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

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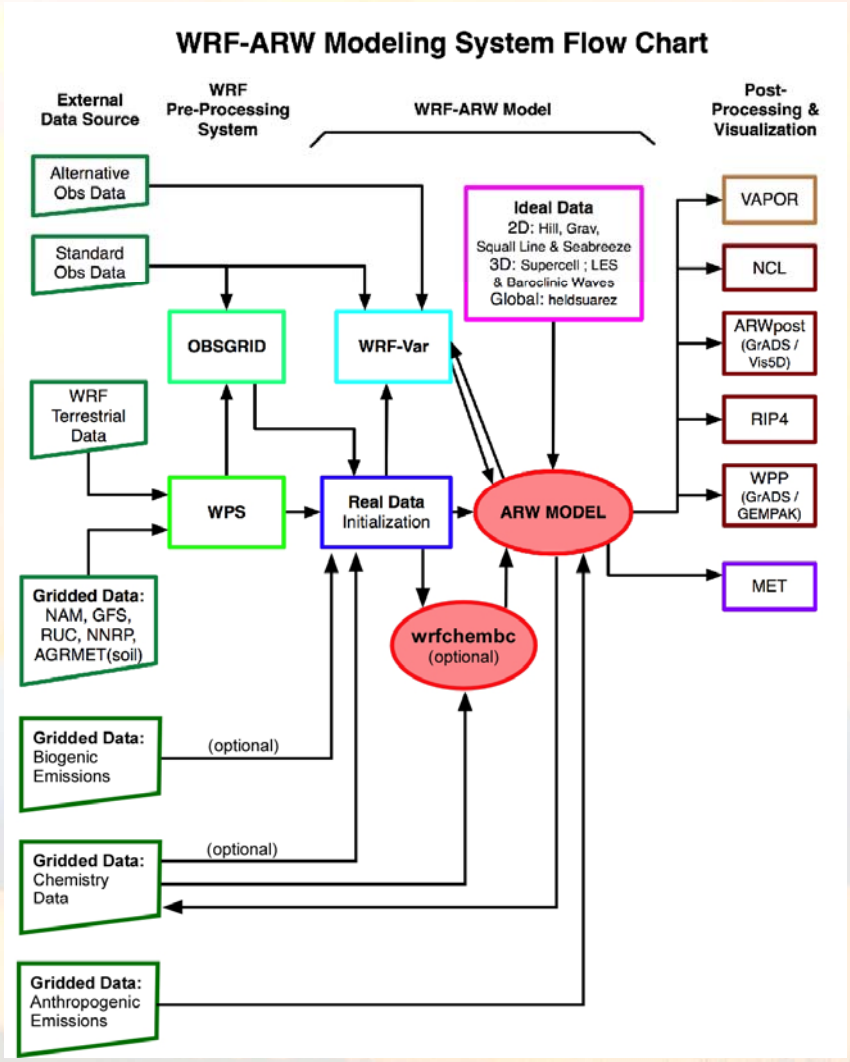
WRF/Chem Model System



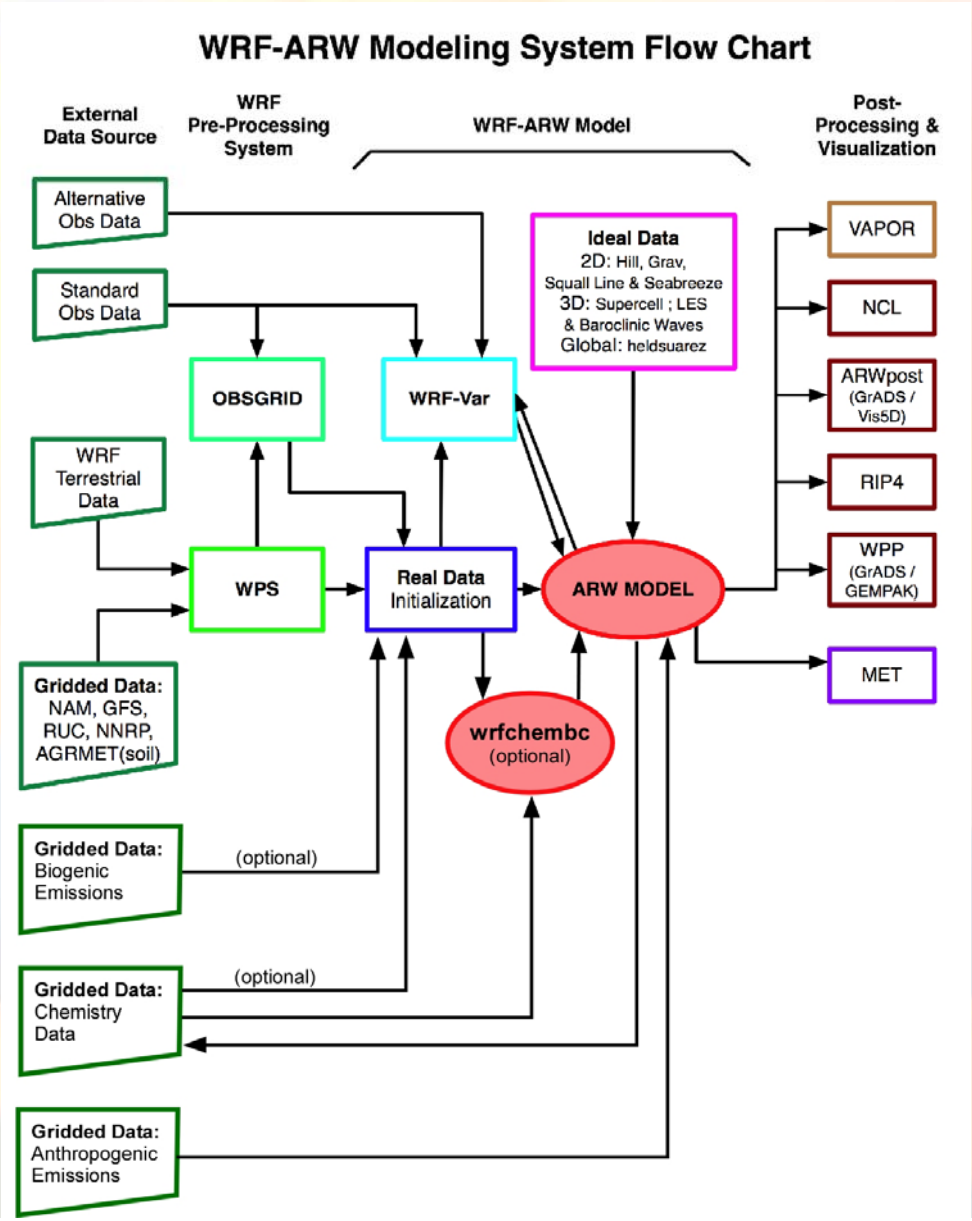
WRF/Chem

- It is assumed that the user of WRF/Chem :
  - is ***very familiar*** with the WRF model system
  - have run WPS
  - and has made more than one weather simulation using WRFV3
- The chemistry code is now available with WRF V3 from NCAR.
  - Send email to WRF/Chem help (wrfchemhelp.gsd@noaa.gov)
  - www.wrf-model.org/WG11
- Test data is available as well
  - Small domain (40x40x35 grid points, 60 km horiz. spacing)

WRF/Chem

- Compile WRF/Chem code
  - Set environmental variables
    - Define which model core to build (use ARW for now).
      - setenv WRF_EM_CORE 1
      - setenv WRF_NMM_CORE 0
    - Chemistry code is to be included in the WRF model build
      - setenv WRF_CHEM 1
    - Kinetic Pre-Processor (KPP) code (later talk by Marc Salzmann)
      - setenv WRF_KPP 1 => if KPP is to be included
      - setenv WRF_KPP 0 => if KPP is NOT to be included
  - 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/Chem Emissions

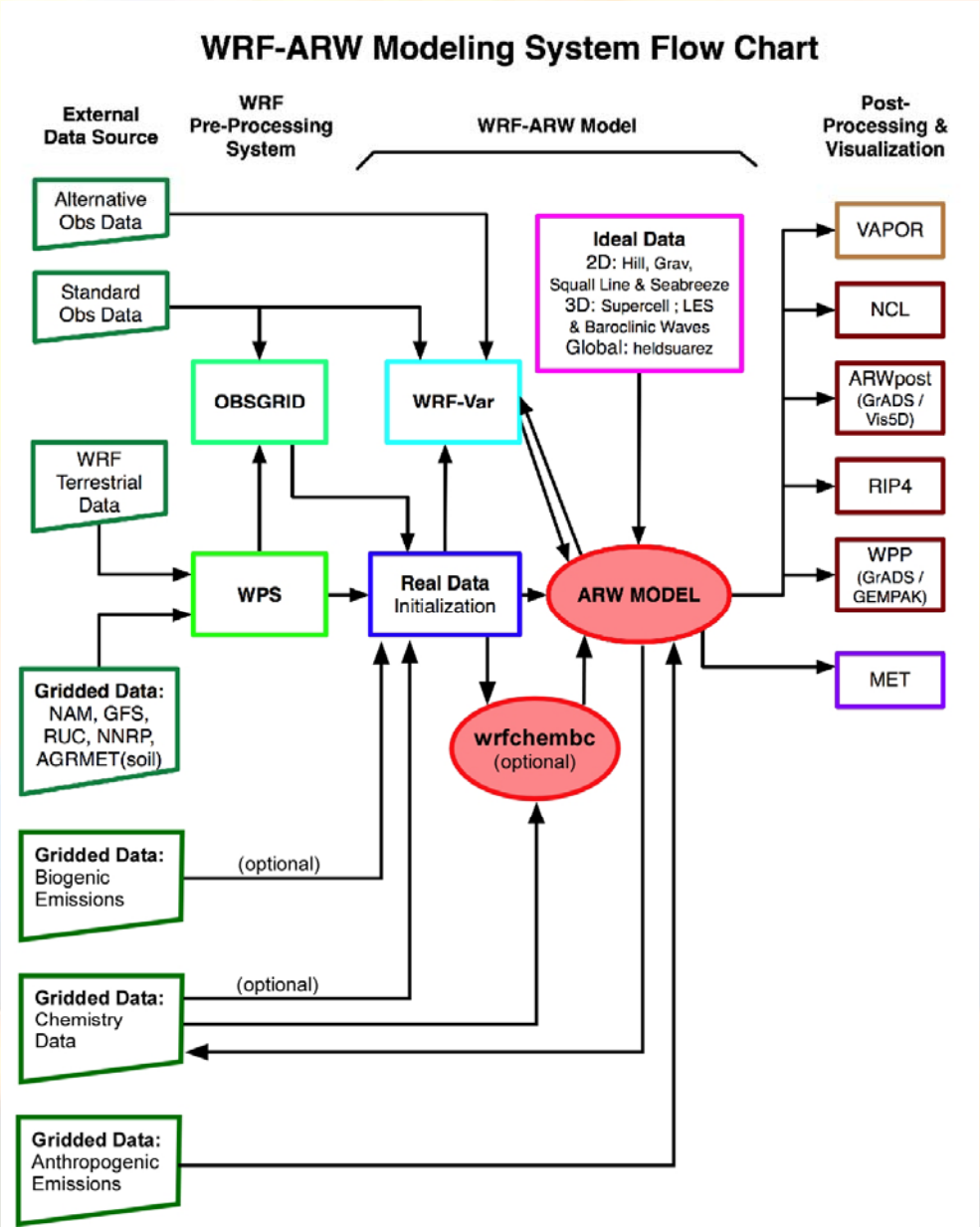
- Two sources of anthropogenic emissions available:
  - NEI-99 for US;
  - RETRO (.5 degree, monthly) and EDGAR (1 degree, annual)
  - Both include programs to map to WRF grid; binary output files

- 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

- Convert emissions data to a WRF netCDF data file
  - compile emi_conv

- Chpt. 3 and Appendix B of User’s Guide for more information

WRF/Chem Biogenic Emissions



WRF/Chem
Biogenic Emissions

- 4 choices for Biogenic emissions
- Option 1: No biogenic emissions (bio_emiss_opt = 0):
  - Provide biogenic emissions through anthropogenic input.
  - No additional input data files.

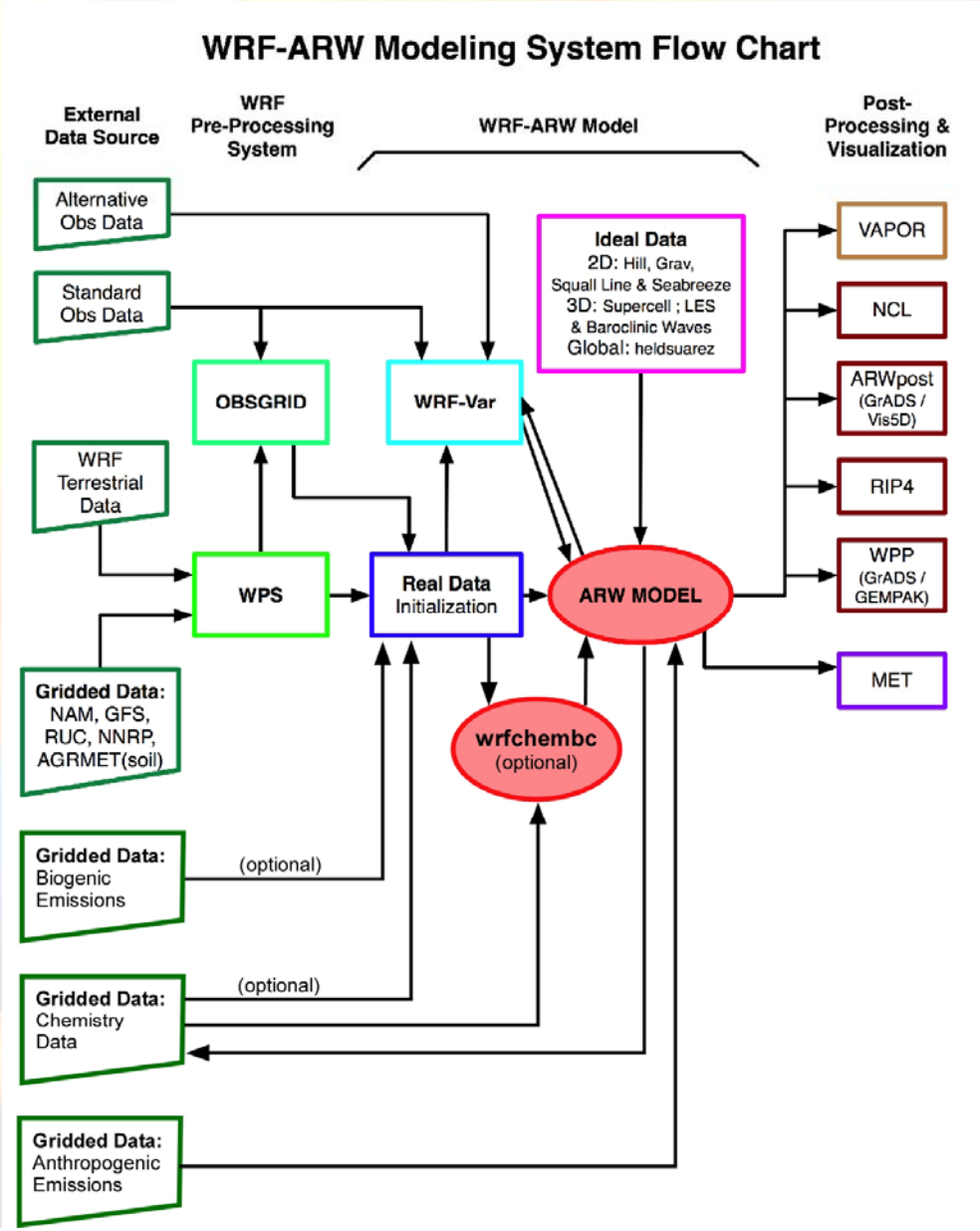
- Option 2 (bio_emiss_opt = 1): (best default option)
  - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
  - No additional input data files.

WRF/Chem
Biogenic Emissions

- Option 3 (bio_emiss_opt = 2):
  - User specified from external data source
    - Biogenic Emissions Inventory System (BEIS) version 3.11 [*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

- Option 4 (bio_emiss_opt = 3): MEGAN

WRF/Chem B.C.s


WRF-ARW Modeling System Flow Chart
External Data Source
WRF Pre-Processing System
WRF-ARW Model
Post-Processing & Visualization
Alternative Obs Data
Standard Obs Data
OBSGRID
WRF-Var
Ideal Data
2D: Hill, Grav, Squall Line & Seabreeze
3D: Supercell ; LES & Baroclinic Waves
Global: heldsuarez
VAPOR
NCL
ARWpost (GrADS / Vis5D)
RIP4
WPP (GrADS / GEMPAK)
MET
WRF Terrestrial Data
WPS
Real Data Initialization
ARW MODEL
Gridded Data: NAM, GFS, RUC, NNRP, AGRMET(soil)
wrfchembc (optional)
Gridded Data: Biogenic Emissions
(optional)
Gridded Data: Chemistry Data
(optional)
Gridded Data: Anthropogenic Emissions

WRF/Chem Chemistry B.C.s

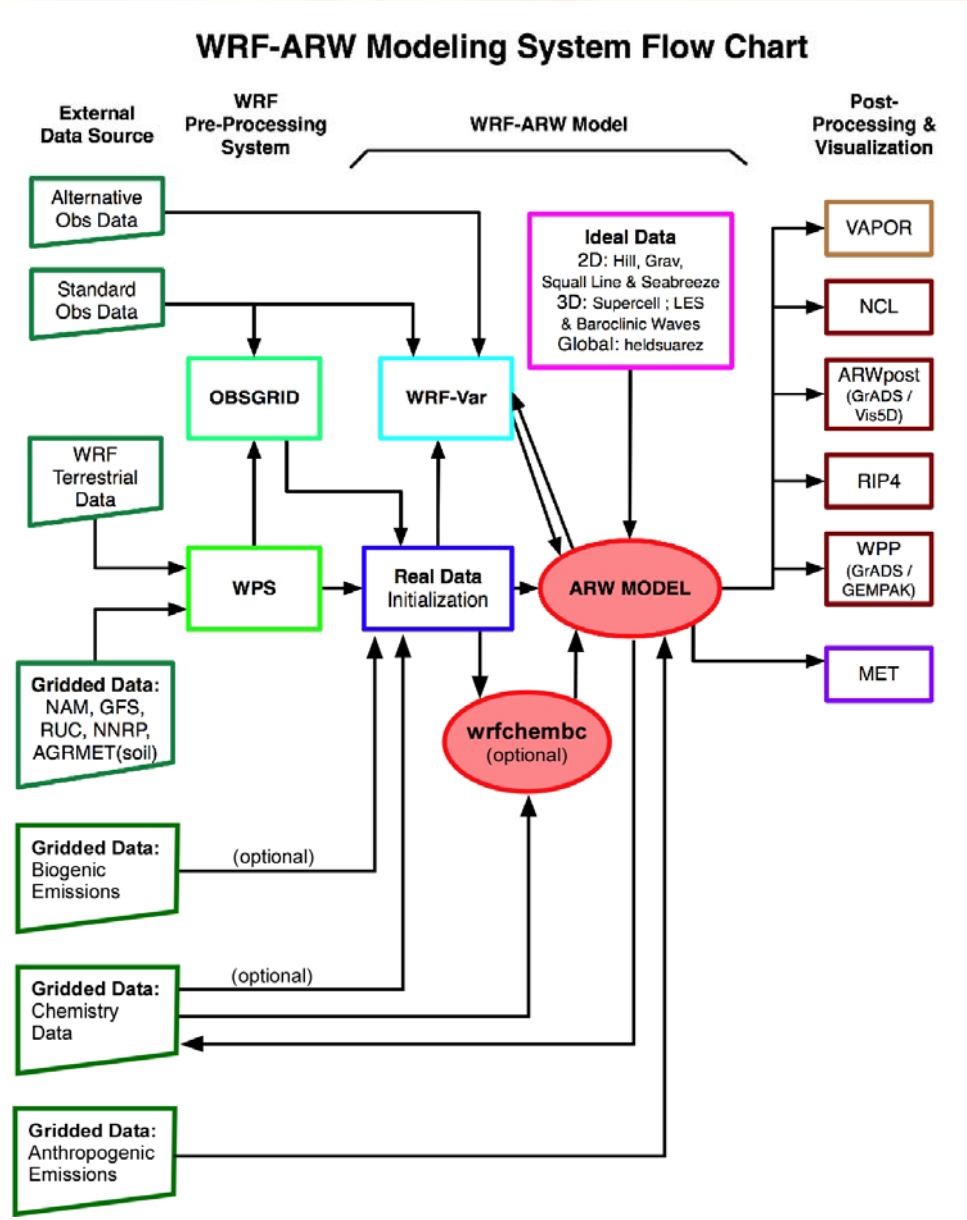
- Tools under development to provide global model data as BC and initial conditions
- Test program available: wrfchembc (Rainer Schmitz - Univ. of Chile)
  - Available code runs with MPI-MATCH & RAQMS data
  - Adds lateral boundary data for chemical species to wrfbdy_d01
  - User specifies which chemical 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
  - One program currently available

- wrfchembc methodology
  - 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 Simulation



WRF/Chem Chemical Data Input

- No chemical initial analysis derived from observations
  - There are no daily 3-D observations (with the exception of a few special occasions)
- Use forecast for initial chemical fields
  - Works well as tropospheric air quality mostly depends on emissions
  - Read in forecast data through real.exe (chem_in_opt = 1)

WRF/Chem Chemical Data Input

- Methodology
  - Set namelist option chem_in_opt = 1
    - Update dates/times of simulation in namelist.input for your forecast
  - Copy or link wrfout file to a “wrf_chem_input” data file

```
ln –s $outdir/wrfout_d01_2007-06-15-12:00:00 wrf_chem_input_d01_2007-06-15-12:00:00
```

  - When you run real.exe
    - A message indicates that model is being initialized with previous forecast

Running WRF/Chem

- Get copy of WRF/Chem code in your home directory

  cp -R /wrfhelp/SOURCE_CODE/WRFV3_CHEM/WRFV3/ WRFV3

  The code is compiled (skip section 1 in the quick start guide).

- Get WPS met data into your WRFV3/test/em_real directory

  tar -xf /wrfhelp/DATA/WRF-CHEM_WPS/met_em.d01.2008071412.tar

- Set options in namelist.input

- Run real.exe with the chemistry turned off (quick start guide #2).
  (Save the wrfinput_d01 data file for use later on.)

- Set the namelist.input options

Running WRF/Chem

- Compile and run the emiss_v03.F program (quick start #3)

```
 INTEGER    :: iproj = 2
REAL       :: rekm = 6371.
REAL       :: dx = 60.E3
REAL       :: dxbigdo = 60.E3
REAL       :: xlatc =  40.00
REAL       :: xlonc = -115.00
REAL       :: clat1 = 40.00
REAL       :: clat2 = -999.
INTEGER    :: inest1 = 0
REAL       :: xnesstr = 1.00
REAL       :: ynesstr = 1.00
INTEGER    :: il = 40
INTEGER    :: jl = 40
INTEGER    :: istart = 12
INTEGER    :: maxhr = 03
```

Set vertical levels (zfa) and vertical wind profile (wind)

- Run convert_emiss.exe
  - Normally produces wrfem60k_00to12Z and wrfem60k_12to24Z binary data files.
  - Tutorial example will produce only 1 file (wrfem60k_12to24Z)

Running WRF/Chem

- Edit the namelist.input file to your test_em_real directory
  - Watch interval_seconds, chem_opt
- run convert_emiss.exe and verify that your wrfchemi_d01 file
  - rename to wrfchemi_12z_d01
- Edit namelist.input file in WRFV3/test/em_real to reset namelist.input and set chem_opt, etc.
- run wrf.exe and verify results.

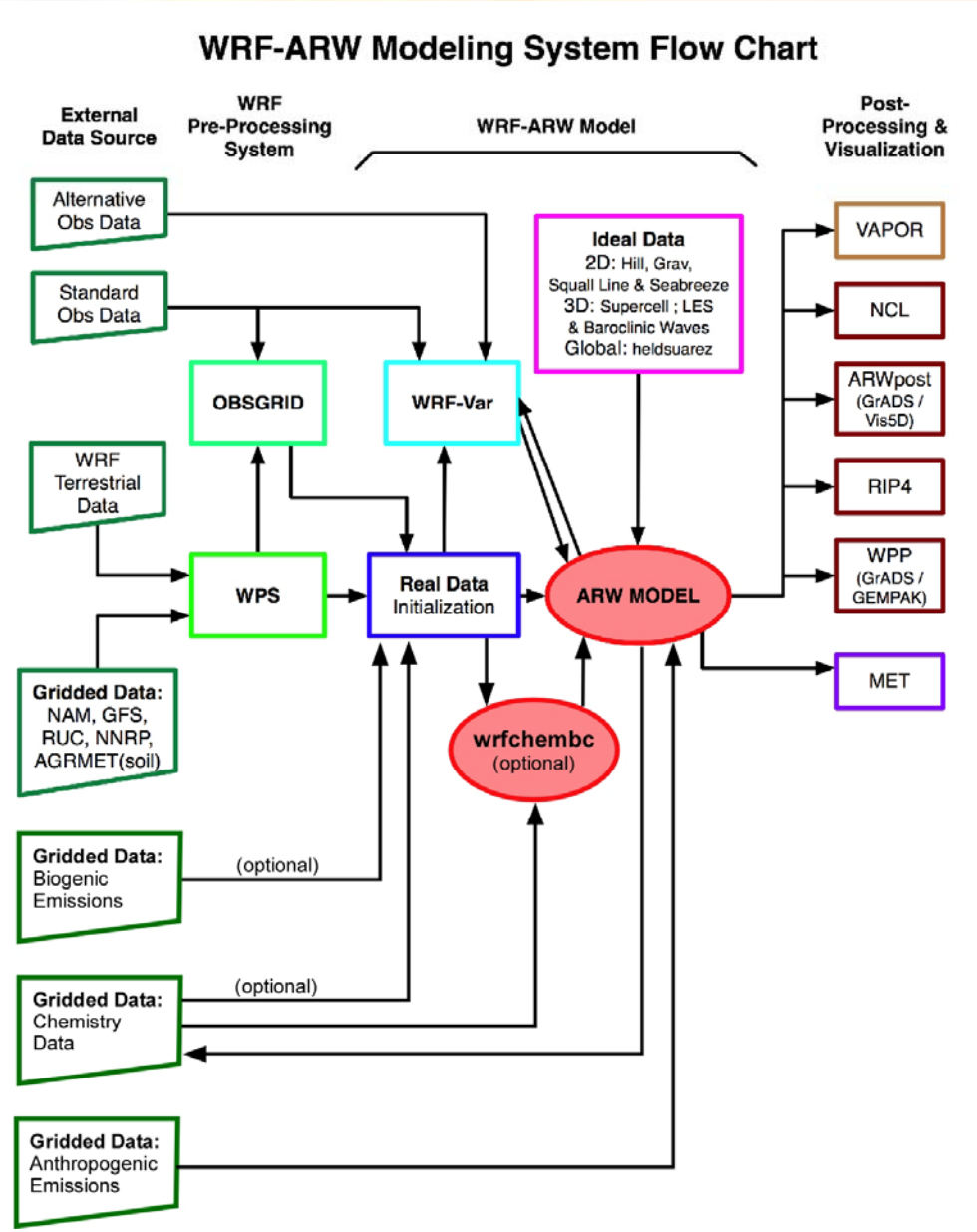
Running WRF/Chem

- After running real.exe, you have:
  - wrfinput_d01 and wrfbdy file
  - Anthropogenic emissions for run domain (wrfchemi_*)
- Set the namelist.input options (may not be necessary)
- Run wrf.exe to produce wrfout data files
  - Use multi-processor compiled code
  - should get messages regarding the reading of
    - anthropogenic emissions
    - If you do not get these messages, an error is likely

Running WRF/Chem

- After running WRF/Chem
  - Check the text output
    - Make sure you are getting the messages you expect
    - Look for any warning/error messages
  - Check the model output (ncview)
    - Confirm that emissions data is being read into simulation
      - Error in kemit will result in no anthropogenic emissions data
      - Error in chem_opt, emiss_inpt_opt? Other namelist options?
  - Make plots of simulation results

WRF/Chem Visualization



WRF/Chem Visualization

- Your favorite netCDF data file viewer to examine results
  - ncview, ncbrowse, etc.
- Other standard WRF visualization tools work with the chemistry variables as well as the meteorology
  - ARWpost (NCL, VIS5D)
  - Grads
  - Etc.

WRF/Chem Visualization

- Now you do it! Several exercises are located under /wrfhelp/WRF-CHEM

  Start with: /wrfhelp/WRF-CHEM/exercise_1/readme.txt

- Easy first one (NEI emissions only)
- 2 – Build and import global emissions
- 3 – full interactive physics
- 4 – Registry change to output new variable
- 5 – you build a new domain, init and build emissions

- Use quick start guide and User's Guide (and ask for help)

Exercise 1 hints (not directions)

- Exercises located at:

/home/gurme/wrfchem_tut/exercises/tutorial_exercises_july08_updated_nov08.tar.gz
or
more /home/gurme/wrfchem_tut/exercises/exercise_1/readme.txt

<tar –zxvf
/home/gurme/wrfchem_tut/exercises/tutorial_exercises_july08_updated_nov08.tar.gz>

- met data at:

/home/gurme/wrfchem_tut/tutorial_data/met_data

- Execute command

mpiexec –n 2 –host compute-0-6 <*filename*>

e.g., mpiexec –n 2 –host compute-0-6 convert_emiss.exe

exercise 1

- Edit the emiss_v03.F:
- POINDIR= ‘/home/gurme/wrfchem_tut/emissions/emissions_data/point/’
- AREADIR= ‘/home/gurme/wrfchem_tut/emissions/emissions_data/’

- Compile:
- mpif90 –free –convert big_endian emiss_v03.F

exercise 2