32	5.70	3.89	190.00	202.02	82.37	60.47
5	7502099999	44.533333	-1.125	2023-01-01 03:00:00	289.25	286.63	4.60	3.35	260.00	196.08	87.76	64.84
6	7502099999	44.533333	-1.125	2023-01-01 04:00:00	287.55	285.94	1.50	2.87	310.00	188.13	92.32	69.34
7	7502099999	44.533333	-1.125	2023-01-01 05:00:00	283.95	285.24	0.90	2.51	999.00	177.70	95.01	73.84
8	7502099999	44.533333	-1.125	2023-01-01 06:00:00	283.15	284.58	1.50	2.33	80.00	165.19	95.74	77.95
9	7502099999	44.533333	-1.125	2023-01-01 07:00:00	282.35	284.56	2.60	2.67	110.00	166.68	94.53	76.80
10	7502099999	44.533333	-1.125	2023-01-01 08:00:00	282.25	285.24	2.10	3.05	100.00	172.42	93.34	71.45
11	7502099999	44.533333	-1.125	2023-01-01 09:00:00	285.15	287.20	3.10	3.58	160.00	178.15	92.40	63.69
12	7502099999	44.533333	-1.125	2023-01-01 10:00:00	286.85	289.43	3.60	4.32	160.00	183.54	89.88	53.76
13	7502099999	44.533333	-1.125	2023-01-01 11:00:00	290.55	291.18	3.60	5.22	170.00	187.63	85.12	46.05
14	7502099999	44.533333	-1.125	2023-01-01 12:00:00	291.85	292.41	5.10	6.04	160.00	190.14	82.95	41.23
15	7502099999	44.533333	-1.125	2023-01-01 13:00:00	291.75	292.79	9.80	6.22	170.00	190.80	83.34	40.05
16	7502099999	44.533333	-1.125	2023-01-01 14:00:00	293.35	292.59	6.70	5.98	160.00	189.67	83.30	40.83
17	7502099999	44.533333	-1.125	2023-01-01 15:00:00	294.25	291.97	8.80	5.58	180.00	187.41	79.66	42.74
18	7502099999	44.533333	-1.125	2023-01-01 16:00:00	291.15	291.13	4.10	5.22	140.00	184.94	85.82	44.53
19	7502099999	44.533333	-1.125	2023-01-01 17:00:00	288.55	290.40	4.60	5.03	150.00	182.92	89.53	45.06
20	7502099999	44.533333	-1.125	2023-01-01 18:00:00	288.15	290.10	3.10	4.99	80.00	181.51	90.49	45.59
21	7502099999	44.533333	-1.125	2023-01-01 19:00:00	286.95	289.43	3.60	4.13	80.00	182.55	92.30	50.68
22	7502099999	44.533333	-1.125	2023-01-01 20:00:00	286.65	288.20	5.10	3.00	160.00	185.37	91.44	60.76
23	7502099999	44.533333	-1.125	2023-01-01 21:00:00	285.55	286.67	1.00	2.07	210.00	193.35	91.12	74.05
24	7502099999	44.533333	-1.125	2023-01-01 22:00:00	288.15	285.65	4.10	1.73	330.00	218.44	93.78	84.55
25	7502099999	44.533333	-1.125	2023-01-01 23:00:00	287.45	285.48	3.60	1.61	330.00	280.04	96.25	90.55
26	7502099999	44.533333	-1.125	2023-01-02 00:00:00	286.75	285.66	3.10	2.17	330.00	314.83	96.83	94.15
27	7502099999	44.533333	-1.125	2023-01-02 01:00:00	286.55	285.67	2.10	2.63	310.00	314.33	96.83	95.08

- Run `extract_and_compute_met_stats.py` to extract model meteorology data along with corresponding ISD data and compute the statistics for each ISD site.

Table 6. Meteorological statistics for WRF model and observational data.

	A	B	C	D	E	F			
1	CC	R2	MBE	MAE	NMB				
2	wind speed	0.58	0.34	0.07	1.59	0.02			
3	wind direction	0.56	0.31	-0.99	35.24	-0.01			
4	temperature	0.95	0.90	-0.70	2.27	0.00			
5	rh	0.80	0.64	-20.69	21.12	-0.23			
6									
	A	B	C	D	E	F	G	H	I
1	Station	Latitude	Longitude	CC	R2	MBE	MAE	MNB	NMB
2	7502099999	44.53	-1.13	0.93	0.86	0.60	1.62	0.00	0.00
3	7535099999	44.75	1.40	0.93	0.87	-0.97	1.80	0.00	0.00
4	7577099999	44.58	4.73	0.90	0.82	-2.42	2.83	-0.01	-0.01
5	7666099999	42.92	3.07	0.94	0.89	-0.08	1.10	0.00	0.00
6	7667099999	43.10	6.15	0.92	0.85	-0.63	1.54	0.00	0.00
7	7754099999	42.53	8.79	0.91	0.83	-2.98	3.06	-0.01	-0.01
8	7768099999	41.60	9.37	0.91	0.82	-1.93	2.10	-0.01	-0.01
9	8085099999	42.77	-1.65	0.93	0.87	-0.63	1.87	0.00	0.00
10	8094099999	42.08	-0.33	0.95	0.89	-0.88	1.71	0.00	0.00
11	8171099999	41.63	0.60	0.94	0.89	-0.27	1.85	0.00	0.00
12	8213099999	40.95	-4.13	0.94	0.88	-1.48	1.82	-0.01	-0.01
13	8231099999	40.07	-2.13	0.95	0.90	-2.40	2.71	-0.01	-0.01
14	8272099999	39.88	-4.05	0.95	0.90	-2.03	2.39	-0.01	-0.01
15	8540099999	39.83	-8.89	0.94	0.88	-0.31	1.37	0.00	0.00
16	8561099999	38.07	-7.92	0.96	0.91	-0.63	1.24	0.00	0.00
17	8924099999	42.30	-1.57	0.40	0.16	-2.80	5.20	-0.01	-0.01
18	8926099999	42.67	0.02	0.70	0.49	-1.13	3.67	0.00	0.00
19	12982099999	46.25	20.10	0.95	0.90	0.09	1.28	0.00	0.00
20	13285099999	44.75	21.52	0.93	0.86	-1.31	2.01	0.00	0.00
21	13384099999	43.93	21.38	0.94	0.88	-1.17	1.91	0.00	0.00
22	13571099999	42.00	20.97	0.85	0.73	-4.09	4.49	-0.01	-0.01
23	13578099999	41.18	20.74	0.90	0.82	-1.66	2.21	-0.01	-0.01

6. Run `spatial_plot_eval.py` for visualization. This script generates spatial evaluation plots across the domain.

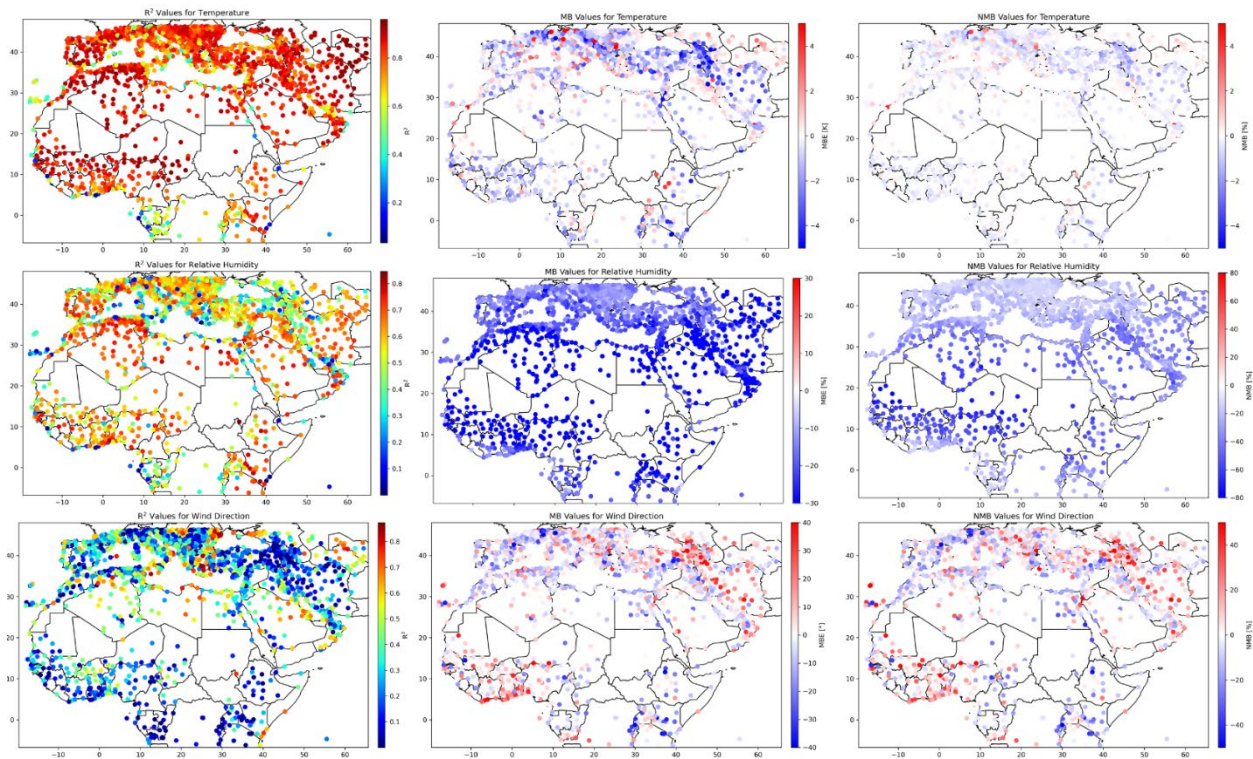


Figure 1. Spatial plot for R^2 , MB, and NMB for WRF outputs.

9.5 PM_{2.5} evaluation

Dataset descriptions: The model's performance can be evaluated using ground observational data, satellite AOD, and reanalysis MERRA-2. Observational air monitoring networks in Africa are sparse, but a few air monitoring networks are publicly accessible, including AirQo (<https://airqo.africa/explore-data>, data is available after July 2023), AirNow (<https://www.airnow.gov/international/us-embassies-and-consulates/>), and SAAQIS for South Africa (<https://saaqis.environment.gov.za/>). In this tutorial, we use AirNow and MERRA-2 (reanalysis data from NASA, <https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/>) to evaluate the WRF-Chem outputs.

Note that all evaluation results in terms of tables and figures were based on initial configurations used during the preliminary testing, they may not be the same as the results based on the final model configurations used in this training.

Scripts for evaluation: Pre-downloaded AirNow and MERRA-2 data are located in the shared folder. Copy scripts from `sharedDrive/evaluation/pm25_evaluation` from the shared directory to your scratch.

1. Copy PM_{2.5} evaluation scripts to your local folder
`/work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/*.py` **/your/folder/path/**
2. Copy AirNow observational data to your local folder `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/2023_Data/` **/your/folder/path/**
3. Copy shapefiles to your local folder `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/shapefiles/` **/your/folder/path/**
4. Run `pm25_eva_apr.py` to extract the PM_{2.5} values from WRF-Chem outputs and AirNow data with respect to temporal and spatial criteria. The script outputs extracted PM_{2.5} from both the model and observation, along with evaluation statistics.

Table 7. Extracted PM_{2.5} from WRF-Chem and AirNow observations.

1	Date_Time	Observation	Model
2	2023-04-06 01:00:00	15.5	8.312355
3	2023-04-06 02:00:00	16.7	8.163019
4	2023-04-06 03:00:00	21.3	7.8404584
5	2023-04-06 04:00:00	20.6	7.3580203
6	2023-04-06 05:00:00	22.3	6.7311463
7	2023-04-06 06:00:00	23.1	5.971729
8	2023-04-06 07:00:00	26.5	5.2735844
9	2023-04-06 08:00:00	28.2	11.810021
10	2023-04-06 09:00:00	26.1	15.36381

Table 8. Statistics for PM_{2.5} output from WRF-Chem and AirNow observations.

	A	B	C	D
1	Location	mbe	mae	nmb
2	Abidjan_IvoryCoast	-12.13	13.62	-58.06
3	Abuja_Nigeria	-1.45	11.03	-5.17
4	Accra_Ghana	-24.84	25.31	-80.23
5	AddisAbabaCentral_Ethiopia	-6.88	13.61	-35.01
6	Algiers_Algeria	-6.76	7.27	-50.92
7	Bamako_Mali	-44.37	45.41	-61.83
8	Cairo_Egypt	-15.33	46.19	-26.45
9	Conakry_Guinea	-12.21	15.93	-43.19
10	Dakar_Senegal	-12.96	23.04	-29.93
11	Kampala_Uganda	-19.52	21.11	-62.01
12	Kinshasa_RepublicOfTheCongo	-2.31	18.77	-9.01
13	Lagos_Nigeria	1.23	8.28	8.01
14	Nairobi_Kenya	-4.42	6.86	-43.57
15	NDjamena_Chad	-134.99	135.59	-76.24
16	Ouagadougou_BurkinaFaso	-30.10	36.76	-43.15

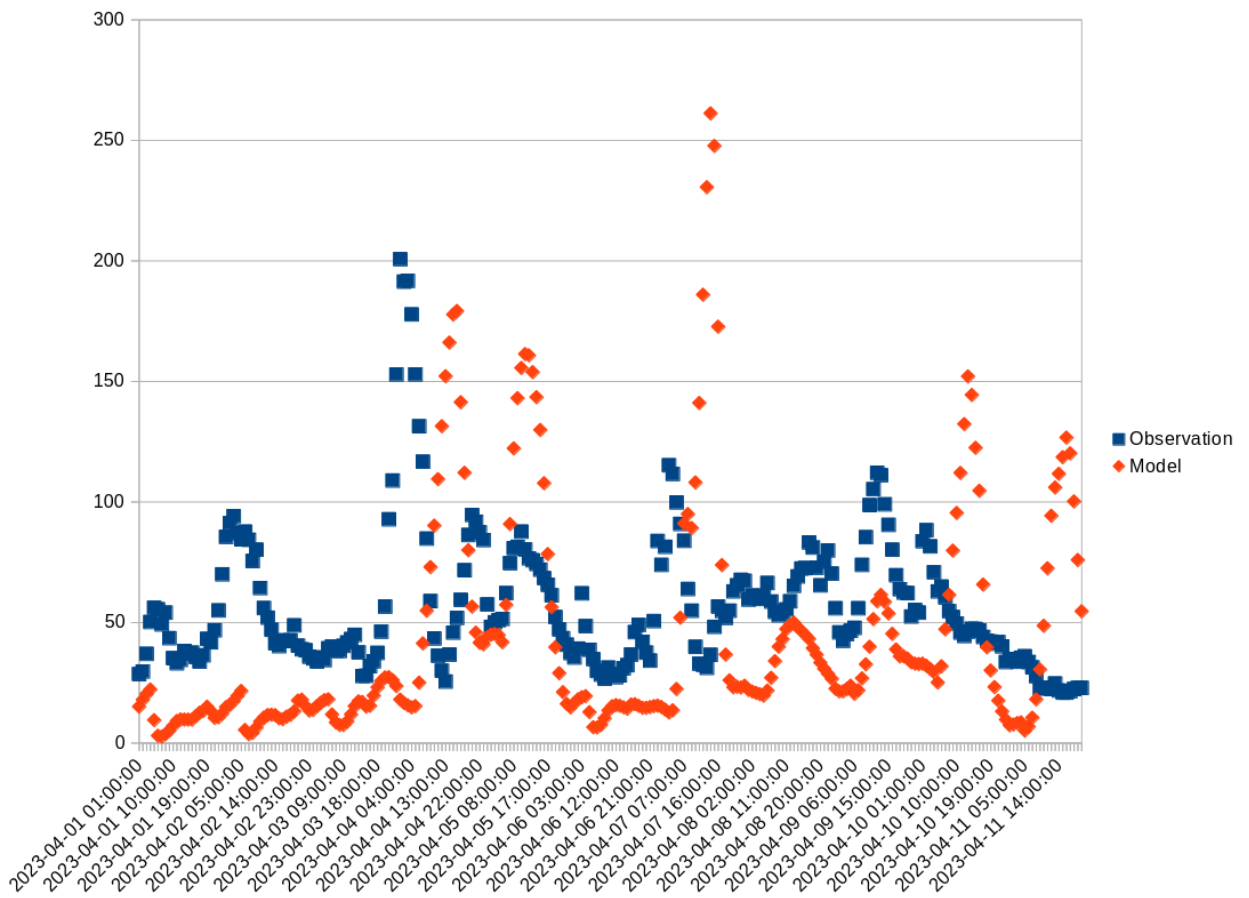


Figure 2. PM_{2.5} time series from Apr 01 to Apr 11, 2023.

- To evaluate the model using MERRA-2 dataset, run `eval_using_merra3.py`. The script calculates the evaluation metrics for the entire domain and generates the spatial plots of the statistic evaluation against the MERRA-2 dataset.

Table 9. Evaluation statistics for PM_{2.5} from WRF-Chem and MERRA-2.

	A	B	C
1	R	MBE	NMB [%]
2		0.54	-16.64
			-42.41

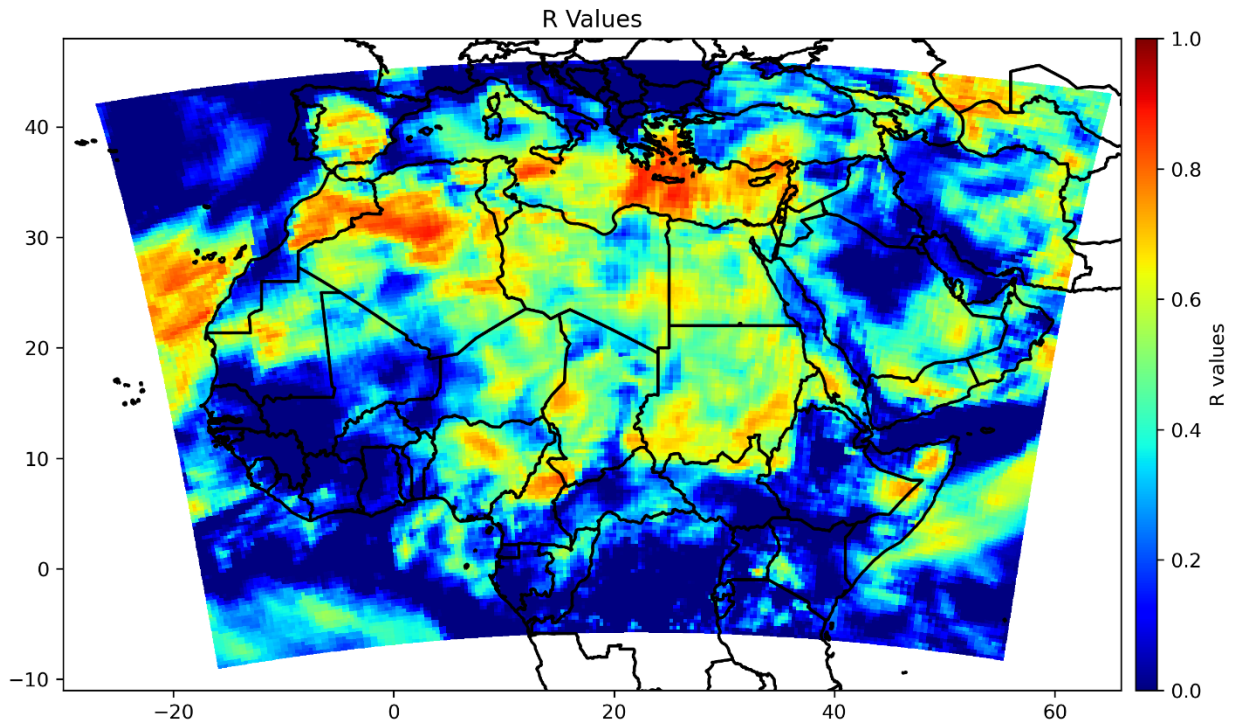


Figure 3. Spatial plot of R value for PM_{2.5} compared to MERRA-2.

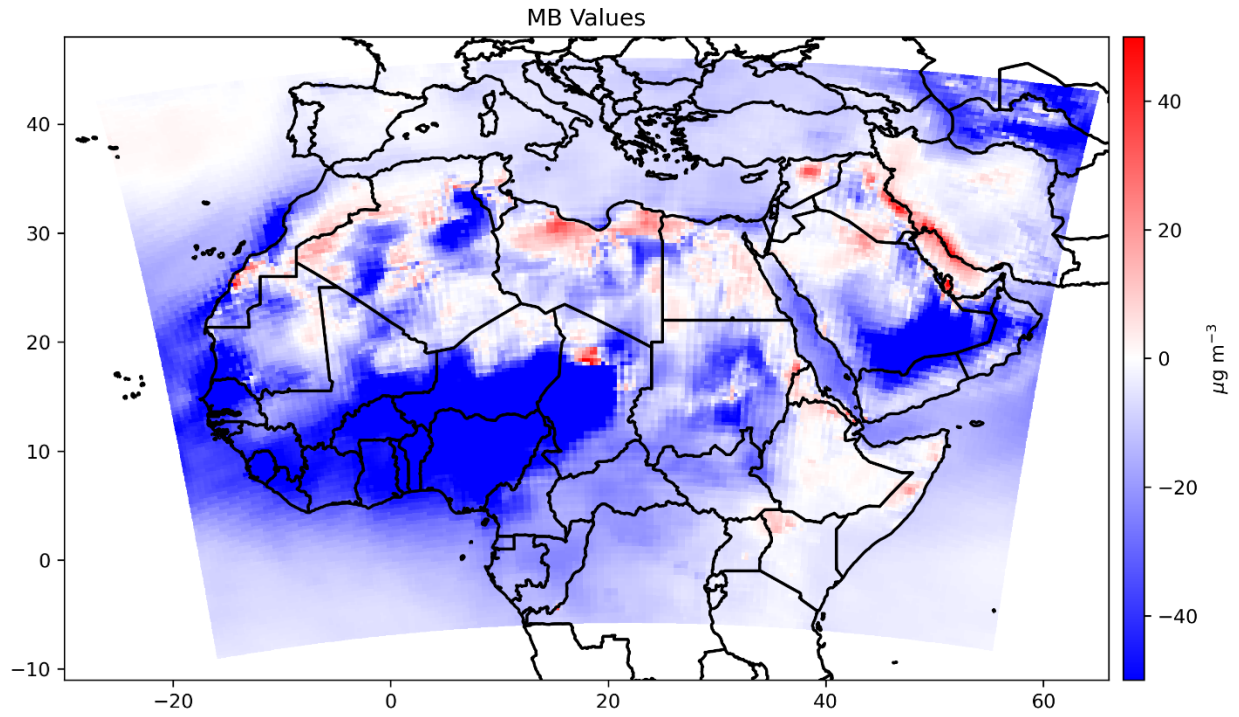


Figure 4. Spatial plot of MB value for PM_{2.5} compared to MERRA-2.

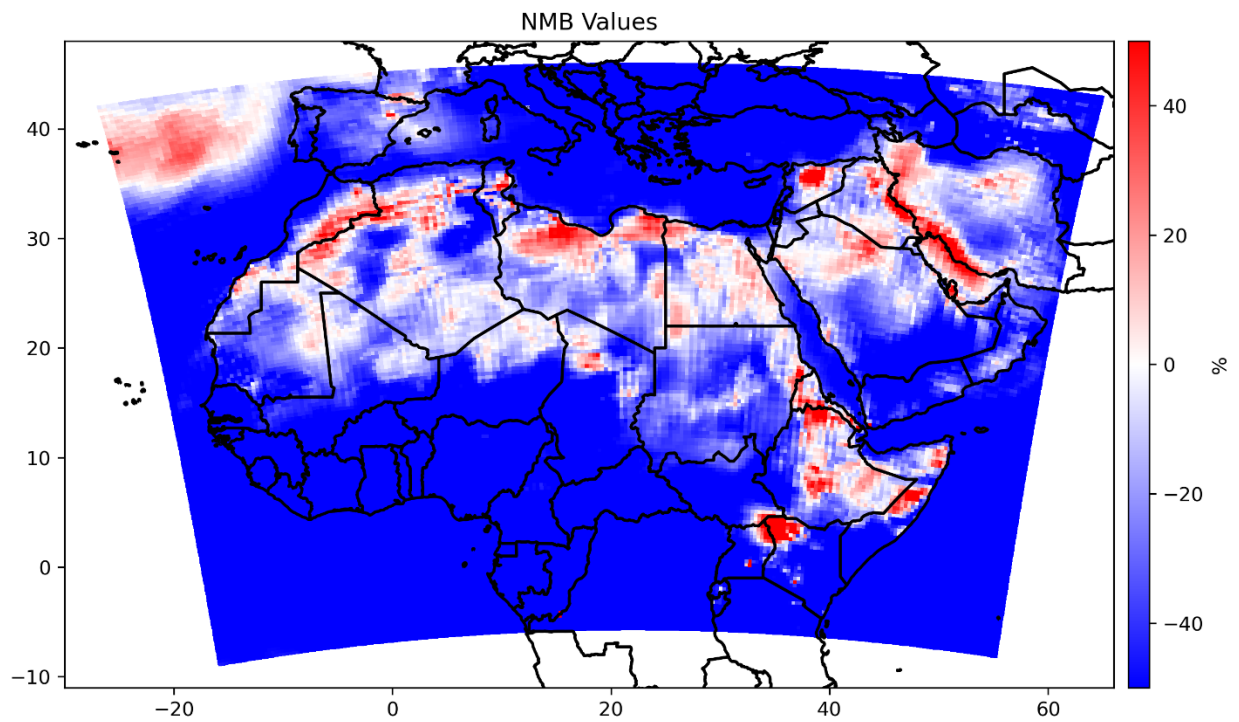


Figure 5. Spatial plot of NMB value for PM_{2.5} compared to MERRA-2.

9.6 Difference plots

We compare the differences in $PM_{2.5}$ concentrations using multiple science schemes and physics. Plotting the spatial differences between scheme 1 and scheme 2 allows us to identify the appropriateness of scheme/physics options applied to a specific region.

Run `pm25DiffPlot.py` to generate the difference plot.

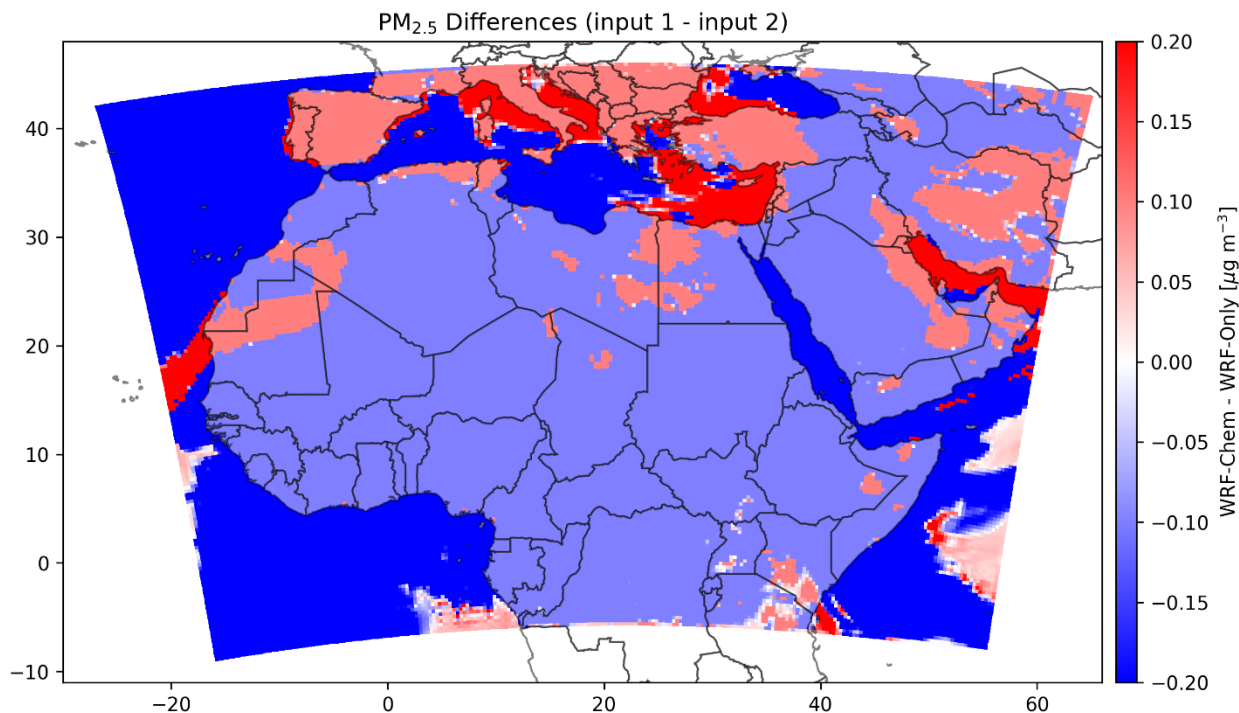


Figure 6. Spatial differences in $PM_{2.5}$ between the two different physics options.

9.7 PM_{10} evaluation

PM_{10} from WRF-Chem output is evaluated against EMA monitoring site in Cairo. The PM_{10} observational data is provided by the EMA for the month of January and April 2023. To evaluate PM_{10} , run `pm10_eval.py` to obtain PM_{10} statistics. Run `pm10_timeseries_plot.py` to generate PM_{10} time series.

Note that all evaluation results in terms of figures were based on initial configurations used during the preliminary testing, they may not be the same as the results based on the final model configurations used in this training.

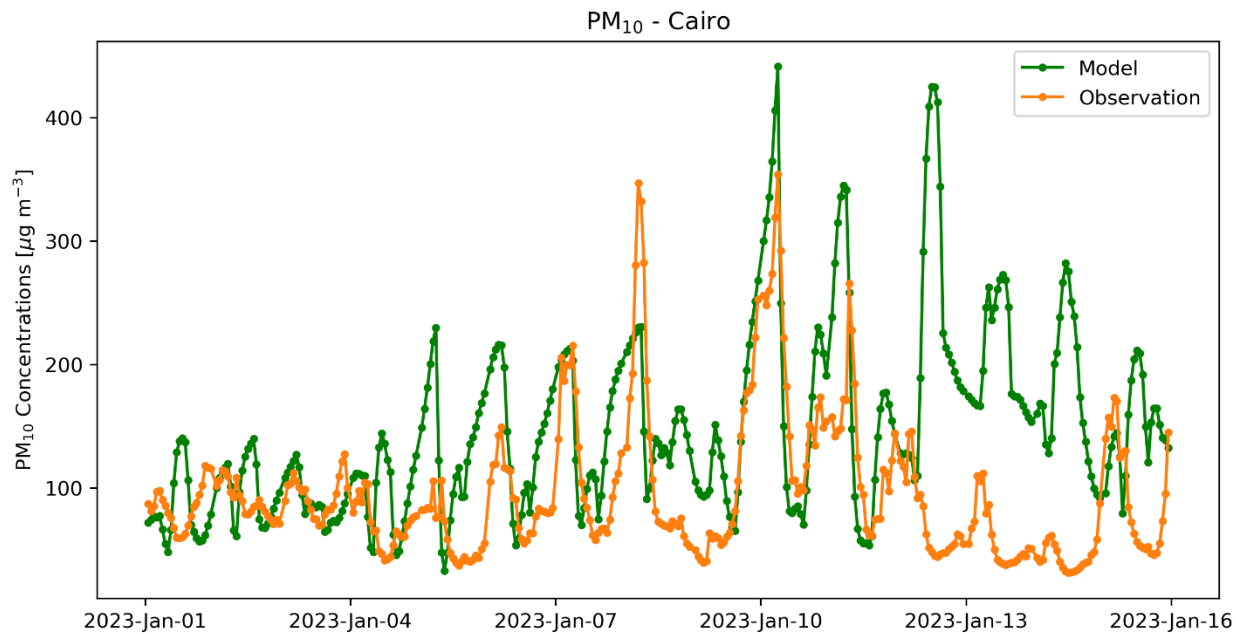


Figure 7. PM₁₀ time series from January 01 to January 15, 2023, for WRF-Chem model and EMA observations in Cairo, Egypt.

9.8 To download the file from HPC server

scp -r [yourAccount@login.discovery.neu.edu:/FilePath/files /DestinationPath/](#)

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