Hands-on Session on Online-Coupled WRF-Chem Version 4.6.0: Model Setup, Simulation, and Pre- and Post-Processing

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Northeastern University, Boston, USA

World Meteorological Organization's

"Training course on Seamless Prediction of Air Pollution in Africa"

October 3-4, 2024

Outline

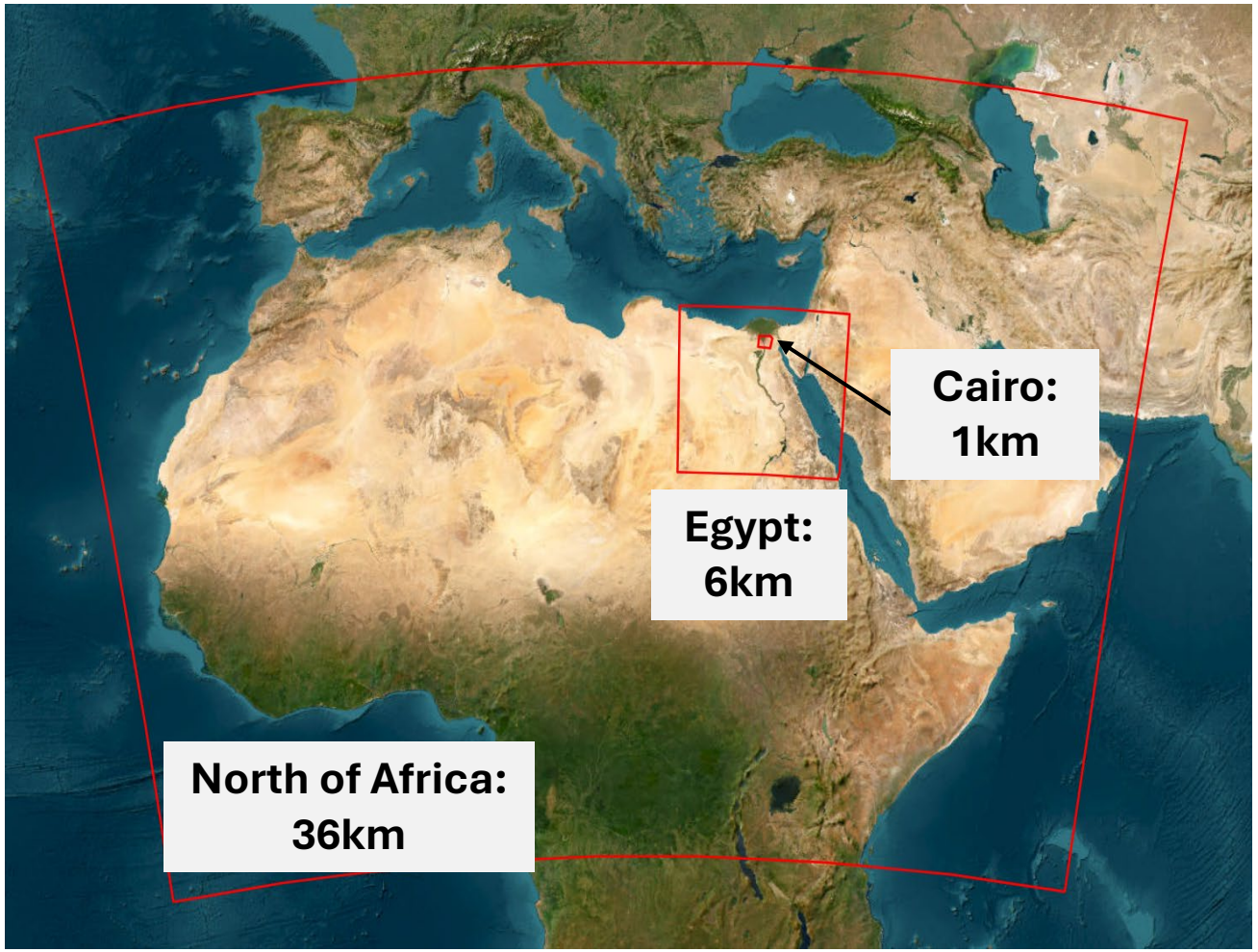
- **Overview (Yang Zhang)**
  - African testbed using WRF-Chem
  - Goal of hands-on Training
  - Training schedule and working groups
- **Input Preprocessing (Daniel Schuch)**
  - Overview of WRF-Chem Inputs
  - Input processing (IC/BC, emissions)
- **Output Post-processing and Analysis (Khanh Do)**
  - WRF-Chem compilation and simulation design
  - WRF-Chem job submission
  - Output post-processing and evaluation
  - Analysis of impacts of different science/physics schemes on predictions

Major sources: WRF and WRF-Chem Users' Guide, WRF-Chem Training Manual (Do et al., 2024), and Zhang et al. (2024)

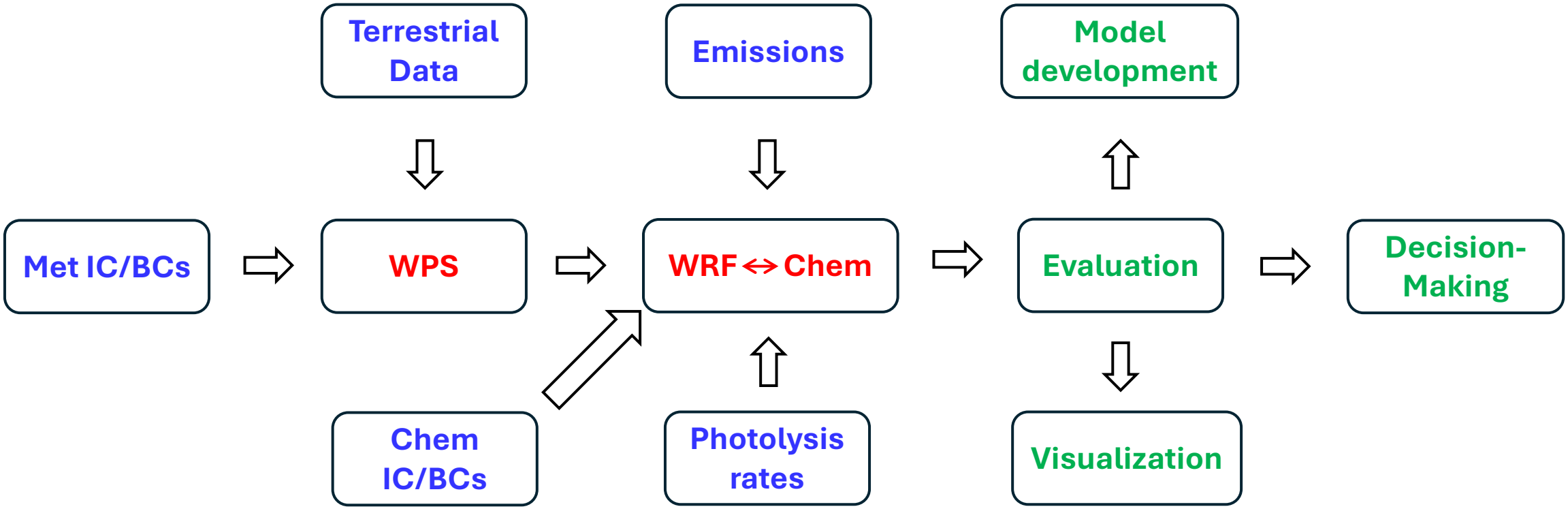
Application of WRF-Chem over Africa (Do et al., 2024; Zhang et al., 2024)

Objectives: Develop model testbed for WMO Training course and demonstrate model performance

- WRF-Chem version 4.6.0 (released in May 2024)
- Simulation Period January and April 2023
- Grid Resolution 36-6-1 km
- Anthropogenic Emissions EDGAR version 8.1
- Initial/Boundary Cond. 10-day spinup, Whole Atmosphere Community Climate Model (**WACCM**)



Overview WRF-Chem Inputs/Outputs



- Inputs: Meteorology and Chemical ICON/BCONs and emissions
- Outputs: 3-D air pollution and 3-D meteorology

WRF-Chem Version 4.6.0: Model Configuration

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) or Lin et al. Scheme
Surface layer	Pleim-Xiu (Pleim, 2006) or Monin-Obukhov scheme
Land surface	Pleim-Xiu Land Surface Model (Pleim & Xiu, 1995, 2003; Xiu & Pleim, 2001)
Boundary layer	ACM2 PBL (Pleim, 2007) or YSU scheme (Hong et al., 2006; Hong, 2010)
Cumulus clouds	Multi–scale Kain–Fritsch Scheme (Zheng et al., 2016) or Tiedtke scheme (Tiedtke, 1989; Zhang et al., 2011)
FDDA	All domains / all layers outside PBL; grid nudging 6h interval for 109 hours; guv = 0.0003 gt = 0.0003 gq = 0.00001
Gas-phase chemistry	2005 Carbon Bond chemistry mechanism (CB05) (Wang et al., 2015)
Photolysis	Fast-J photolysis (Barnard, 2004; Wild et al., 2000)
Aerosol chemistry	Modal aerosol dynamics model for Europe (MADE) (Ackermann et al., 1998)
Secondary organic aerosol	Volatility Basis Set (VBS) (Ahmadov et al., 2012)
Dust emissions	GOCART[a] dust emissions with AFWA[b] modifications (LeGrand et al., 2019) or Shao et al. (2011)
Sea salt emissions	GOCART sea salt emission scheme (Gong, 2003)

[a] Global Ozone Chemistry Aeroso; Radiation and Transport; [b] Air Force Weather Agency (U.S.)

Goal of WMO Hands-on Model Training

Objective:

Acquire knowledge on WRF-Chem and hands-on training on its application in Africa

- Learn considerations of model simulation design and application
- Learn the input choices and namelist options
- Learn all input data need to run the model
  - initial and lateral boundary conditions
  - emission sources
- Learn major steps to compile code and run the model
- Learn how to process observation/reanalysis data for model evaluation
- Learn fundamental on model performance evaluation
- Learn post-processing of multiple simulations for comparison and analysis

Training Schedule and Content

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

Training Simulations and Working Groups

Time period	Model configuration	Simulation and 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

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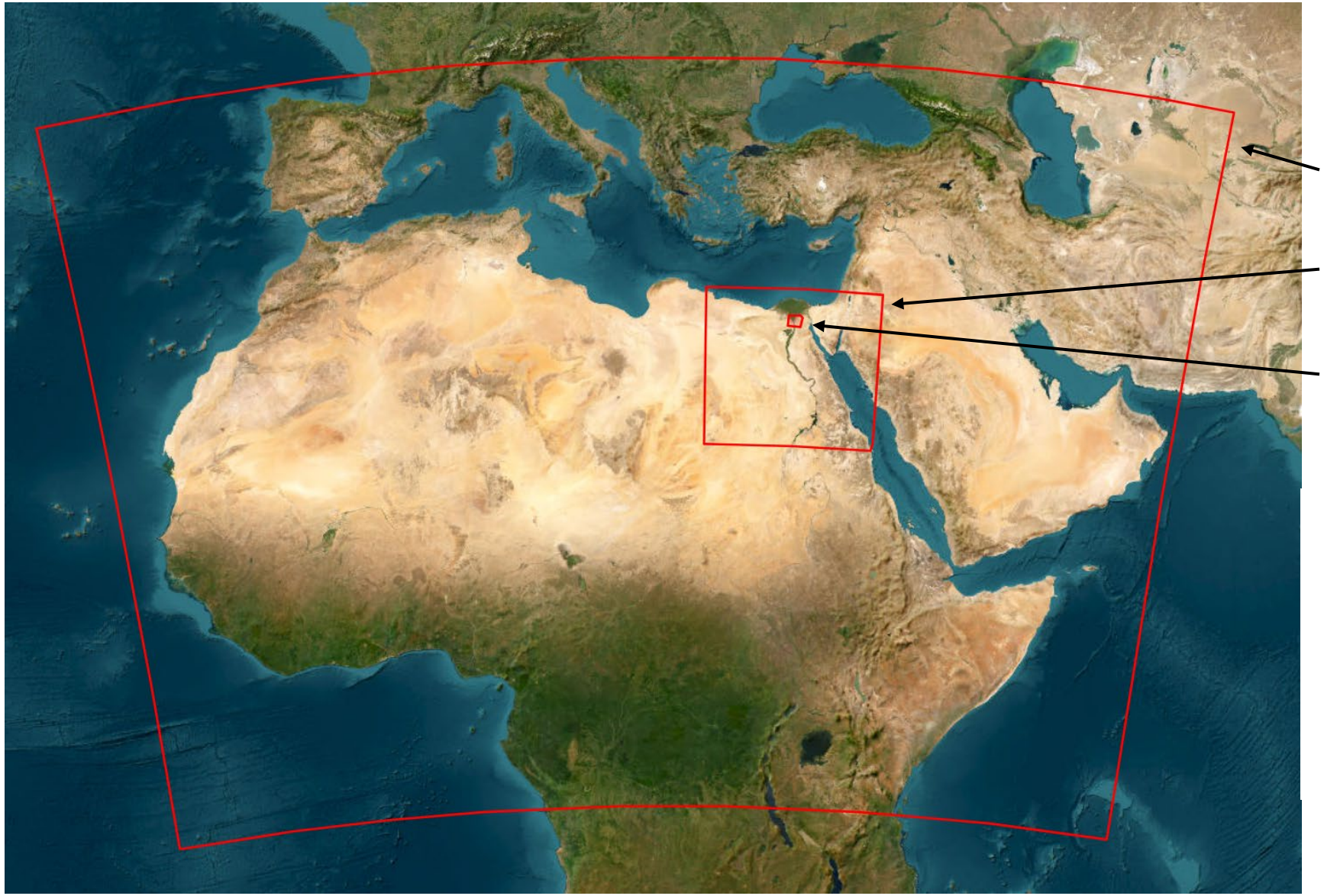
Major sources: WRF and WRF-Chem Users' Guide, WRF-Chem Training Manual (Do et al., 2024), and Zhang et al. (2024)

WRF-Chem Inputs used for the Testbed

Inputs	Sources of Inputs
Meteorology IC/BC	NCEP Final analysis 0.25 degree (NCEP-FNL, 2020)
Geographical data	WPS V4 Geographical Static Data
Land use data	MODIS
Gas and aerosol IC/BC	WACCM (Gettelman et al., 2019)
Anthropogenic emissions	EDGAR 8.1 (Crippa et al., 2024)
Biogenic emissions	Model of Emissions of Gases and Aerosols from Nature (MEGAN 2) (Guenther et al., 2006)
Fire emissions	Fire Inventory from NCAR (FINN) (Wiedinmyer et al., 2011)

Initial and Boundary Conditions for Gases and Aerosols



ICs/BCs

- **North of Africa: 36-km**
  Based on a global CTM
- **Egypt: 6-km**
  Based on 36-km predictions
- **Cario: 1-km**
  Based on 6-km predictions

Download WACCM outputs

(https://rda.ucar.edu/datasets/d313006/dataaccess)

Whole Atmosphere Community Climate Model (WACCM) Model Output

d313006 | DOI: 10.5065/G643-Z138 ☆

DESCRIPTION | DATA ACCESS | CITATION | DOCUMENTATION | SOFTWARE | METRICS

ASK A QUESTION >

Mouse over the underlined table headings for detailed descriptions

DATA DESCRIPTION		DATA FILE DOWNLOADS		CUSTOMIZABLE DATA REQUESTS	NCAR-ONLY ACCESS
		Web Server Holdings	Globus Transfer Service (GridFTP)	Subsetting	Central File System (GLADE) Holdings
UNION OF AVAILABLE PRODUCTS		Web File Listing	Globus Transfer	Get a Subset *(login required)*	GLADE File Listing
PRODUCTS	6-hourly 0.9x1.25 degree global WACCM files for 2019	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
	6-hourly 0.9x1.25 degree global WACCM files for 2020	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
	6-hourly 0.9x1.25 degree global WACCM files for 2021	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
	6-hourly 0.9x1.25 degree global WACCM files for 2022	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
	6-hourly 0.9x1.25 degree global WACCM files for 2023	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
	6-hourly 0.9x1.25 degree global WACCM files for 2024	Web File Listing		Get a Subset *(login required)*	GLADE File Listing

Download MOZBC Preprocessor:

(https://www.acom.ucar.edu/wrf-chem/download.shtml)

MOZBC source code

Click to download:

mozbc | bio_emiss | bio_emiss input files | preprocessor | anthro_emiss | EDGAR-HTAP | EPA_ANTHRO_EMIS

You may need to press your browser's 'Back' button to return and download another package.

MOZBC – Step by Step

1. *Download* and compile mozbc pre-processor

```
mkdir MOZBC; cd MOZBC
tar xvf mozbc.tar
chmod +x make_mozbc
./make_mozbc
```

This will generate the executable **mozbc**.

2. Link files from WPS and copy the input files for WRF to MOZBC folder

```
ln –s $WPS_FOLDER/met_em.d0?.*.nc .
cp $WRF_FOLDER/wrfbdy_d01 $WRF_FOLDER/wrfinput_d0? .
```

3. *Download* output from the WACCM model and combine the inputs using `ncrcat` command

```
ncrcat f.e22.beta02.*.cam.h3.2023-01-*.nc waccm_01.nc
```

The waccm_01.nc file will be used by mozbc

4. Run mozbc

```
./mozbc < cb05_d01.inp > log.mozbc
```

`Log.mozbc` is the log file and `wrfbdy_d01`, `wrfinput_d01`, and `wrfinput_d02` will be updated

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```

`Log.mozbc` is the log file and `wrfbdy_d01`, `wrfinput_d01`, and `wrfinput_d02` will be updated

cb05_d01.inp

```
&control
 do_bc           = .true.
 do_ic           = .false.
 def_missing_var = .true.
 domain          = 1
 dir_wrf         = './'
 dir_moz         = './waccm/'
 fn_moz          = 'waccm_01.nc'
 moz_var_suffix  = ''
 spc_map = 'o3 -> O3',
  'no -> NO',
  'no2 -> NO2',
  'n2o5 -> N2O5',
  'nh3 -> NH3',
  'hno3 -> HNO3',
  'h2o2 -> H2O2',
  'ch4 -> CH4',
  'co -> CO',
  'so2 -> SO2',
  'no3 -> NO3',
  'oh  -> OH',
  'ho2 -> HO2',
  'tol -> TOLUENE',
  'cres -> CRESOL',
  'mgly -> CH3COCHO',
  'xyl -> XYLENES',
  'isop -> ISOP',
  'form -> CH2O',
  'aldx -> 0.62000*[CH3CHO]',
  'ald2 -> 0.38000*[CH3CHO]',
  'etha -> C2H6',
  'meoh -> CH3OH',
  'par -> C3H8+BIGALK',
  'iole -> 0.5*BIGENE',
  'ole -> C3H6+MVK+0.5*BIGENE',
  'eth -> C2H4',
  'eci->bc_a1+bc_a4;0.113571e9',
  'ecj->bc_a1+bc_a4;0.264125e9',
  'p25i->4.66064*[dst_a2];1.e9',
  'p25j->4.66064*[dst_a1];1.e9',
  'soila->4.66064*[dst_a3];1.e9',
  'aacd -> CH3COOH',
  'mgly -> CH3COCHO',
  'ntr -> ONITR',
  'pacd -> CH3COOH',
  'open -> BIGALD',
  'pan -> PAN',
  'ispd -> MACR',
  'so4ai -> so4_a2;1.e9',
  'so4aj -> so4_a1;1.e9',
  'orgpaj -> pom_a1;1.e9',
 /
```

Biogenic Emissions Processing using MEGAN 2

(https://ruc.noaa.gov/wrf/wrf-chem/wrf_tutorial_2012/wrfchem_tutorial_biogenic.pdf)

- **MEGAN**:
  Model of Emissions of Gases and Aerosols from Nature
  - Guenther et. al., *Atmospheric Chemistry and Physics*, 2006
  - 134 emitted chemical species
    - Isoprene
    - Monoterpenes
    - Oxygenated compounds
    - Sesquiterpenes
    - Nitrogen oxide
  - 1 km^2 resolution
  - Input files available at:

MEGAN Framework: Calculation of emissions

$$EM = \varepsilon \bullet \gamma_{CE} \bullet \gamma_{age} \bullet \gamma_{SM} \bullet \rho$$

$$\gamma_{CE} = \gamma_{LAI} \bullet \gamma_{P} \bullet \gamma_{T}$$

EM: Emission ($\mu g\ m^{-2}\ hr^{-1}$)
ε: Emission Factor ($\mu g\ m^{-2}\ hr^{-1}$)
γ_{CE}: Canopy Factor
γ_{age}: Leaf Age Factor
γ_{SM} : Soil Moisture Factor
ρ: Loss and Production within plant canopy
γ_{LAI} : Leaf Area Index Factor
γ_{P} : PPFD Emission Activity Factor (light-dependence)
γ_{T}: Temperature Response Factor

Download Source Code and Inputs

(https://www.acom.ucar.edu/wrf-chem/download.shtml)

BIO_EMISS source code

Inputs

Click to download:

mozbc | bio_emiss | bio_emiss input files | preprocessor | anthro_emiss | EDGAR-HTAP | EPA_ANTHRO_EMIS

You may need to press your browser's 'Back' button to return and download another package.

Megan_bio_emiss – Step by Step

1. *Download* and compile megan_bio_emiss pre-processor and input data:

```
mkdir MEGAN; cd MEGAN
tar xvf megan_bio_emiss.tar
make megan_bio_emiss
```

This will generate the executable **`megan_bio_emiss`**.

2. Copy the input files for WRF to MEGAN folder

```
cp $WRF_FOLDER/wrfinput_d0? .
```

3. Untar MEGAN data on MEGAN folder:

```
tar xvf megan.data.tar.gz
```

4. Run megan_bio_emiss

```
./megan_bio_emiss < bioemiss.inp > log.megan
```

`log.megan` is the log file and `wrfbiochemi_d01` and `wrfbiochemi_d02` are the biogenic emissions

Megan_bio_emiss – Step by Step

1. *Download* and compile megan_bio_emiss pre-processor and input data:

```
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tar xvf megan_bio_emiss.tar
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```

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```

4. Run megan_bio_emiss

```
./megan_bio_emiss < bioemiss.inp > log.megan
```

`log.megan` is the log file and `wrfbiochemi_d01` and `wrfbiochemi_d02` are the biogenic emissions

bioemiss.inp

```
&control
 domains = 2,
 start_lai_mnth = 1,
 end_lai_mnth   = 3,
 wrf_dir    = './',
 megan_dir = './'
/
```

Fire Emissions Processing Based on FINN v2.5

(https://ruc.noaa.gov/wrf/wrf-chem/wrf_tutorial_2012/wrfchem_tutorial_biogenic.pdf)

Daily fire emissions calculated with FINNv1

Wiedinmyer et al., *Geoscientific Model Development*, 2011, http://www.geosci-model-dev.net/4/625/2011/gmd-4-625-2011.html

- Daily global fire emissions
  - GHG, CO, NOx, VOCs, SO2, NH3, Particulate Matter
- Spatial resolution ~ 1km^2
- Available for hindsight and forecast model applications

Download INPUTS:
(https://rda.ucar.edu/datasets/ds312.9/dataaccess

Fire Inventory from NCAR version 2 Fire Emission

d312009 | DOI: 10.5065/XNPA-AF09

DESCRIPTION | DATA ACCESS | CITATION | DOCUMENTATION | SOFTWARE | METRICS | ASK A QUESTION

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PRODUCTS	modis: FINNv2.5 modis fire emissions, daily, the base, MOZART, SAPRC, GEOSCHEM compounds based on MODIS data, 0.1x0.1 degree, global	Web File Listing		Get a Subset *(login required)*	GLADE File Listing
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PRODUCTS	eachfire modis: Global daily emissions for each fire at 1 km resolution, the base and speciated VOCs based on MODIS data (txt.gz)	Web File Listing			GLADE File Listing
PRODUCTS	eachfire modisviirs: Global daily emissions for each file at 1 km resolution, the base and speciated VOCS based on MODISVIIRS data (txt.gz)	Web File Listing			GLADE File Listing

Download Source-Code (https://www.acom.ucar.edu/Data/fire/)

Source code and static input

Gridding program - updated June 2020

- (●) fire_emis fortran program to grid the FINN (v1.5 and v2) text files to netcdf files for use in WRF-Chem or global models.
- ( ) vegetation data files used in creating WRF-Chem gridded emissions (not needed for global grids).

Security question: What is 3 plus 4 ? 7

Submit download request here: Submit Cancel

13450 downloads since 2013-08-29.

Fire_emis – Step by Step

1. *Download* and compile fire_emis pre-processor:

```
mkdir FINN2.5; cd FINN2.5
tar xvf fire_emis.tgz
cd grid_finn_fire_emis_v2020/src/
./make_fire_emis
cd ..
ln -s src/fire_emis .
```

This will generate the executable **`fire_emis`**.

2. Untar the static inputs:

```
tar xvf fire_emis_input.tar
```

3. *Download* and gunzip FINN files on `grid_finn_fire_emis_v2020` folder:

```
gunzip FINNv2.5.1_modvrs_MOZART_202301_c20240521.txt.gz
```

4. Run megan_bio_emiss

```
./fire_emis < finn_wrf.inp > log.fire
```

`log.fire` is the log file and `wrffirechemi_d01_2023-04-??_??:00:00` are the emissions from fires

Fire_emis – Step by Step

1. *Download* and compile fire_emis pre-processor:

```
mkdir FINN2.5; cd FINN2.5
tar xvf fire_emis.tgz
cd grid_finn_fire_emis_v2020/src/
./make_fire_emis
cd ..
ln -s src/fire_emis .
```

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```

4. Run megan_bio_emiss

```
./fire_emis < finn_wrf.inp > log.fire
```

`log.fire` is the log file and `wrffirechemi_d01_2023-04-??_??:00:00` are the emissions from fires

`finn_wrf.inp`

```
&control
fire_directory   = './',
fire_filename(1) = 'FINNv2.5.1_modvrs_MOZART_202301_c20240521.txt',
fire_filename(2) = 'FINNv2.5.1_modvrs_MOZART_202302_c20240521.txt',
fire_filename(3) = 'FINNv2.5.1_modvrs_MOZART_202303_c20240521.txt',
fire_filename(4) = 'FINNv2.5.1_modvrs_MOZART_202304_c20240521.txt',
fire_filename(5) = 'FINNv2.5.1_modvrs_MOZART_202305_c20240521.txt',
start_date       = '2023-04-01',
end_date         = '2023-04-30',
output_timing    = 'daily',
Model            = 'WRF',
wrf_directory    = './',
domains          = 2,
defaultUnits     = 'molecules/cm^2/s',
FinnVers         = '2.5',

wrf2fire_map = 'co -> CO', 'no -> NO', 'so2 -> SO2', 'bigalk -> BIGALK',
               'bigene -> BIGENE', 'c2h4 -> C2H4',
               'c2h6 -> C2H6', 'c3h8 -> C3H8','c3h6 -> C3H6','ch2o -> CH2O',
               'ch3cho -> CH3CHO', 'ch3coch3 -> CH3COCH3', 'ch3oh -> CH3OH',
               'mek -> MEK', 'toluene -> TOLUENE',
               'nh3 -> NH3', 'no2 -> NO2',
               'ch3cooh -> CH3COOH','cres -> CRESOL','glyald -> GLYALD',
               'acetol -> HYAC',
               'isop -> ISOP','macr -> MACR', 'mvk -> MVK',
               'oc -> OC;aerosol','bc -> BC;aerosol'
/
```

Anthropogenic Emissions Processing based on EDGARv8.1

Introduction

EDGARv8.1 provides emissions not only for the greenhouse gases per sector and country but also for the air pollutants:

- Ozone precursor gases: Carbon Monoxide (CO), Nitrogen Oxides (NO_X), Non-Methane Volatile Organic Compounds (NMVOC) and Methane (CH_4)
- Acidifying gases: Ammonia (NH_3), Nitrogen oxides (NO_X) and Sulfur Dioxide (SO_2)
- Primary particulates: Fine Particulate Matter (PM_{10} and $PM_{2.5}$) and Carbonaceous speciation (BC, OC)

Emissions from large scale biomass burning with Savannah burning, forest fires, and sources and sinks from land-use, land-use change and forestry (LULUCF) are excluded.

For the energy related sectors the activity data are primarily based on IEA data (2022) World Energy Balances, (www.iea.org), all rights reserved, as modified by Joint Research Centre, European Commission, whereas the activity data for the agricultural sectors originate primarily from FAO (2022) (www.fao.org/faostat).

Novelties of EDGARv8.1 compared to the previous EDGARv6.1 release are:

- updates of all activity data up to 2022
- updates of technology penetration, abatement measures and emission factors for power plant emissions and residential emissions in Europe
- new spatial proxies as described in Crippa et al. (2024)

Download inputs and additional information:
Global air pollutants Emissions (*version 8.1*):
(https://edgar.jrc.ec.europa.eu/dataset_ap81)

Global GHG pollutants (*version 8.0*):
(https://edgar.jrc.ec.europa.eu/dataset_ghg80)

Download EDGARv8.1 monthly sector-specific gridmaps

PAGE CONTENTS

Monthly sector-specific gridmaps (2000-2022)

— Click to expand

Monthly emission gridmaps (2000-2022) are provided for all substances and sectors using the temporal distribution profiles described in Crippa et al. (2020).

Sectors definition:

- Power Industry - Power and heat generation plants (public & autoproducers)
- Industrial combustion - Combustion for industrial manufacturing
- Buildings - Small scale non-industrial stationary combustion
- Transport - Mobile combustion (road & rail & ship & aviation)
- Agriculture - Agricultural soils, crop residues burning, enteric fermentation, manure management, indirect N2O emissions from agriculture
- Fuel exploitation - Production, transformation and refining of fuels
- Processes - Industrial processes (e.g. emissions from the production of cement, iron and steel, aluminum, chemicals, solvents, etc.)
- Waste - Solid waste disposal and waste water treatment

Files format:

- Emissions: Mg/month gridmaps at 0.1x0.1degree resolution, .NetCDF file per year, substance and sector is produced including the emissions for the 12 months.
- Emission fluxes: kg/m2/s at 0.1x0.1degree resolution, .NetCDF file per year, substance and sector is produced including for each sector the emission fluxes for the 12 months.
- Note that OC emission and fluxes are expressed in amount of C.

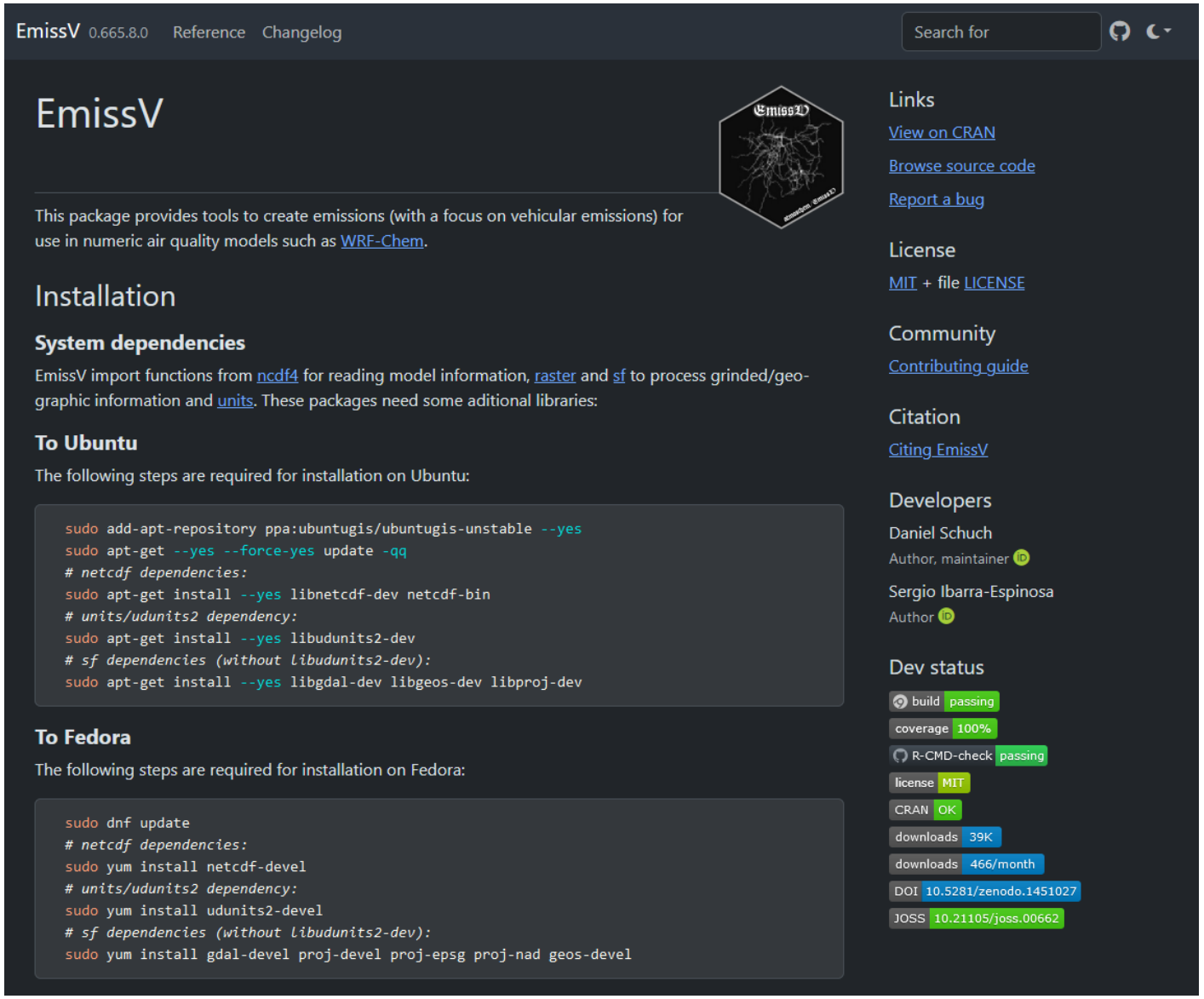
- **Agriculture**
  IPCC 1996: 4A+4B+4C+4D+4F+4G / IPCC 2006: 3A+3C+5A

EDGAR BC - NETCDF (emi) (AGRICULTURE_emi_nc.zip)
English (687.89 Mb - ZIP) Download

EDGAR BC - NETCDFD (fluxes) (AGRICULTURE_flx_nc.zip)
English (700.96 Mb - ZIP) Download

Anthropogenic Emissions Processing Using R-package EmissV

Atmoschem: is organization of software developers focusing on air quality modeling.
https://github.com/atmoschem



Dev: https://github.com/atmoschem/EmissV
Official: https://CRAN.R-project.org/package=EmissV
Doc: https://atmoschem.github.io/EmissV

Anthropogenic Emissions Processing Using R-package EmissV

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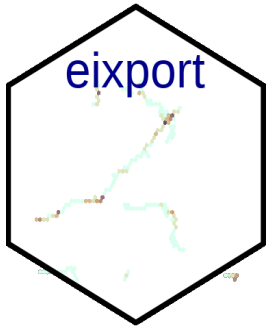
https://github.com/atmoschem

eixport 0.6.0 Reference Changelog

eixport

build unknown | build passing | coverage 100% | DOI 10.5281/zenodo.10044992
CRAN 0.6.0 | downloads 34K | JOSS 10.21105/joss.00607 | Github 27



Exporting emissions to atmospheric models, eixport: 0.6.0

Emissions are mass that affects atmosphere in complex ways, not only physical, but also, in the health of humans, ecosystems, economically, etc.

There are several models whose inputs are emissions, such as R-Line or WRF-Chem. This R-Package provide functions to read emissions from VEIN and from other models in different formats and export the emissions into the appropriate format suitable to other models.

Install

To install the CRAN version:

```
install.packages("eixport")
```

To install the development version:

```
devtools::install_github("atmoschem/eixport")
```

Links

View on CRAN
Browse source code
Report a bug

License

MIT + file LICENSE

Community

Contributing guide
Code of conduct

Citation

Citing eixport

Developers

Sergio Ibarra-Espinosa
Author, maintainer

Daniel Schuch
Author

More about authors...

Dev: https://github.com/atmoschem/eixport
Official: https://CRAN.R-project.org/package=eixport
Dev: https://atmoschem.github.io/eixport

Anthropogenic Emissions Processing Using R-package EmissV

1. Download **EDGAR** and install the R-packages **EmissV** and **eixport**
2. The function `read()` is used read EDGAR 8.1 emission files
3. The function `gridinfo()` Extract the domain information from a **wrfinput** file
4. The function `emission()` interpolates and converts the units for WRF-Chem
5. The functions `wrf_create()` create the emission file
6. The functions `wrf_put()` and `to_wrf()` write the emissions

Outline

- **Overview (Yang Zhang)**
  - African testbed using WRF-Chem
  - Goal of hands-on Training
  - Training schedule and working groups
- **Input Preprocessing (Daniel Schuch)**
  - Overview of WRF-Chem Inputs
  - Input processing (IC/BC, emissions)
- **Output Post-processing and Analysis (Khanh Do)**
  - WRF-Chem compilation and simulation design
  - WRF-Chem job submission
  - Output post-processing and evaluation
  - Analysis of impacts of different science/physics schemes on predictions

Major sources: WRF and WRF-Chem Users' Guide, WRF-Chem Training Manual (Do et al., 2024), and Zhang et al. (2024)

Basic Linux Commands

- **`ls`** – list the contents
- **`pwd`** – print full path
- **`cd/cd ..`** – navigate directory
- **`mkdir`** – make new directories/files
- **`rm`** – delete file /folders
- **`mv`** – change name files/directories
- **`cp`** – copy files / directories
- **`vim`** – edit files using VIM text editor
- **`tar`** – compress / uncompress files
- **`grep`** – search for files / keywords
- **`find`** – search for a file in a directory
- **`tail`** – print the last few lines from files
- **`diff`** – compare the differences 2 files
- **`wget`** – download files from internet
- **`history`** – show previous command
- **`export`** – export the environment vars

WRF-Chem Dependencies

- `HDF5, zlib, netCDF, JasPer, libpng, yacc, mpi`
- No need to compiled these environments
  - Load from Discovery modules (e.g., `module load intel/compiler`)
  - Export from compiled libraries (e.g., `export NETCDF=/path/to/NETCDF/`)
- Set up environments for Intel compiler
  - e.g., `export CC=icx, export F77=ifort`
- Set up flags for WRF-Chem compilation
  - e.g., `export WRF_CHEM=1, export WRF_KPP=1`

Compile WRF-Chem

- Compile WRF-Chem version 4.6.0
  - `git clone --recurse-submodules https://github.com/wrf-model/WRF`
  - `./configure` and choose option 16 for Intel compiler
  - `./compile em_real 2>&1 | tee compile.log`
- Compile WPS
  - `git clone https://github.com/wrf-model/WPS`
  - `export WRF_DIR=../WRF-4.2.1/`
  - Export JASPERLIB, JASPERINC, and other libraries
  - `./configure` and choose option 16 for Intel compiler
  - `./compile 2>&1 | tee compile.log`

Simulation Design

Simulation period	Model config	Namelists	Run scripts	Node #	Group #
January 1-7, 2023	Baseline	namelist_base	runWRFChem3000	d[3073-3075]	1
January 1-7, 2023	YSU PBL scheme+Monin-Obukhov surface layer scheme	namelist_pbl	runWRFChem3000	d[3076-3078]	2
January 1-7, 2023	Lin scheme	namelist_micro	runWRFChem3000	d[3079-3081]	3
January 1-7, 2023	Tiedtke cumulus scheme	namelist_cu	runWRFChem4000	d[4019-4021]	4
January 1-7, 2023	Dust	namelist_dust	runWRFChem4000	d[4016-4018]	
April 1-7, 2023	Baseline	namelist_base	runWRFChem4000	d[4001-4003]	5
April 1-7, 2023	YSU PBL scheme+Monin-Obukhov surface layer scheme	namelist_pbl	runWRFChem4000	d[4004-4006]	6
April 1-7, 2023	Lin scheme	namelist_micro	runWRFChem4000	d[4007-4009]	7
April 1-7, 2023	Tiedtke cumulus scheme	namelist_cu	runWRFChem4000	d[4010-4012]	8
April 1-7, 2023	Dust	namelist_dust	runWRFChem4000	d[4013-4015]	9

Exercise 9.1: Login to Discovery

- Linux and MAC system
  - Use terminal to log in Discovery
  - `ssh username.login.discovery.neu.edu`
- Windows computer
  - 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 the "Host Name"
    - Login with your username and password
- Inputs located in the shared folder on Discovery
  - Anthropogenic, fire, biogenic emissions, GFS, run scripts, and namelists
  - `/work/zhanglab/kdo/sharedDrive`

Exercise 9.2.1: Run WPS

- WPS generates grided meteorological files for WRF
- We will skip this exercise and use preprocessing met_em
- You can try in you own time by following the training manual

Download files from Discovery

scp -r **yourAccount**@login.discovery.neu.edu:/**FilePath/files /DestinationPath/**

View PNG from PowerShell

```
start file.png
```

Load 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`

Exercise 9.2.2: Run WRF-Chem

1. Copy the compiled WRF to your scratch
   ```
   1.  cp -r /work/zhanglab/kdo/sharedDrive/WRFv4_6/WRF/ .
   ```
2. cd to your em_real folder located at `/WRF/test/em_real`
3. Copy the namelist.input from sharedDrive. Use the right namelist that designed for your group. The link for January is different.
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/namelists/namelist_base/* .
   ```
4. Copy emissions from the sharedDrive to the working WRF folder
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/emissions/* .
   ```
5. Copy fire emissions to the working WRF folder
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/fire/* .
   ```
6. Copy biogenic emissions to the working WRF folder
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/megan/* .
   ```
7. Copy preprocessed met_em*
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/met_em/* .
   ```
8. Copy met ICON/BCONS
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/ICBC/* .
   ```
9. Copy chem ICON/BCONS for warm start
   ```
   1.  cp /work/zhanglab/kdo/sharedDrive/aprilData/output/* .
   ```
10. Copy the run script to the working folder
    ```
    1.  cp /work/zhanglab/kdo/sharedDrive/namelists/run_WRF-Chem_aprilData_node4000.sh .
    ```
11. Modified your **`run_WRF-Chem_aprilDate_node4000.sh`** based on slide 33 for node number
12. Submit the jobs: `sbatch` **`run_WRF-Chem_aprilDate_node4000.sh`**

For January group, change /aprilData/ to /januaryData/

Exercise 9.3: Load Libraries for Evaluation

1. Move to compute node

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

   or

   ```
   srun --time=8:00:00 --job-name=WRF_AFRICA --ntasks=10
   --partition=zhang --nodelist=d4024 --pty /bin/bash
   ```

2. Load anaconda module

   ```
   module load anaconda3/2022.05
   ```

3. Activate anaconda environment

   ```
   source activate
   /work/zhanglab/kdo/sharedDrive/WRFChemWorkshop
   ```

Monitor the jobs

- Monitor the queue

  ```
  squeue –u username
  ```

- Monitor the progress

  ```
  tail –f rsl.err.0000
  ```

- Delete the job

  ```
  scancel jobID
  ```

Data used for the African Testbed Evaluation

- Meteorology – NOAA Global Hourly Integrated Surface Database
  - 20,000 stations worldwide
  - Data includes wind speed (WS), wind direction (WD), temperature (T), and dew point temperature (DT)
- Air quality
  - **AirNow**: ground observations for $PM_{2.5}$
  - **EMA:** ground observationPM_{10} data
  - **MERRA-2**: reanalysis data for $PM_{2.5}$

Exercise 9.3: Load Libraries for Evaluation

1. Move to compute node

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

   or

   ```
   srun --time=8:00:00 --job-name=WRF_AFRICA --ntasks=5 --partition=zhang --nodelist=d4024 --pty /bin/bash
   ```

2. Load anaconda module

   ```
   module load anaconda3/2022.05
   ```

3. Activate anaconda environment

   ```
   source activate /work/zhanglab/kdo/sharedDrive/WRFChemWorkshop
   ```

Exercise 9.4: Meteorology Evaluation

1. Create meteorology evaluation folder in your scratch
    1. `mkdir met_evaluation && cd met_evaluation`
2. Copy evaluation scripts from sharedDrive to your local folder
    1. `cp /work/zhanglab/kdo/sharedDrive/evaluation/met_evaluation/*.py` **`/your/folder/path/`**
    2. `cp /work/zhanglab/kdo/sharedDrive/evaluation/met_evaluation/*.csv` **`/your/folder/path/`**
    3. `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/met_evaluation/shapefiles/` **`/your/folder/path/`**
3. **Rember to change the paths and the dates in python scripts**
4. Run `./extract_model_and_ISD_data_points.py` to extract model meteorological data along with observational data
5. Run `./extract_and_compute_met_stats.py` to extract model meteorological data along with observations and calculate the statistics for each IDS site
6. Run `./spatial_plot_eval.py` for visualization

Exercise 9.5: $PM_{2.5}$ Evaluation

1. Create PM evaluation folder in your scratch
   1. `mkdir pm_evaluation && cd pm_evaluation`
2. Copy PM2.5 evaluation scripts to your local folder `cp /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/*.py` **`/your/folder/path/`**
3. Copy AirNow observational data to your local folder `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/2023_Data/` **`/your/folder/path/`**
4. Copy PM_{10} observational data to your local folder `cp /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/pm10_cai_2023_for_WMO_course.csv` **`/your/folder/path/`**
5. Copy shapefiles to your local folder `cp -r /work/zhanglab/kdo/sharedDrive/evaluation/pm25_evaluation/shapefiles/` **`/your/folder/path/`**
6. Run `./pm25_eval_`**`apr`**`.py` to extract the $PM_{2.5}$ values from WRF-Chem outputs and AirNow data
7. Evaluate the model with MERRA-2 (Optional), run `./eval_using_merra3.py`
8. **Rember to change the paths and dates in python scripts**

Exercise 9.6: Difference Plots

- Open `./pm25DiffPlot.py` and change directories for input1 and input2 as the baseline and you WRF-Chem output
- Run `./pm25DiffPlot.py` to generate the difference plot between scheme 1 and scheme 2

Exercise 9.7: PM_{10} Evaluation

- Run `./pm10_eval.py` to obtain PM_{10} statistics
- Run `./pm10_timeseries_plot.py` to generate PM_{10} time series

Exercise 9.8: Download the file from HPC server

scp -r **yourAccount**@login.discovery.neu.edu:/**FilePath/files /DestinationPath/**

Rember to change the paths in python scripts

References

- WRF (ARW) Version 4.5 User's Guide,2024, http://www2.mmm.ucar.edu/wrf/users/
- WRF-Chem Version 4.4 User's Guide, https://ruc.noaa.gov/wrf/wrf-chem/Users_guide.pdf
- Do, K., D. Schuch, and Y. Zhang, 2024, 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, October 3-4, 2024, Cario, Egypt.
- Zhang, Y., D. Schuch, and K. Do, 2024, Multi-Scale Air Quality Modeling Using WRF-Chem-GHG over Northeastern Africa, oral presentation at the 23rd Annual CMAS Conference, Chapel Hill, NC, October 21-23, 2024.