

WRF-Chem:
A Quick Review Of How To
Set-Up & Run

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WRF-Chem

- It is assumed that the user of WRF-Chem :
 - is *very familiar* with the WRF model system
 - have run WPS and a weather simulation using WRFV3
 - know FORTRAN and C and can edit code, recompile, etc.
- The chemistry code is available from WRF web page.
 - Questions: Send email to WRF-Chem help (wrfchemhelp.gsd@noaa.gov)
 - Web page: www.wrf-model.org/WG11
- Test data is available as well (tutorial exercises)
 - Small domain (41x41x31 grid points, 100 km horiz. spacing)

WRF-Chem

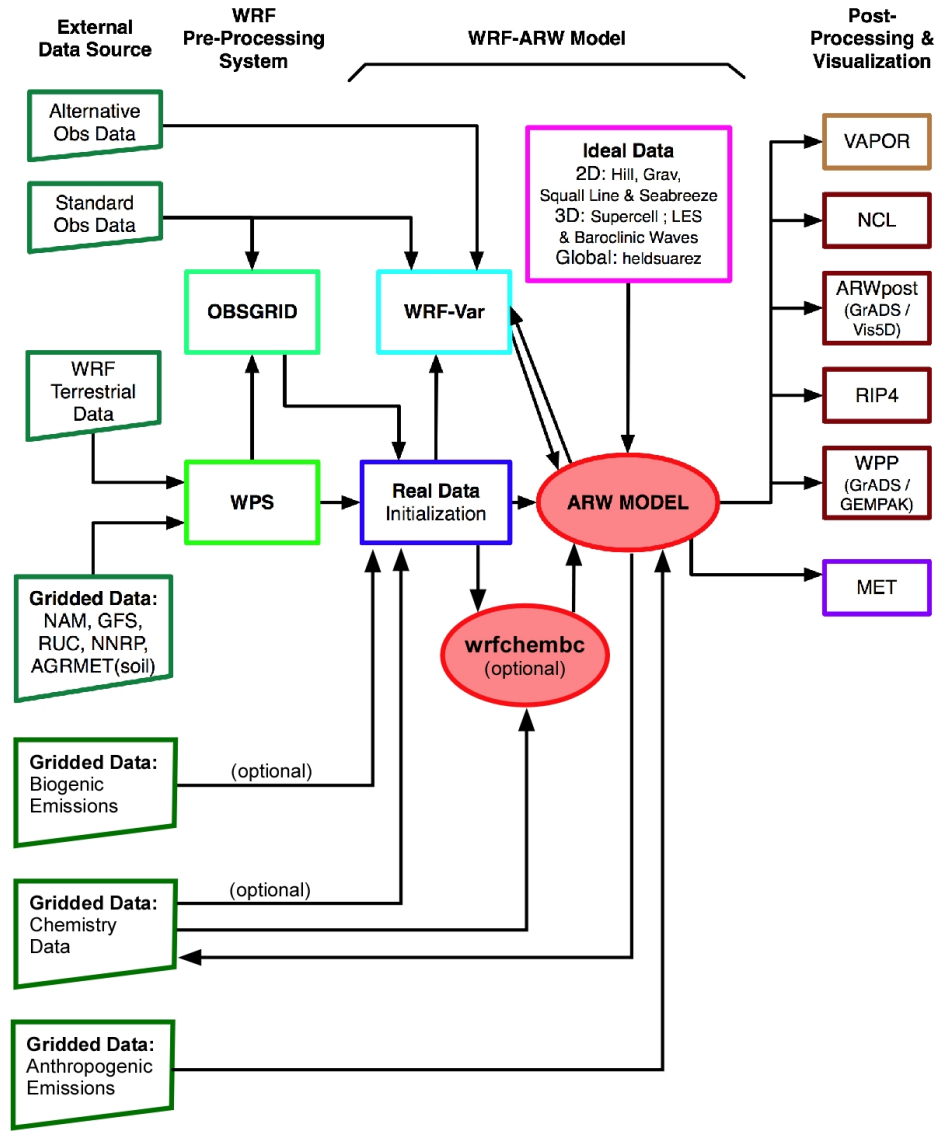
- **GOAL:** To understand how:
 - to make a WRF simulation that includes chemistry
 - Navigate all of the input choices and namelist options
- **To accomplish this goal:**
 - Learn steps to compile code,
 - Learn how to include emission sources,
 - Anthropogenic
 - Biogenic
 - Biomass Burning
 - Dust
 - Learn about modifying initial and lateral boundary conditions
 - Become familiar with some namelist.input settings

WRF-Chem: Compile code

- Compile WRF-Chem code (already done for tutorial)
 - Set environmental variables
 - Define which model core to build (use ARW only).
 - `setenv EM_CORE 1`
 - Chemistry code is to be included in the WRF model build
 - `setenv WRF_CHEM 1`
 - Kinetic Pre-Processor (KPP) code
 - `setenv WRF_KPP 1` => if KPP is to be included
 - `setenv WRF_KPP 0` => if KPP is NOT to be included
 - `setenv FLEX_LIB_DIR /usr/lib`
 - `setenv YACC '/usr/bin/yacc -d'`
 - Configure and issue “`compile em_real`” command
 - Save compile output to file
 - Check results for errors and check known problems web page if no `wrf.exe`

WRF-Chem Emissions

WRF-ARW Modeling System Flow Chart



WRF-Chem Emissions

- Two sources of anthropogenic emissions available on WRF-Chem ftp site:
 - RETRO (.5 degree, monthly) and EDGAR (1 degree, annual)
 - Run Prep_sources_chem (Tutorial exercise 2)
 - National Emissions Inventory (NEI-2005) for U.S.
 - Run without chemistry first as mean wind profile is needed!
 - Both include programs to map to WRF grid; binary output files
- Can use other external emissions data
 - Start with “raw” emissions data
 - Specify the speciation for the desired chemical mechanism
 - Prepared the 3-D (or 2-D) anthropogenic emissions data set
 - Map data onto your WRF-Chem simulation domain
 - Output data
 - Goal: have data in a WRF data file to run with model

WRF-Chem Emissions

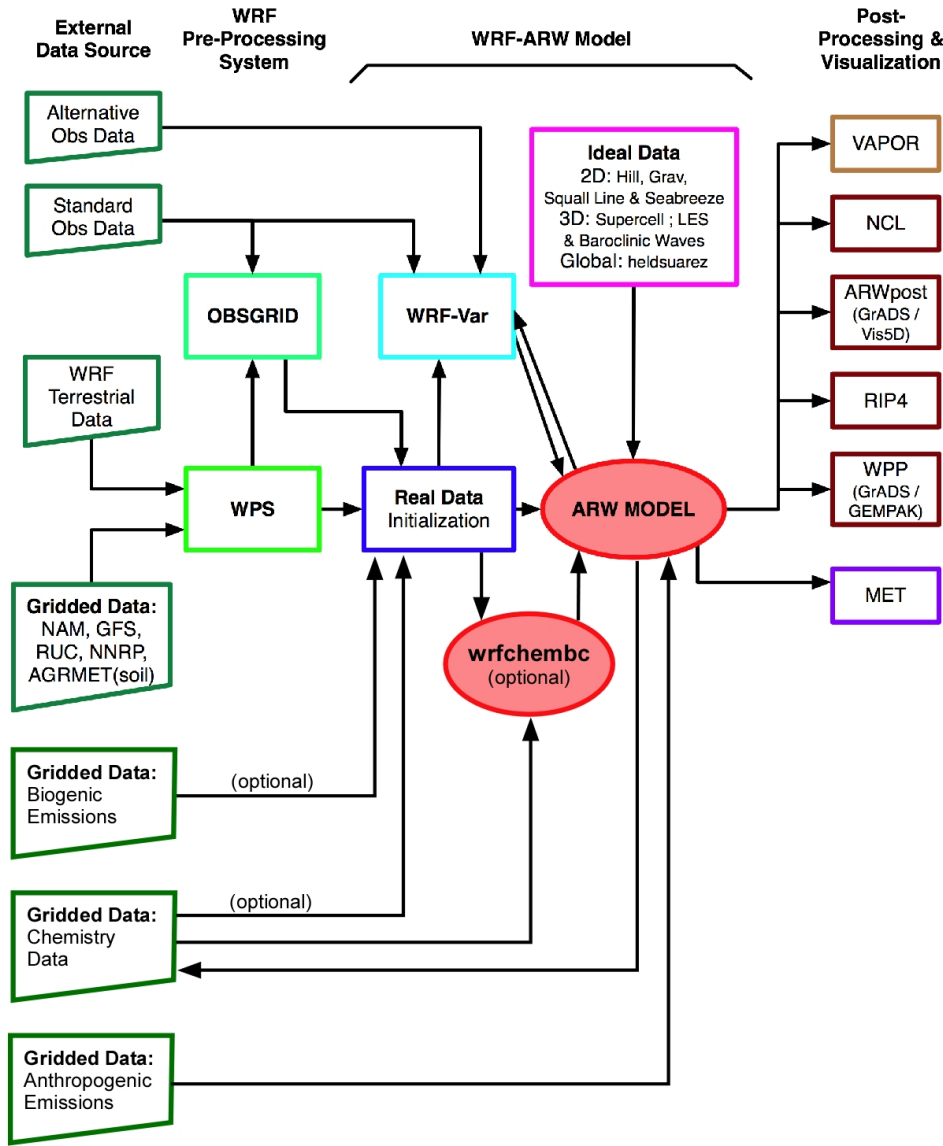
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WRF-Chem Emissions

- The “available” methodology for emissions uses a convert program
 - Program called `convert_emiss.exe` (compile `emi_conv`)
 - Reads header information from a WRF input file
 - Reads binary emissions data
 - Writes a WRF netCDF data file
- `convert_emiss` is very simple. Uses just a few namelist settings.
 - `emiss_opt=3` – NEI emissions for U.S.A.
 - `emiss_opt=5` – RETRO/EDGAR global emission
- Data is read in via `auxinput5` when running `wrf.exe`
 - `auxinput5_inname` = ‘`wrfchemi_<hr>z_d<domain>`’, (optional)
 - `io_form_auxinput5` = 2,
- Chpt. 3 and Appendix B of User’s Guide for more information
- Users can create input data files through any other methodology

WRF-Chem Biogenic Emissions

WRF-ARW Modeling System Flow Chart



WRF-Chem

Biogenic Emissions

- 4 choices for Biogenic emissions
- Option 1: No biogenic emissions ($\text{bio_emiss_opt} = 0$):
 - Provide biogenic emissions through anthropogenic input.
 - No additional input data files.
- Option 2 ($\text{bio_emiss_opt} = 1$): (good default option)
 - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
 - No additional input data files.
 - Small number of vegetation types (errors?)

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Biogenic Emissions

- Option 3 (bio_emiss_opt = 2):
 - User specified from external data source
 - Biogenic Emissions Inventory System (BEIS) version 3.14 [*Vukovich and Pierce, 2002*] with land-use obtained from the Biogenic Emissions Landuse Database version 3 (BELD3) [*Pierce et al., 1998*].
 - Static 2-D surface data provided in input data file and are modified according to the environment
 - Data is read in via auxinput6 when running real.exe
 - auxinput6_inname = 'wrfbiochemi_d01',
 - io_form_auxinput6 = 2,

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Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN (best choice?!)
 - Separate program made available by NCAR/ACD
 - Global data with base resolution of ~ 1 km
 - Leaf Area Index, vegetation type, emission factors
 - Steps:
 1. Download MEGAN code from NCAR/ACD
 - megan_bio_emiss.tar
 - megan.data.tar.
(when uncompressed ~ 28 GB)

<http://acd.ucar.ued/~guenter/MEGAN/MEGAN.html>

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Biogenic Emissions

- Option 4 (`bio_emiss_opt = 3`): MEGAN
 - Steps:
 2. Compile `megan_bio_emiss`
 3. Create `wrfbiochemi_d01` data file using:
 - `wrfinput`,
 - RAW MEGAN data files,
 - settings in `megan_bio_emiss.input` file
 - About 10 Gb of memory

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Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN
 - Steps:
 4. View wrfbiochemi_d01 data file to verify data is correct
 5. Run real.exe and wrf.exe
 - Add ne_area setting to the WRF chemistry namelist!!!
 - » ne_area = number of chemical species in chem_opt

<http://acd.ucar.ued/~guenter/MEGAN/MEGAN.html>

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Biomass Burning Emissions

- 2 choices for biomass burning emissions
- Option 1: No biomass emissions (`biomass_burn_opt = 0`):
 - No additional input data files.
- Option 2 (`biomass_burn_opt = 1`):
 - Use `prep_chem_sources` program to read WFABBA, or MODIS data
 - Convert binary data to `wrffirechemi_d01` input file
 - Data read in through `auxinput7` when running `real.exe`

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Dust Emissions

- 3 choices for dust emissions
- Option 1: No dust emissions (`dust_opt = 0`):
 - No additional input data files.
- Option 2 (`dust_opt = 1`):
 - Need to include surface erosion data in WPS
 - Use new GEOGRID table for running `geogrid.exe`
 - Dust data included in `wrfinput` file
- Option 3 (`dust_opt = 3`)
 - AFWA scheme uses same method as option 2
- Work tutorial exercise 1 for more information.

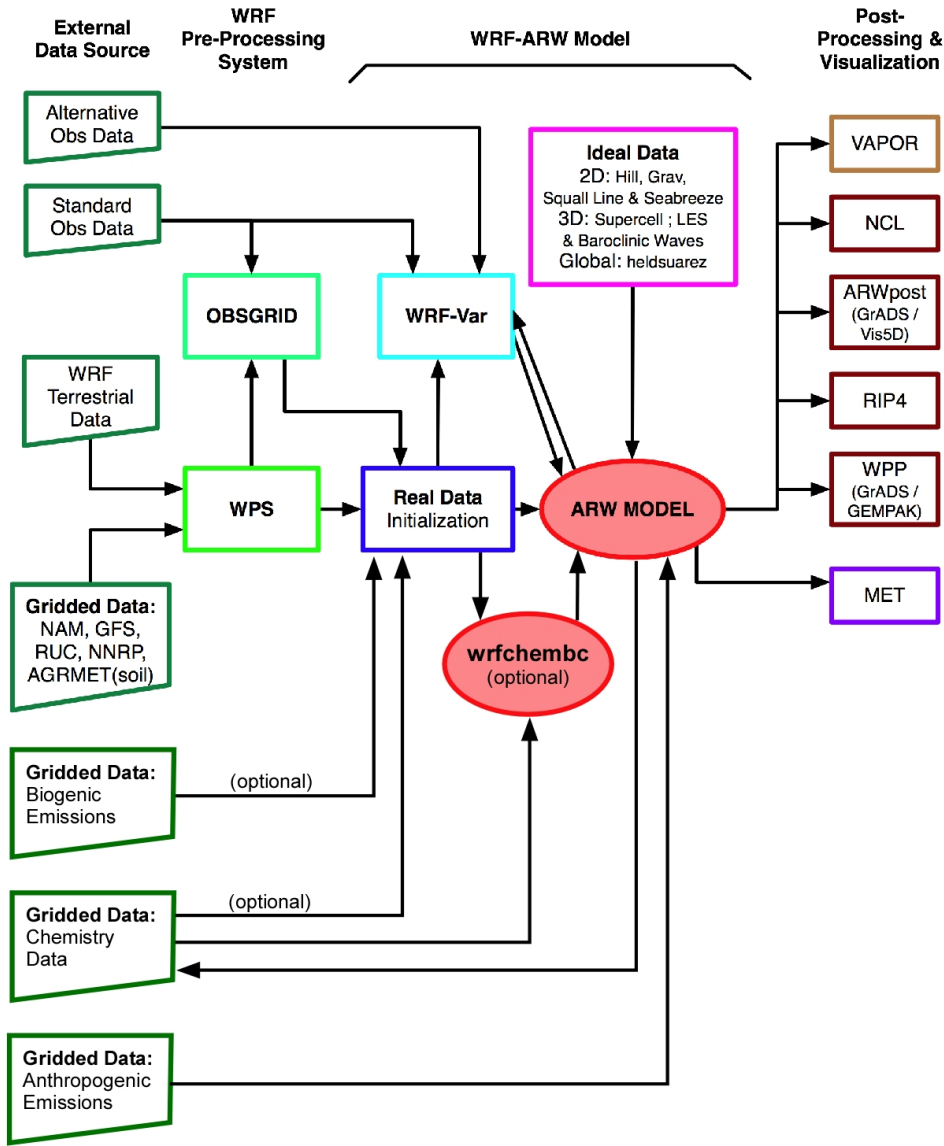
WRF-Chem

GOCART Background Data

- Includes DMS as well as GOCART
 - From running `prep_chem_sources` with GOCART included
 - Planned to be moved to WPS one of these days
- Run `prep_chem_sources` program to produce external binary data files
- Convert binary data files to WRF input files
 - `chem_opt = 300` or `301` and/or `dmsemis_opt=1`
- Data read by `real.exe` through `auxinput8`
 - File name `wrfchemi_gocart_bg_d01`

WRF-Chem Boundary Conditions

WRF-ARW Modeling System Flow Chart



WRF-Chem Chemistry B.C.s

- External tools under development to provide global model data as BC and initial conditions
- Test program available: wrfchembc (Rainer Schmitz - Univ. of Chile)
 - Available code runs with MPI-MATCH & RAQMS data
 - Adds lateral boundary data for chemical species to wrfbdy_d01
 - User specifies which chemical species to use
 - Need to choose chemical species from global model
 - Need to speciate global model data for WRF-Chem chemistry
 - Requires knowledge from user regarding chemistry (not turn-key)
- wrfinput_d01 not modified
 - Can result in differences near boundaries at start of simulation

WRF-Chem Chemistry B.C.s

- Other groups are exploring other possible ways to generate input/B.C. data for WRF-Chem
 - NCAR/ACD has a program available if using MOZART
- MOZBC sets space and time-varying chemical initial (IC) and boundary conditions (BC)
 - global model output (MOZART-4 or CAM-Chem)

MOZBC : <http://www.acd.ucar.edu/wrf-chem/download.shtml>

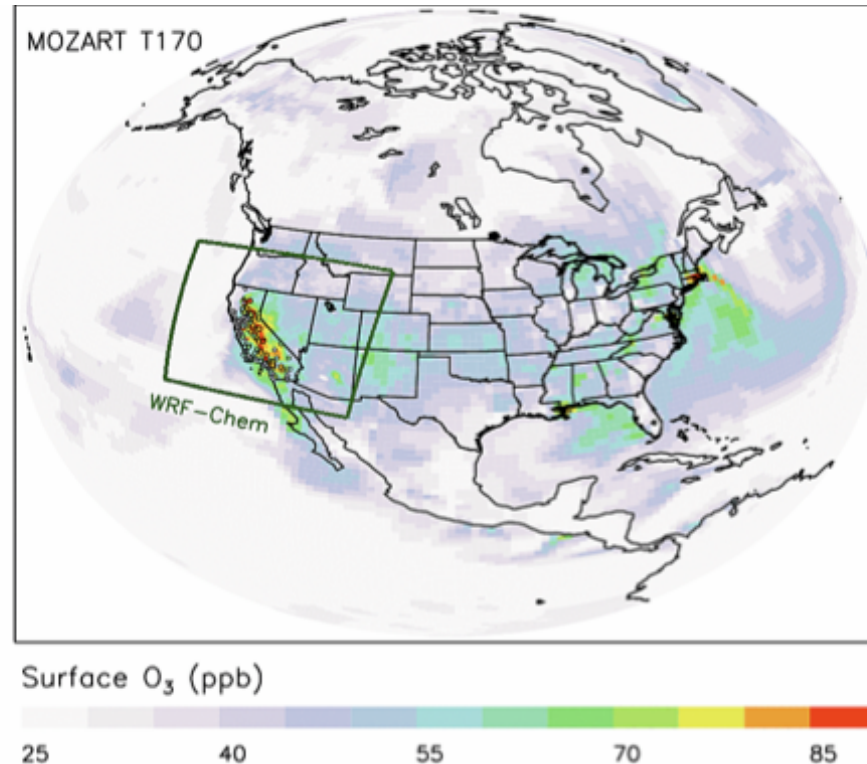
MOZART data (2004-2008):

<http://www.acd.ucar.edu/wrf-chem/mozart.shtml>

- Note: MOZART/CAM-Chem data are interpolated only in space.

WRF-Chem Chemistry B.C.s

- Program will fill the chemical fields in your `wrfinput_d<nn>` and `wrfbdy_d<nn>` files with global model output.



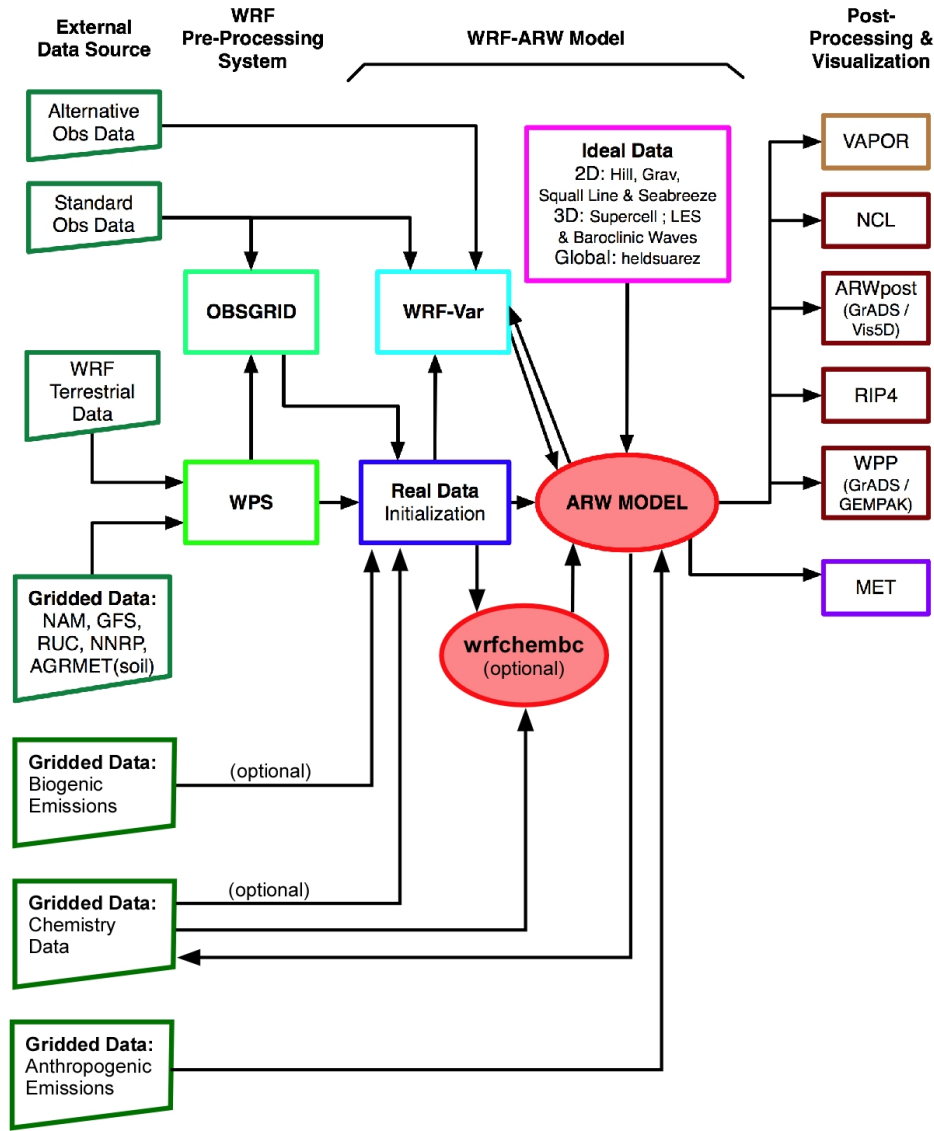
- To enable chemical IC and BC when running WRF-Chem set in `namelist.input`:
have_bcs_chem = .true.

WRF-Chem Chemistry B.C.s

- What if you have different GCM data?
- Methodology is the same
 - Read global model chemistry data
 - Skip over if not a desired chemistry species
 - Determine grid point location on WRF-Chem grid
 - If at boundary, interpolate data to WRF-Chem grid
 - Once completed reading/interpolating global data:
 - Open wrfbdy_d01 data file
 - Write boundary data to wrfbdy_d01

WRF-Chem Namelist

WRF-ARW Modeling System Flow Chart



WRF-Chem Namelist

- **Time control namelist options**
- A few of the chemistry related namelist options
 - More details provided in Chapter 4 of User's Guide

WRF-Chem Namelist

- Time control namelist
 - Chemistry input fields come in through auxiliary input ports
 - Biogenic emissions use auxinput 6 for example

&time_control

...

```
auxinput6_inname      = 'wrfbiochemi_d<domain>',  
auxinput6_interval_m = 1440,  
io_form_auxinput6    = 2,
```

Recall:

Defining a variable-set for an I/O stream

- **Fields are added to a variable-set on an I/O stream at compile-time with Registry**

#	Type	Sym	Dims	Use	Tlev	Stag	IO	Dname	Descrip
state	real	u	ikjb	dyn_em	2	X	i01rhusdf	"U"	"X WIND COMPONENT"

IO is a string that specifies if the variable is to be subject to initial, restart, or history I/O. The string may consist of 'h' (subject to history I/O), 'i' (initial dataset), or 'r' (restart dataset). The 'h', 'r', and 'i' specifiers may appear in any order or combination.

The 'h' and 'i' specifiers may be followed by an optional integer string consisting of '0', '1', ..., '9'. Zero denotes that the variable is part of the principal input or history I/O stream. The characters '1' through '9' denote one of the auxiliary input or history I/O streams.

WRF-Chem Registry

- Thus, in registry.chem

```
state real - i+jf emis_ant - - - - "Anthropogenic Emissions" ""
state real e_iso i+jf emis_ant 1 Z i5r "E_ISO" "Isoprene EMISSIONS" "mol km^-2 hr^-1"
state real e_so2 i+jf emis_ant 1 Z i5r "E_SO2" "EMISSIONS" "mol km^-2 hr^-1"
state real e_no i+jf emis_ant 1 Z i5r "E_NO" "EMISSIONS" "mol km^-2 hr^-1"

#
state real e_bio ijo misc 1 Z r "E_BIO" "EMISSIONS" "ppm m/min"
state real sebio_iso ij misc 1 - i6r "sebio_iso" "Reference biog emiss" "mol km^-2 hr^-1"
state real sebio_oli ij misc 1 - i6r "sebio_oli" "Reference biog emiss" "mol km^-2 hr^-1"

# additional arrays needed for biomass burning emissions input
state real - i|j|f ebu_in - - - - "Biomass burnung input" ""
state real ebu_in_no i|j|f ebu_in 1 - i{7} "ebu_in_no" "EMISSIONS" "mol km^-2 hr^-1"
state real ebu_in_co i|j|f ebu_in 1 - i{7} "ebu_in_co" "EMISSIONS" "mol km^-2 hr^-1"

# Input for GOCART: Background chemistry, erodible surface emissions map
state real backg_oh ikj misc 1 - i8r "BACKG_OH" "Background OH" "volume mixing ratio"
state real backg_h2o2 ikj misc 1 - i8r "BACKG_H2O2" "Background H2O2" "volume mixing ratio"
```

WRF-Chem Namelist

- For the chemistry variables to come in via auxiliary port
 - Registry set for input via auxiliary port

Auxiliary port number	Description
5	Anthropogenic emissions
6	Biogenic emissions
7	Surface biomass burning data
8	GOCART background fields
12	External chemistry fields (wrfout data from previous run)
13	Volcanic Ash emissions
14	Aircraft emissions
15	Green House Gas emissions

WRF-Chem Namelist

- For the chemistry variables to come in via auxiliary ports (cont.)
 - Namelist set in time_control

```
&time_control
...
auxinput6_inname = 'wrfbiochemi_d01',
auxinput7_inname = 'wrffirechemi_d<domain>',
auxinput8_inname = 'wrfchemi_gocart_bg_d<domain>',
auxinput12_inname = 'wrf_chem_input',
auxinput13_inname = 'wrfchemv_d<domain>',
auxinput5_interval_m = 86400, 86400, 60,
auxinput7_interval_m = 86400, 86400, 60,
auxinput8_interval_m = 86400, 86400, 60,
auxinput13_interval_m = 86400, 86400, 60,
io_form_auxinput2 = 2,
io_form_auxinput5 = 2,
io_form_auxinput6 = 0,
io_form_auxinput7 = 0,
io_form_auxinput8 = 0,
io_form_auxinput12 = 0,
io_form_auxinput13 = 0,
```

WRF-Chem Namelist

A few of the chemistry namelist options

- More details provided in Chapter 4 of WRF-Chem User's Guide

WRF-Chem Namelist

- Chemistry control namelist

Chem_opt	Description
0	No chemistry
1 - 40	Chemical mechanisms (RADM2, CBMZ), tracer options (chem_opt=13 to 17)
101 - 200	Options covering RADM2, CBMZ, MOZART, SAPRC99, NMHC9 chemical mechanisms using KPP.
300 – 303	GOCART aerosol options
400 – 403	Dust and Volcano options (volcanic and surface lofted)
501 – 504	CBMZ and MAM aerosols (run with CAM5 physics)

WRF-Chem Namelist

emiss_opt	Description
0	no anthropogenic emissions
2	use radm2 anthropogenic emissions
3	use radm2/MADE/SORGAM anthropogenic emissions
4	use CBMZ/MOSAIC anthropogenic emissions
5	GOCART RACM_KPP emissions
6	GOCART simple emissions
7	MOZART emissions .
8	MOZCART (MOZART + GOCART aerosols) emissions
13	SAPRC99 emissions
16	CO2 tracer emissions
17	Green House Gas emissions

Remember: emiss_opt sets emissions structure (registry.chem)

#emission package definitions

```
package eradmsorg    emiss_opt==3
emis_ant:e_iso,e_so2,e_no,e_no2,e_co,e_eth,e_hc3,e_hc5,e_hc8,e_xyl,e_ol2,e_olt,e_oli,e_tol,e_csl,e_hch
o,e_ald,e_ket,e_ora2,e_nh3,e_pm25i,e_pm25j,e_pm_10,e_eci,e_ecj,e_orgi,e_orgj,e_so4i,e_so4j,e_no3i,e_
no3j,e_naaj,e_naai,e_orgi_a,e_orgj_a,e_orgi_bb,e_orgj_bb
```

```
package ecptec      emiss_opt==5
emis_ant:e_iso,e_so2,e_no,e_no2,e_co,e_eth,e_hc3,e_hc5,e_hc8,e_xyl,e_ol2,e_olt,e_oli,e_tol,e_csl,e_hch
o,e_ald,e_ket,e_ora2,e_nh3,e_pm_25,e_pm_10,e_oc,e_sulf,e_bc
```

Anthropogenic CO₂, CO and CH₄ emissions:

```
package eco2        emiss_opt==16    emis_ant:e_co2,e_co2tst,e_co
```

```
package eghg        emiss_opt==17    emis_ant:e_co2,e_co2tst,e_co,e_cotst,e_ch4,e_ch4tst
```

WRF-Chem Namelist

cu_rad_feedback

Description

.false.

No feedback from the parameterized convection to the atmospheric radiation and the photolysis schemes. (logical)

.true.

Feedback from the parameterized convection to the radiation schemes turned on. (logical) - use Grell cumulus scheme

progn

0

Turns off prognostic cloud droplet number in the Lin et al. microphysics

1

Prognostic cloud droplet number included in the Lin et al. This effectively turns the Lin et al. scheme into a second-moment microphysical scheme. If set with chem._opt=0 a default prescribed aerosol concentration is used.

WRF-Chem Namelist

cldchem_onoff

Description

- 0 cloud chemistry turned off in the simulation, also see the “chem_opt” parameter
- 1 cloud chemistry turned on in the simulation, also see the “chem_opt” parameter

wetscav_onoff

- 0 wet scavenging turned off in the simulation, also see the “chem_opt” parameter
- 1 wet scavenging turned on in the simulation, also see the “chem_opt” parameter

NAMELIST CHOICES

Dust only

&chem

chem_opt = 401,

chemdt = 5,

dust_opt = 1

/

NAMELIST CHOICES

GOCART (simple)

```
&time_control  
io_form_auxinput5      = 2,  
io_form_auxinput6      = 0,  
io_form_auxinput7      = 2,  
io_form_auxinput8      = 2,  
/  

```

```
&chem  
kemit                  = 1,  
chem_opt               = 300,  
chemdt                 = 60,  
io_style_emissions    = 1,  
emiss_opt              = 5,  
dust_opt               = 1,  
seas_opt               = 1,  
biomass_burn_opt      = 1,  
plumerisefire_freq    = 30,  
aer_ra_feedback       = 1,  
aer_op_opt             = 1,  
opt_pars_out          = 1,  
/  

```

NAMELIST CHOICES

RACM-SOA_VBS

```
&time_control  
io_form_auxinput5      = 2,  
io_form_auxinput6      = 2,  
io_form_auxinput7      = 2,  
io_form_auxinput8      = 2,  
/  

```

```
&chem  
chem_opt                = 108,  
chemdt                  = 0,  
gas_drydep_opt          = 1,  
aer_drydep_opt          = 1,  
bio_emiss_opt           = 3,  
ne_area                 = 104,  
wetscav_onoff           = -10,  
cldchem_onoff           = 0,  
vertmix_onoff           = 1,  
chem_conv_tr            = 1,  
conv_tr_wetscav         = 1,  
conv_tr_aqchem          = 1,  
seas_opt                = 0,  
dust_opt                = 0,  
aer_op_opt              = 0,  
/  

```

Questions?

Go to:

<http://ruc.noaa.gov/wrf/WG11/Tutorial.html>

Near the bottom:

Online Tutorial Exercises

Tutorial Exercises For **Learning to Run WRF-Chem version 3.5**