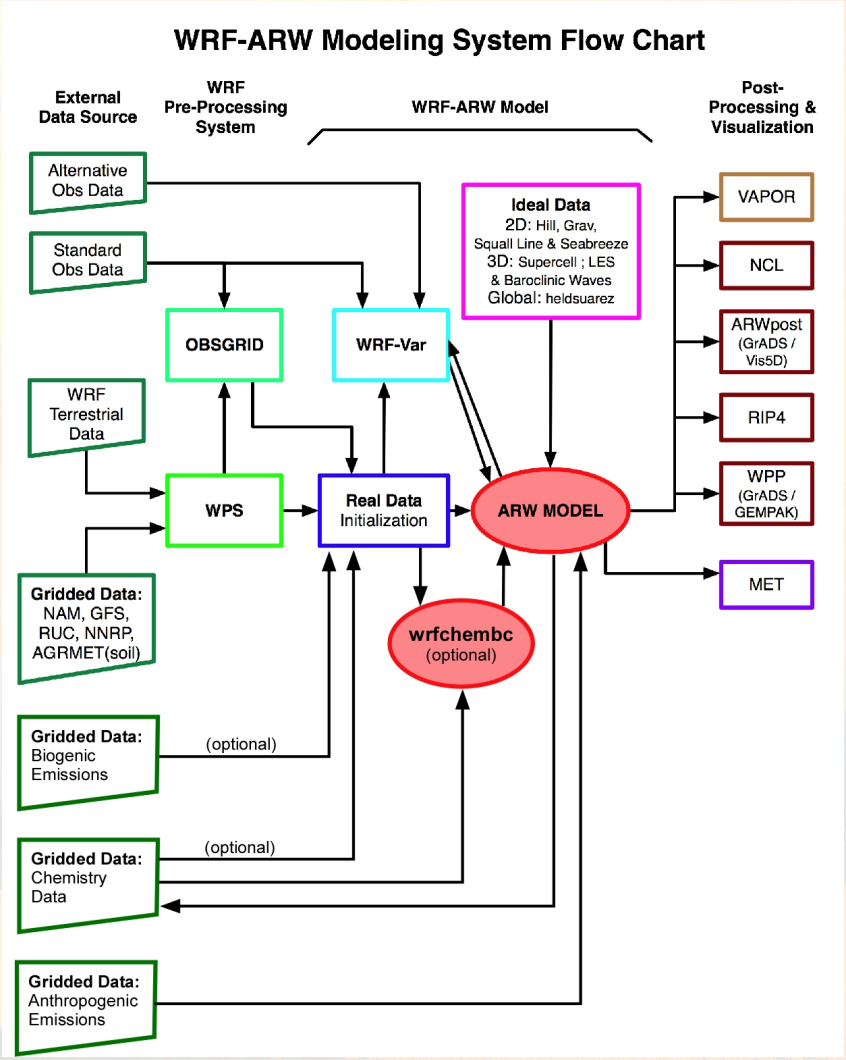
WRF/Chem V3.3: A Quick Review Of How To Set-Up & Run

Steven Peckham

WRF/Chem Model System



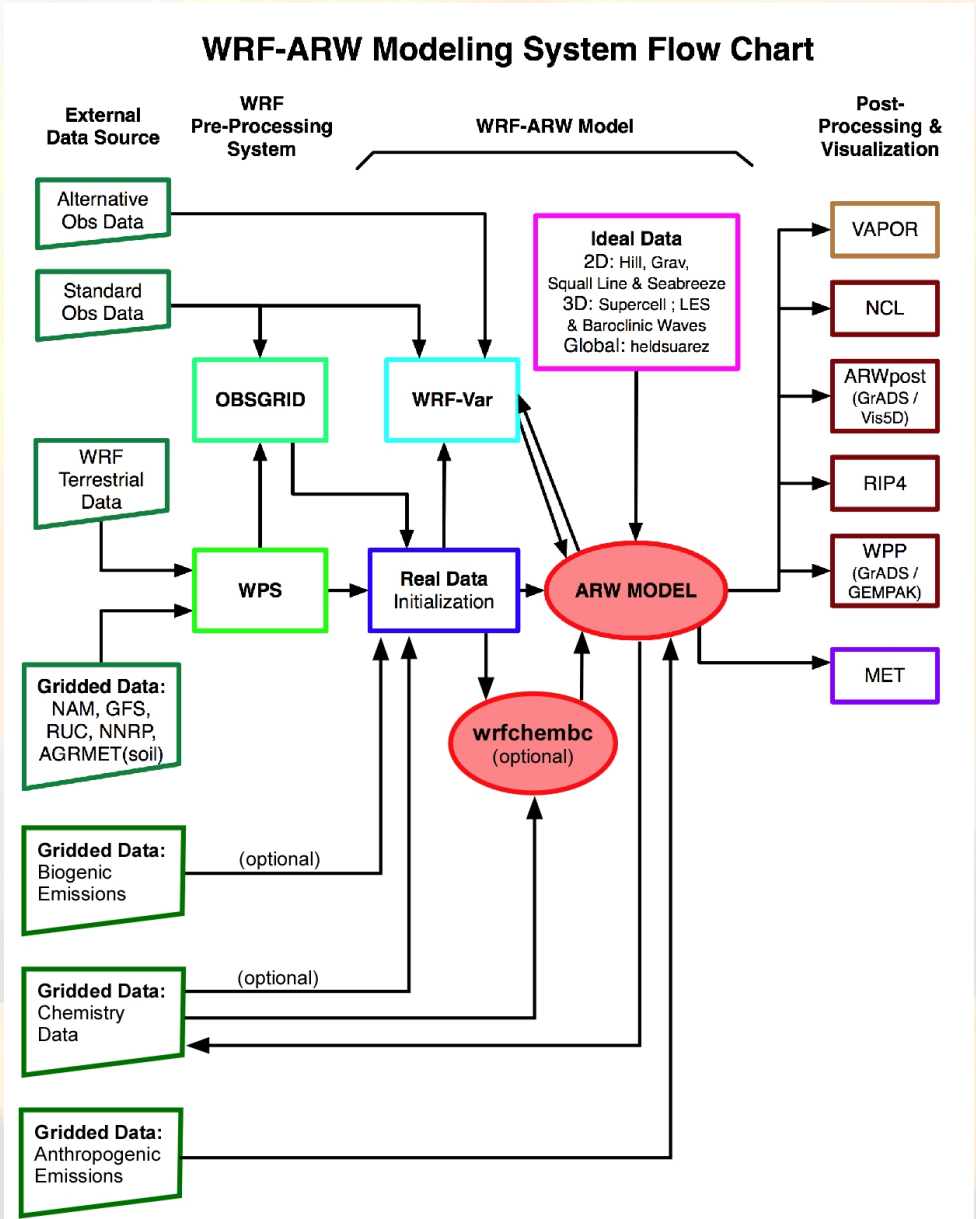
WRF/Chem

- 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 (already done)
  - 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
      - 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/Chem Emissions

- Two sources of anthropogenic emissions available:
  - National Emissions Inventory (NEI-2005) for U.S.
    - Run without chemistry first as mean wind profile is needed!
  - RETRO (.5 degree, month) and EDGAR (10 degree, annual)
    - Run Prep_sources_chem (Tutorial exercise 2)
  - 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

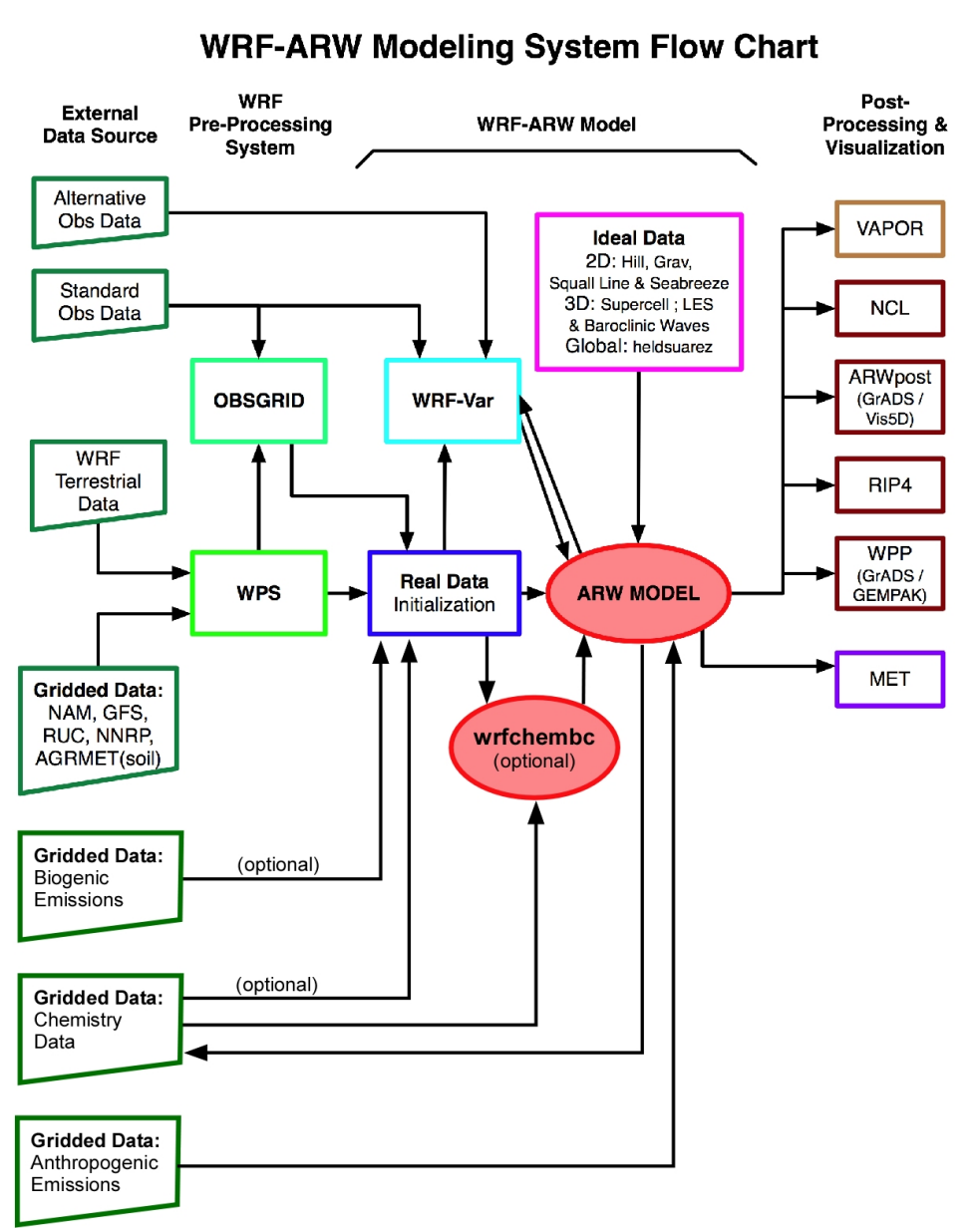
- One methodology is available emissions + convert program
  - Reads header information from a WRF input file
  - Reads binary emissions data to a WRF netCDF data file
  - compile emi_conv

- Convert program 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

- 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/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
  - Data is read in via auxinput6 when running real.exe
    - auxinput6_inname = 'wrfbiochemi_d01',
    - io_form_auxinput6 = 2,

WRF/Chem
Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN
  - Separate program made available by NCAR/ACD
  - Global data with base resolution of ~ 1 km
    - Leef Area Index, vegetation type, emission factors
  - Steps:
    - 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

WRF/Chem
Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN
  - Steps:
    - Compile megan_bio_emiss
    - Create wrfbiochemi_d01 data file using:
      - wrfinput,
      - RAW MEGAN data files,
      - settings in megan_bio_emiss.input file
    - View wrfbiochemi_d01 data file to verify data is correct.

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

WRF/Chem
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

WRF/Chem
Dust Emissions

- 2 choices for dust emissions
- Option 1: No dust emissions (dust_opt = 0):
  - No additional input data files.

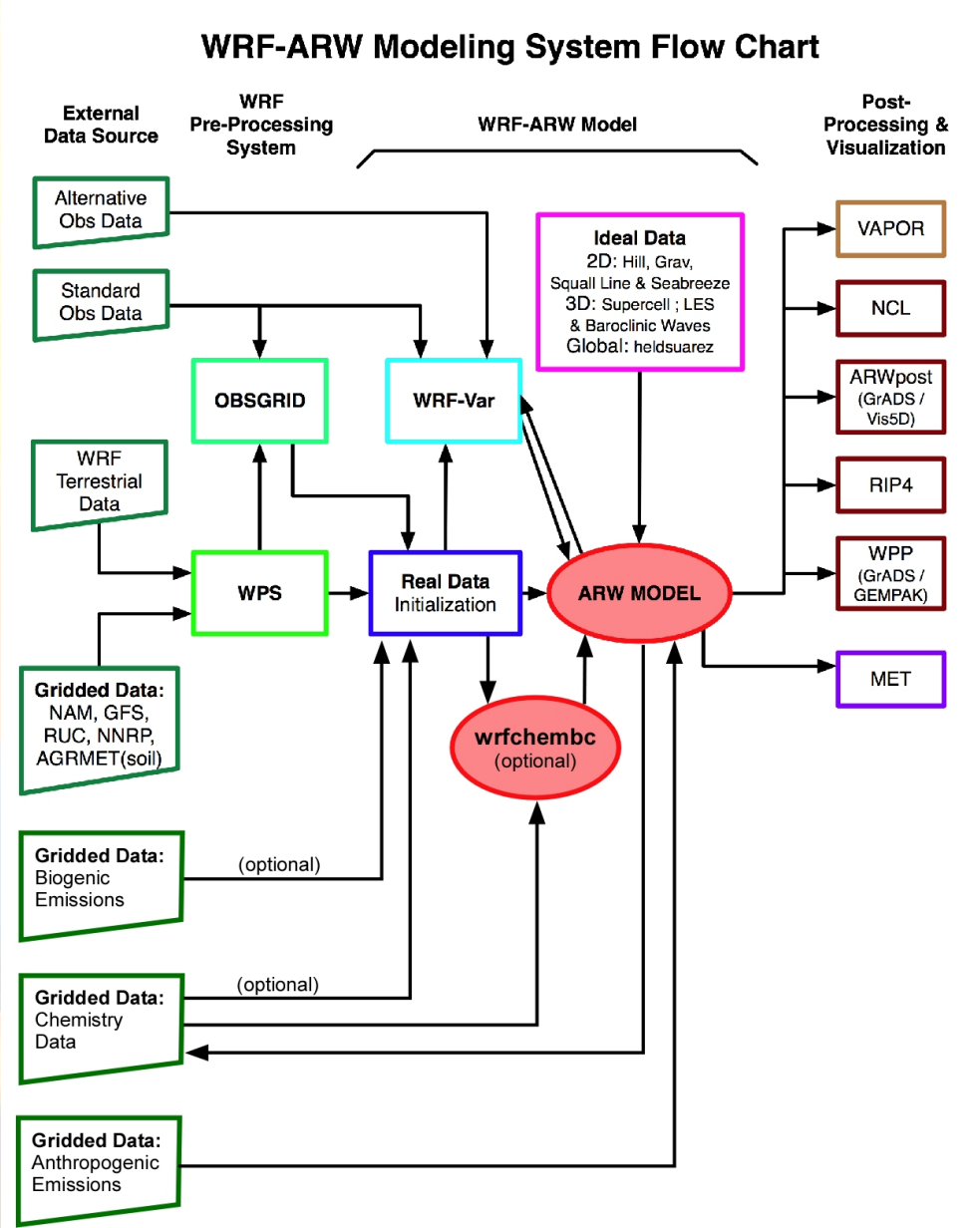
- Option 2 (dust_opt = 1):
  - Need to include surface erosion data in WPS
  - Use new GEOGRID table for running geogrid.exe
  - Dust data included in wrfinput file

- Work tutorial exercise 3 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
- 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 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
WRF Terrestrial Data
Gridded Data: NAM, GFS, RUC, NNRP, AGRMET(soil)
Gridded Data: Biogenic Emissions
Gridded Data: Chemistry Data
Gridded Data: Anthropogenic Emissions
OBSGRID
WRF-Var
WPS
Real Data Initialization
ARW MODEL
wrfchembc (optional)
Ideal Data
2D: Hill, Grav, Squall Line & Seabreeze
3D: Supercell ; LES & Baroclinic Waves
Global: heldsuarez
(optional)
(optional)
VAPOR
NCL
ARWpost (GrADS / Vis5D)
RIP4
WPP (GrADS / GEMPAK)
MET

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)

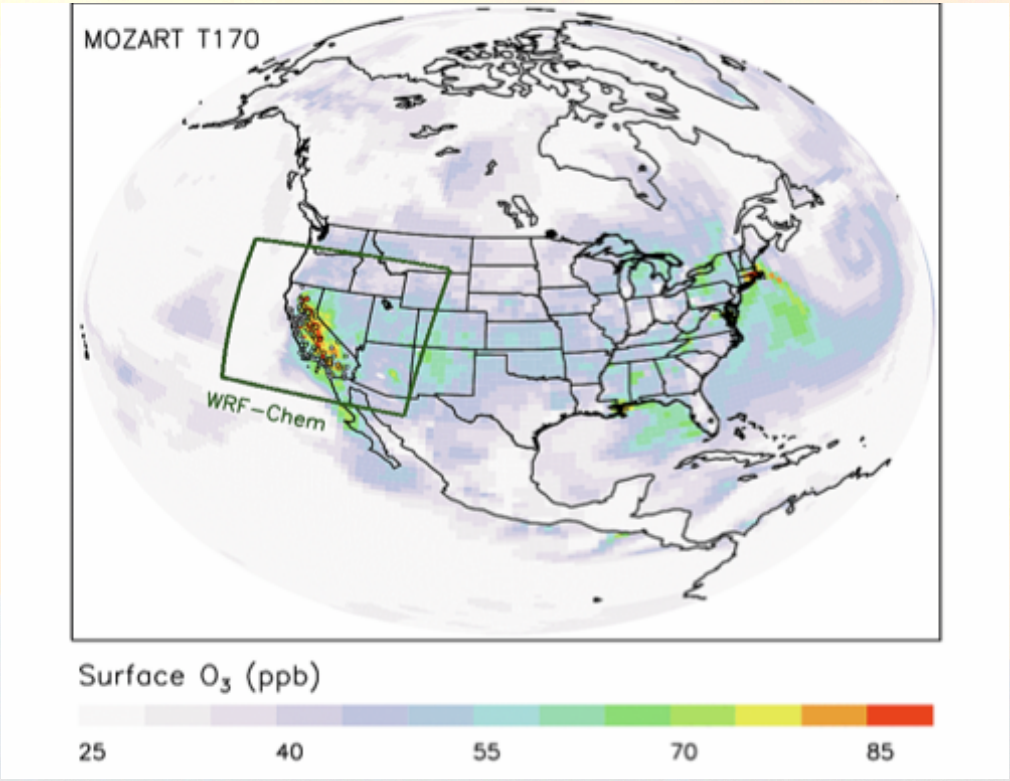
MOZBC : http://www.acd.ucar.edu/wrf-chem/download.shtml

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.

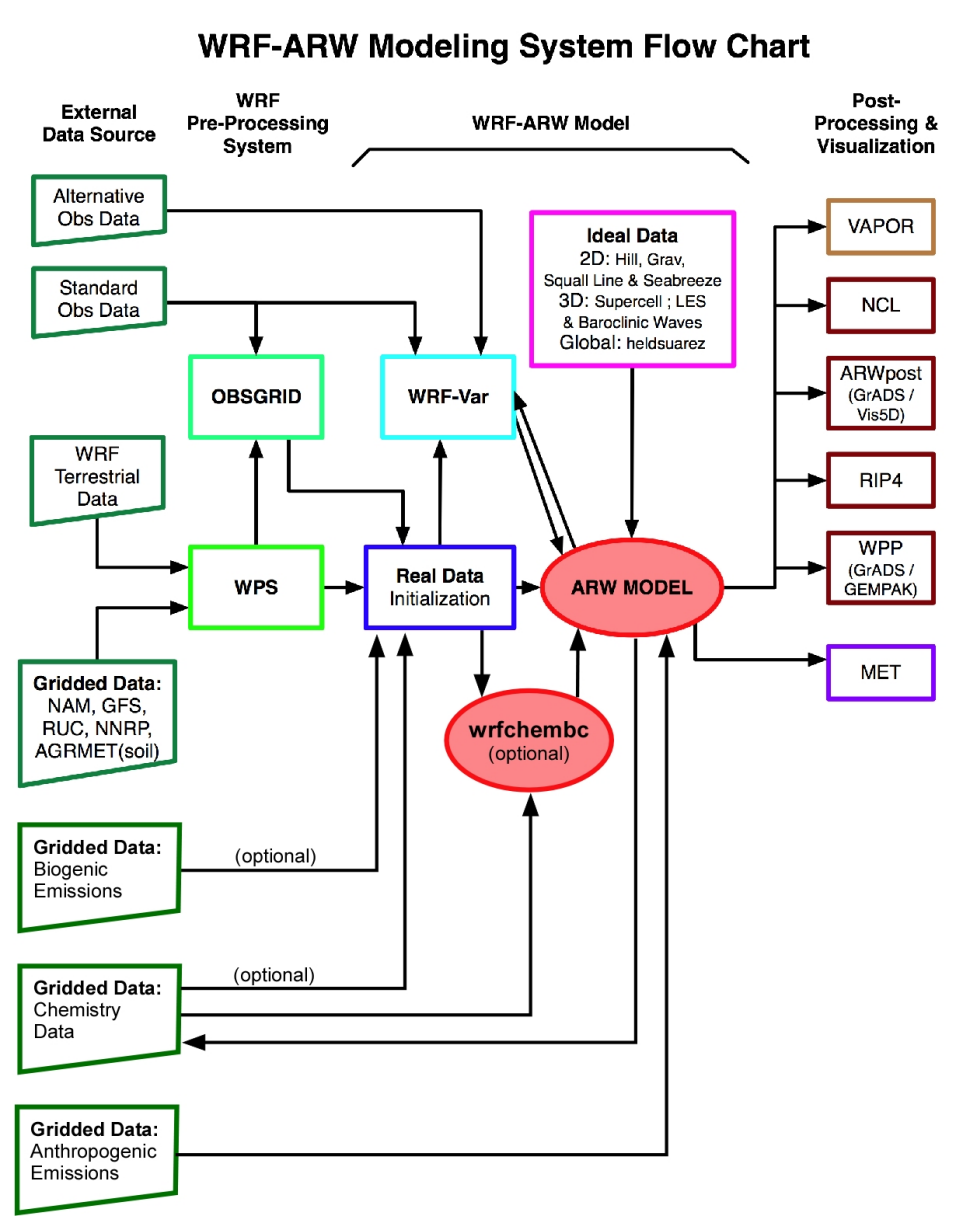


- To enable chemical IC and BC when running WRF-Chem set in namelist.input:
  have_bcs_chem = .true.

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 Simulation



WRF/Chem Namelist

- **Time control namelist options**

- A few of the Chemistry 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]jf    ebu_in      -       -     -     -              "Biomass burnung input "       ””””
state    real  ebu_in_no    i]jf    ebu_in      1       -     i{7}  "ebu_in_no"      "EMISSIONS"         "mol km^-2 hr^-1”
state    real  ebu_in_co    i]jf    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)

WRF/Chem Namelist

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

```
&time_control
…
auxinput6_inname          = ‘wrfbiochemi_d<domain>,
auxinput7_inname          = ‘wrffirechemi_d<domain>,
auxinput8_inname          = ‘wrfchemi_gocart_bg_d<domain>,
auxinput5_interval_m      = 60,
auxinput7_interval_m      = 1440,
auxinput8_interval_m      = 1440,
io_form_auxinput2         = 2,
io_form_auxinput5         = 2,
io_form_auxinput6         = 2,
io_form_auxinput7         = 2,
io_form_auxinput8         = 2,
io_form_auxinput12        = 0,
```

WRF/Chem Namelist

- Time control namelist options

- **A few of the Chemistry namelist options**
  - More details provided in Chapter 4 of User's Guide

WRF/Chem Namelist

- Chemistry control namelist

Chem_opt	Description
0	No chemistry
1 - 40	RADM2, CBMZ chemical mechanism options
101 - 200	Options covering RADM2, CBMZ, MOZART, SAPRC99, NMHC9 chemical mechanisms using KPP.
300 – 301	GOCART aerosol options
400 – 401	Dust options (volcanic and surface lofted)

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

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)
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.

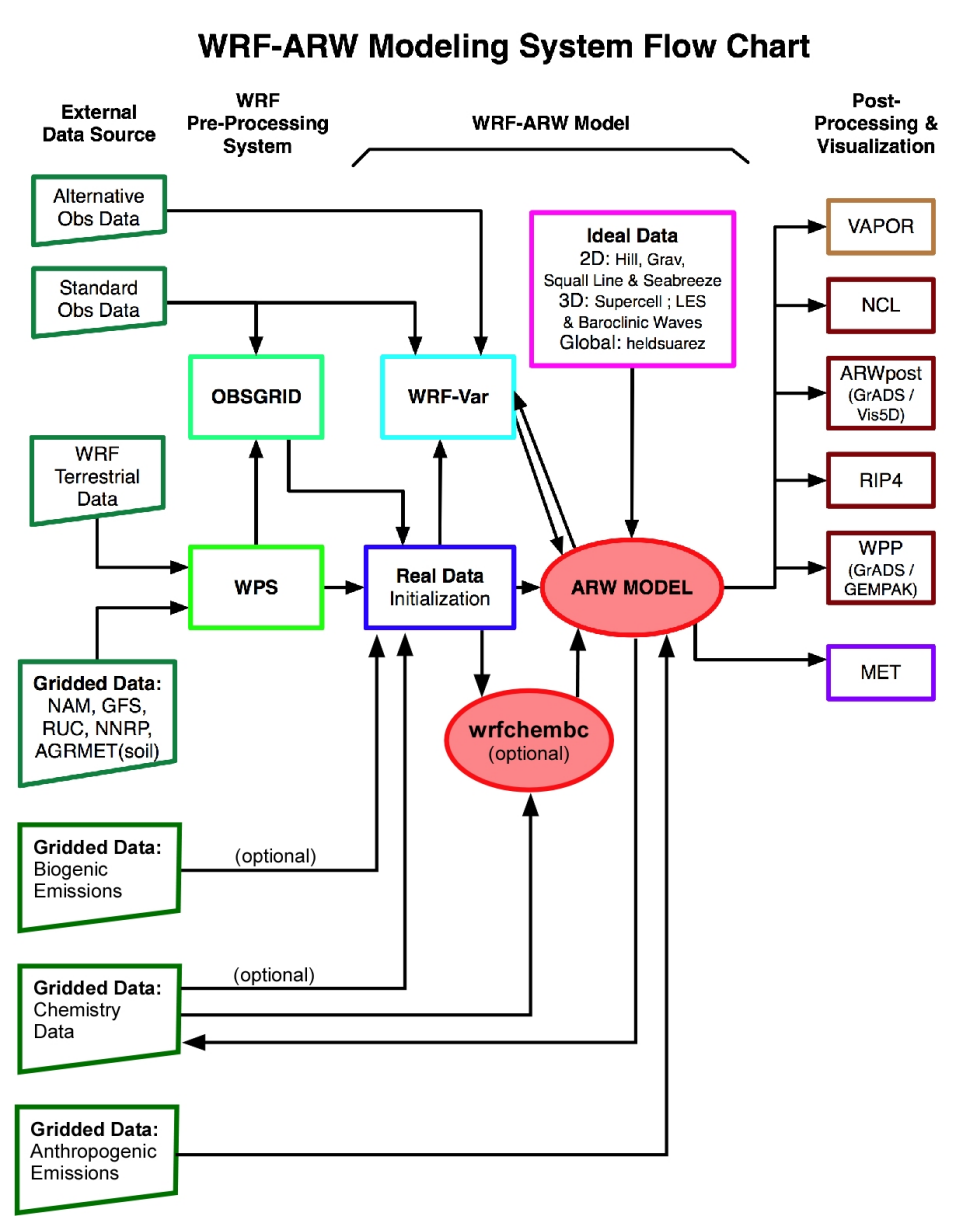
WRF/Chem Namelist

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
-10	

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)
  - Default initial state for N. America summer (chem_in_opt = 0)
- Use forecast for initial chemical fields
  - Works well as lower tropospheric air quality mostly depends on emissions
  - real.exe reads in forecast data through auxinput12 (chem_in_opt = 1)

Running WRF/Chem



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
  - Set auxinput12 namelist options

```
ln –s $outdir/wrfout_d01_2007-06-15-12:00:00 wrf_chem_input_d01
```

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

Running WRF/Chem

Step 1: run case without chemistry

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

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

  The tutorial code is pre-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

Step 2: Get emissions for your domain

- Set hourly wind profile for plume rise calculation (wind speed and elevation)
- Set vertical levels for your domain (elevation array - zfa)
- 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
```

Running WRF/Chem

Step 2: Get emissions for your domain (cont.)

- Keep the wrfinput file for your meteorology only run
- Set namelist options
  - Auxiliary input stream 5 for anthropogenic emissions
    - auxinput5_interval = 60
    - io_form_auxinput5 = 2
    - chem_opt = 2
    - emiss_opt=3
- Run convert_emiss.exe
  - Normally produces wrfem_00to12Z and wrfem_12to24Z binary data files.
  - Tutorial example will produce only 1 file (wrfem_12to24Z)

Running WRF/Chem

- Edit the namelist.input file to your test_em_real directory
  - Watch auxinput5_interval, io_form_auxinput5, chem_opt
- run convert_emiss.exe and verify that your emissions file name
  - wrfchemi_12z_d01
- Edit namelist.input file in WRFV3/test/em_real to set chem_opt, etc.
- run wrf.exe and verify results.

Running WRF/Chem

- Step 3: Run real.exe to include chemistry
- If including fixed surface emissions (biogenic, fire, GOCART background, etc.):
  - Set namelist options to include additional inputs
    - Auxinput6 – biogenic emissions
    - Auxinput7 – biomass burning emissions
    - Auxinput8 – GOCART background fields
    - Auxinput12 – Include previous run's chemistry fields
- Run real.exe
  - Get wrfinput_d01 and wrfbdy files with chemistry fields
  - Should get messages showing chemistry is in run.

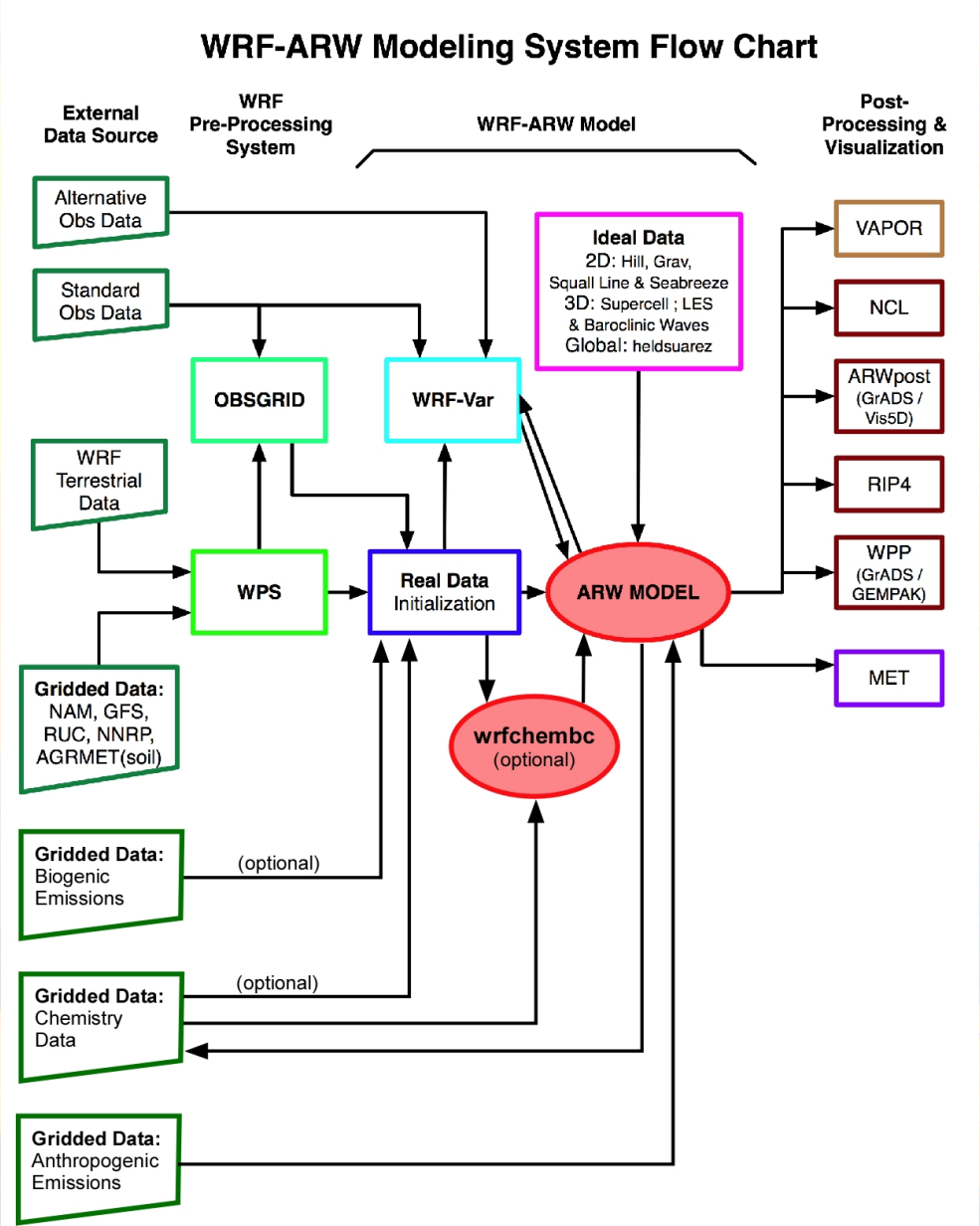
Running WRF/Chem

- Step 4: Run wrf.exe to produce wrfout data files
  - Set namelist options to include additional inputs
    - Auxinput5 – anthropogenic emissions
  - Turn off namelist options that are excluded
    - Auxinput7 – biomass burning emissions
    - Auxinput8 – GOCART background fields
    - Auxinput12 – Include previous run's chemistry fields
  - Should get messages regarding the reading of
    - Anthropogenic emissions
    - If you do not get these messages, an error is likely

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, io_form_auxinput5? 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 Exercises

- Now you do it! Several exercises are located on the WRF/ Chem web page (linked to on tutorial web page).

  First exercises: Building and using anthropogenic emissions

- 1 – NEI emissions
  - USA only, but need to understand methodology)

- 2 – Global emissions
  - Includes building GOCART, biomass burning emissions
  - Most likely choice for domains outside USA

WRF/Chem Exercises

- 3 – Dust only simulation
  - Use global dust erosion data set
  - May2010 dust transport event
- 4 – Full interactive physics
  - understand namelist choices
- 5 – Edit registry.chem and add a new output variable
- Use quick start guide (Appendix A) and User's Guide (and ask for help)