WRF-Chem V3.4: 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 has made more than one weather simulation using WRFV3
  - know FORTRAN and C and can edit code, recompile, etc.

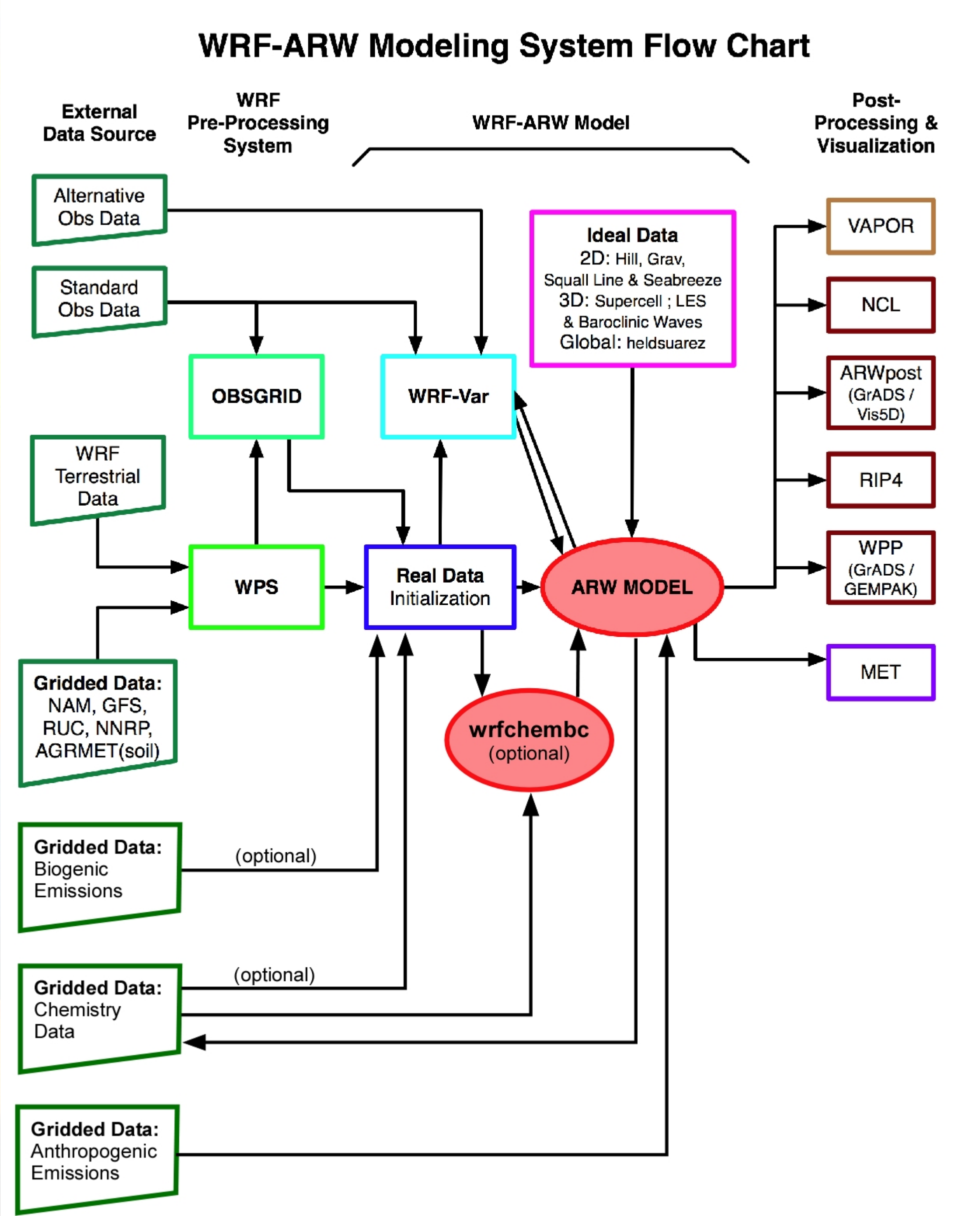
- The chemistry code is available from WRF web page.
  - Questions: Send email to WRF-Chem help (wrfchemhelp.gsd@noaa.gov)
  - Web page: www.wrf-model.org/WG11

- Test data is available as well (tutorial exercises)
  - Small domain (41x41x31 grid points, 100 km horiz. spacing)

WRF-Chem

- Compile WRF-Chem code (already done for tutorial)
  - Set environmental variables
    - Define which model core to build (use ARW only).
      - 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
      - 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 on ftp site:
  - RETRO (.5 degree, monthly) and EDGAR (10 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

- 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

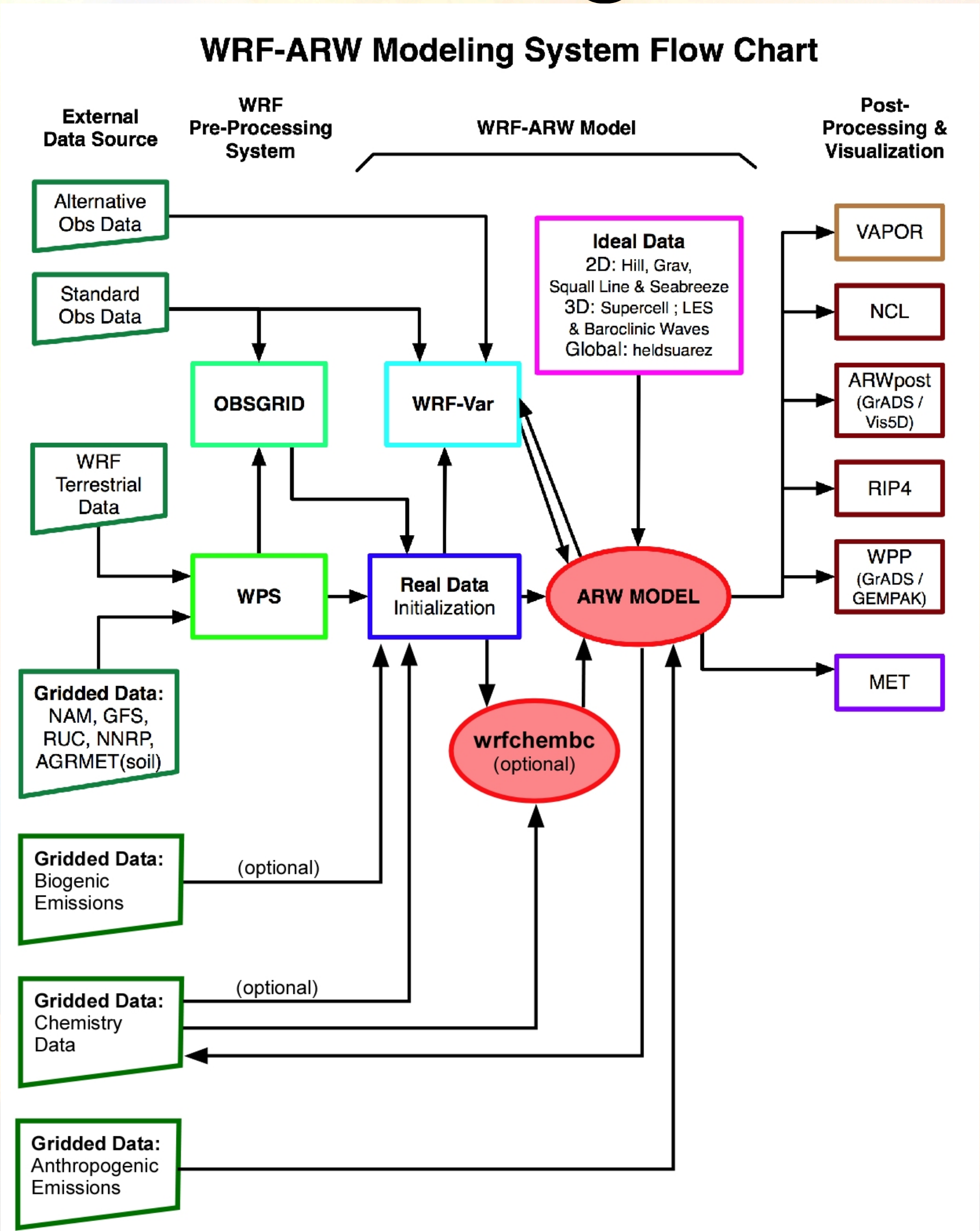
- convert_emiss is very simple. Uses just a few namelist settings.
  - emiss_opt=3 – NEI emissions for U.S.A.
  - emiss_opt=5 – RETRO/EDGAR global emission

- 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-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): (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?)

WRF-Chem 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,

WRF-Chem
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

WRF-Chem 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

WRF-Chem
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

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

- 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

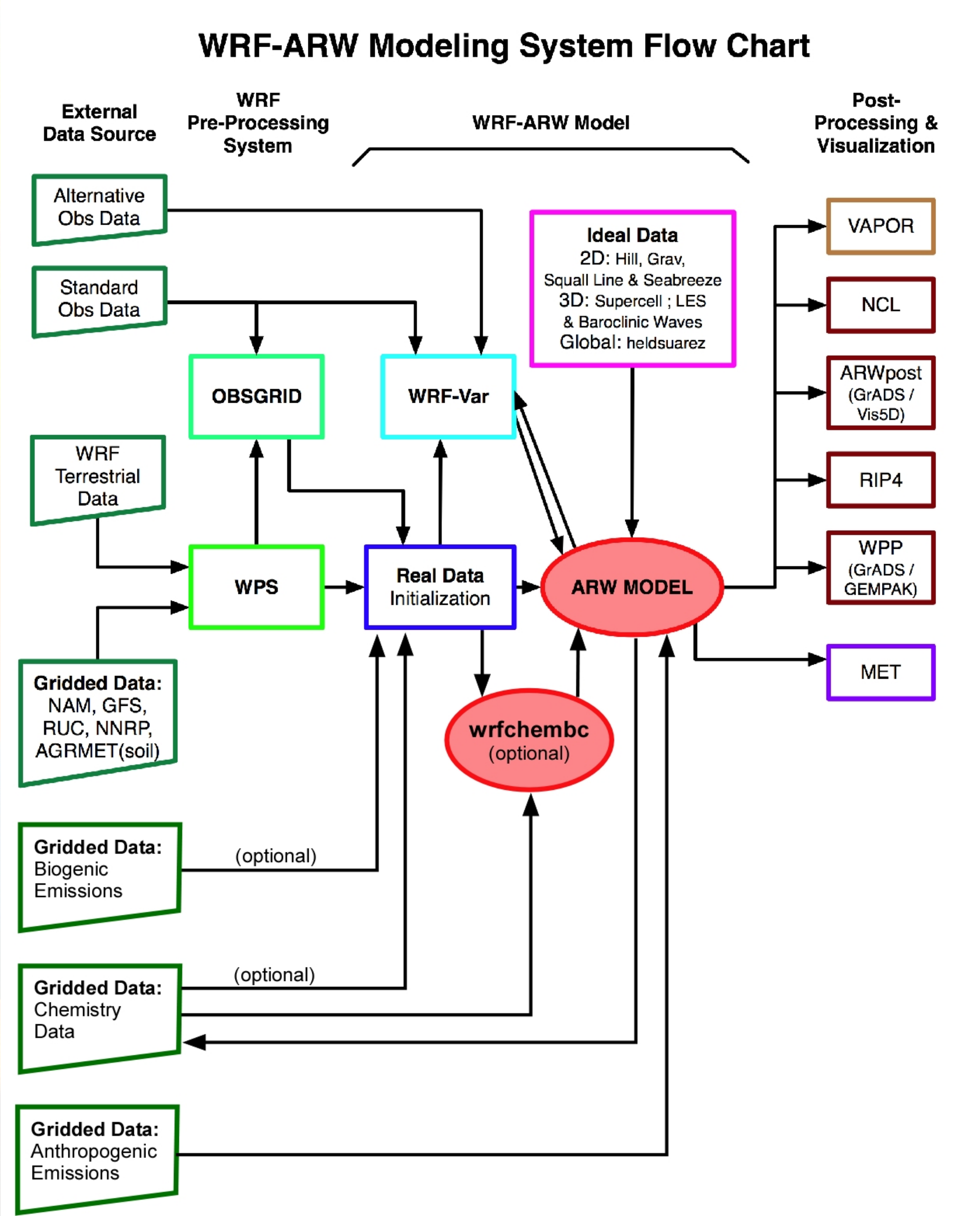
- Includes DMS as well as GOCART
  - From running prep_chem_sources with GOCART included
  - Planned to be moved to WPS one of these days

- 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 Initial Conditions



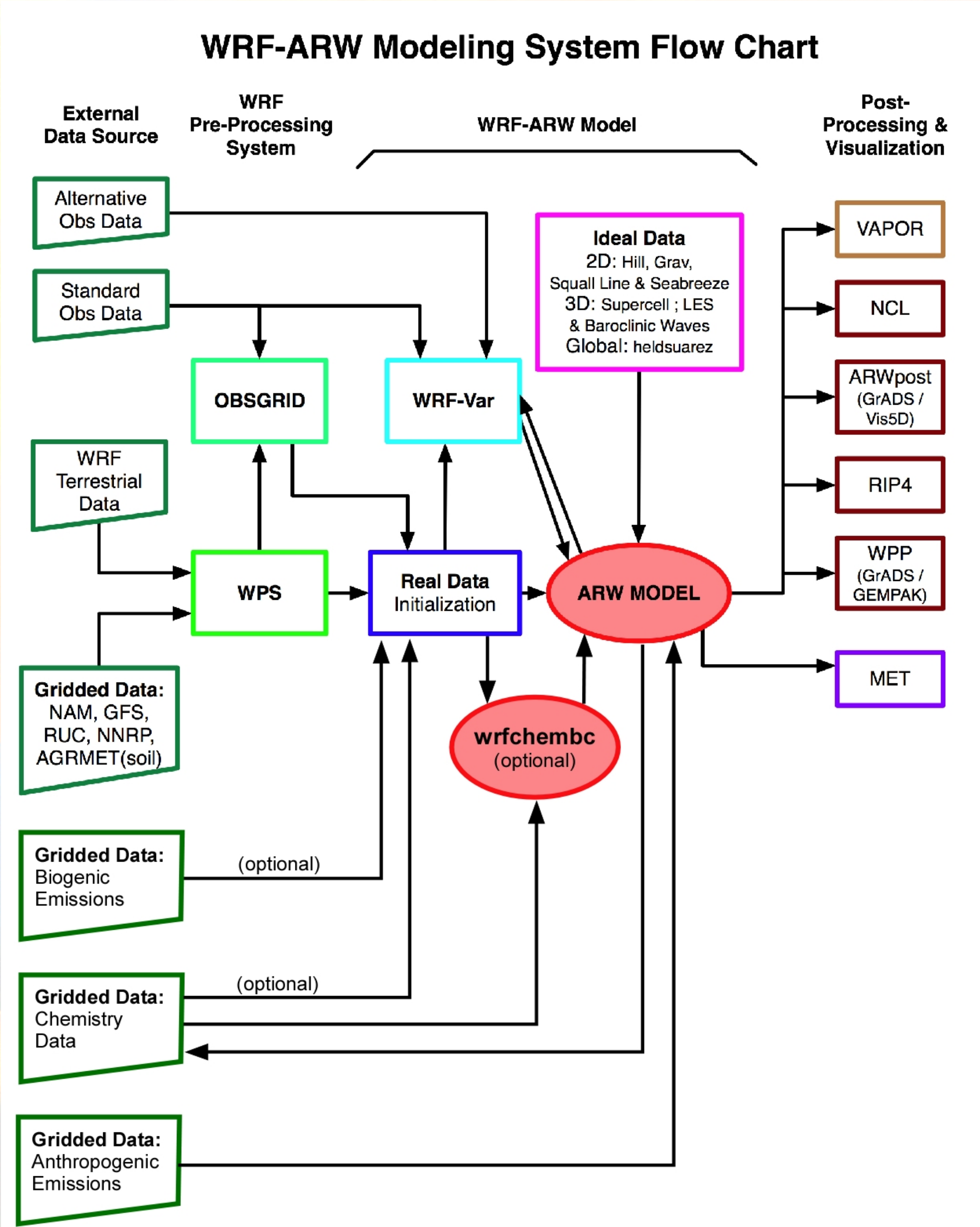
WRF-Chem Chemical I.C.s

- WPS gives meteorology I.C.s
- Problem: Need 3-D state of atmospheric chemistry for model initialization
  - Every 12 hours balloons used to measure state of atmosphere
    - Instruments rarely measure chemistry
      - Temperature, relative humidity, wind speed and direction
      - Occasionally measure ozone
  - No other consistent measurements of chemistry
  - Satellites measure AOD
    - Vertical integral
    - Distinguish between type (carbon, sulfate, etc.) aerosols?
- Solution: WRF-Chem model provides chemical I.C.s

WRF-Chem Chemical I.C.s

- Option 1 – Idealized profile
  - Every grid point gets same chemical profile
  - Assumes August in North America for I.C.
  - Set chem_in_opt = 0 in namelist, run real.exe
- Option 2 – WRF/Chem Forecast
  - Use previous forecast for chemistry I.C.
  - Set chem_in_opt = 1 in namelist, run real.exe
- Option 3 – Use other model data for I.C.
  - User needs to modify the wrfinput file after running real.exe
  - No chem_in_opt setting necessary (chem_in_opt=0 default)

WRF-Chem Boundary Conditions



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)

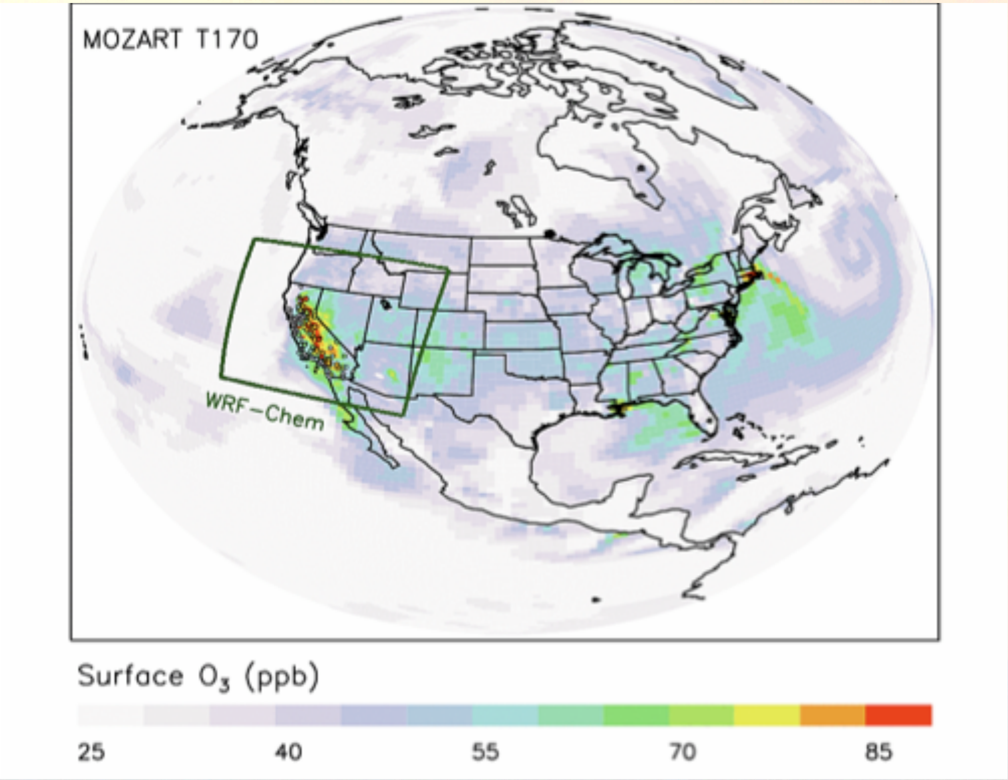
MOZBC : http://www.acd.ucar.edu/wrf-chem/download.shtml

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.



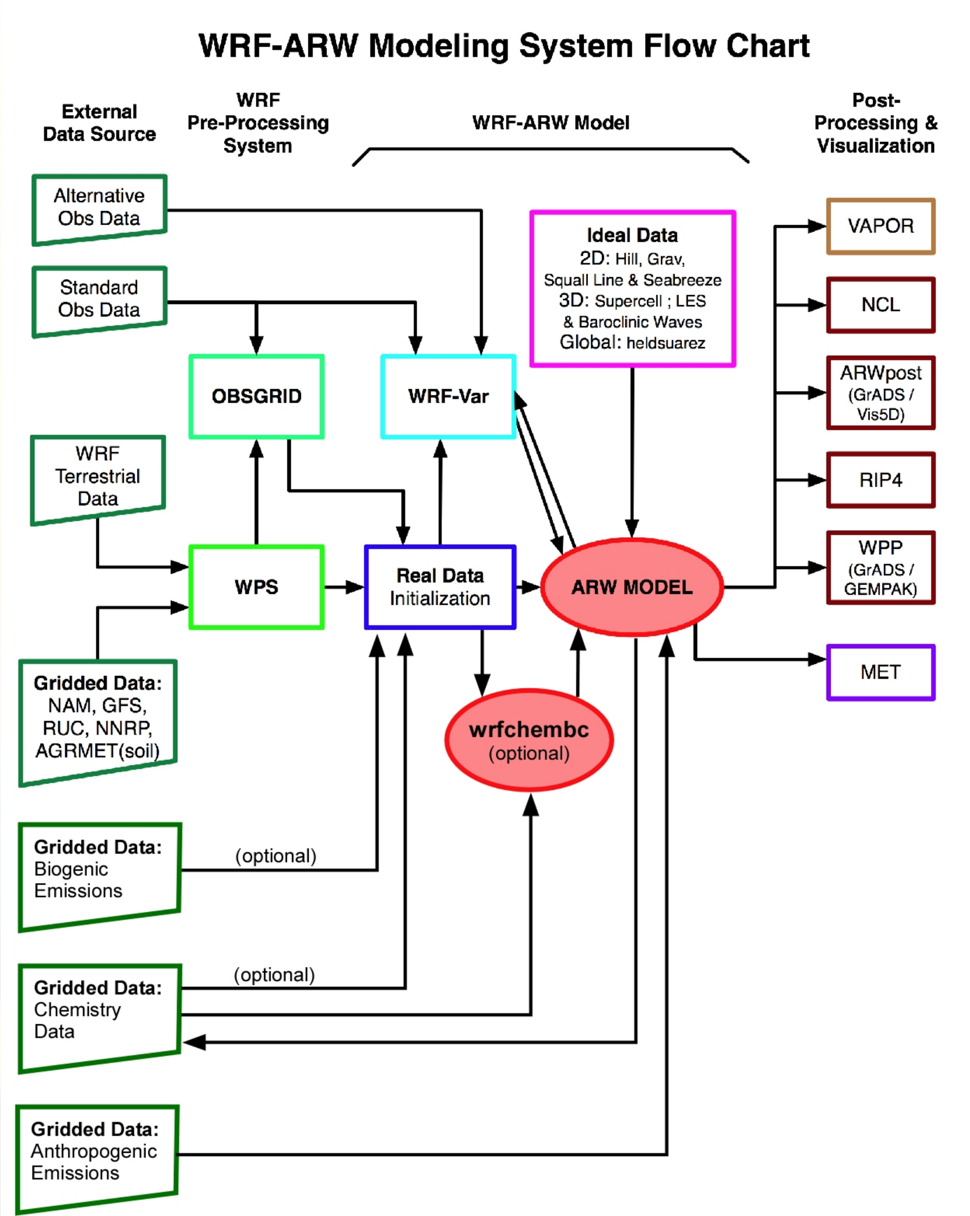
- To enable chemical IC and BC when running WRF-Chem set in namelist.input:
  have_bcs_chem = .true.

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-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)
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)

WRF-Chem Namelist

emiss_opt	Description
0	no anthropogenic emissions
2	RADM2 anthropogenic emissions
3	RAM2/MADE/SORGAM anthropogenic emissions
4	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_hcho,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_hcho,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

WRF-Chem Namelist

- chem_in_opt = 0
  - No chemical initial analysis derived from observations
  - Default initial state for N. America summer
- chem_in_opt=1
  - Use forecast for initial chemical fields
  - Good choice for real time forecast runs
  - Works well as lower tropospheric air quality mostly depends on emissions
  - real.exe reads in forecast data through auxinput12

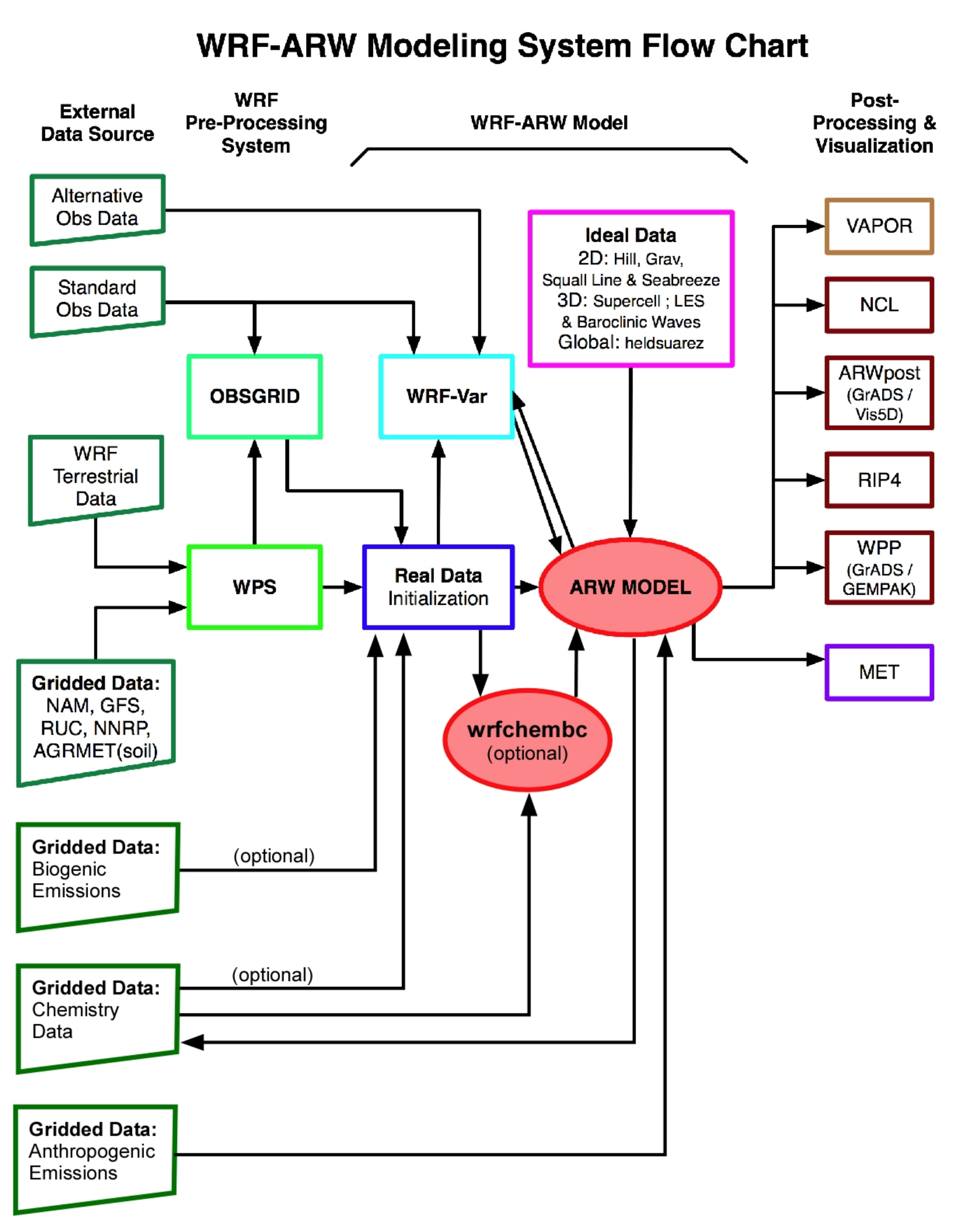
WRF-Chem Namelist

- chem_in_opt=1: additional 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

    - Real.exe gives a message indicates that model is being initialized with previous forecast
  - Do tutorial exercise 5 to better understand methodology

WRF-Chem Simulation



Running WRF-Chem

Option 1: Run without chemistry

- Get copy of WRF code in your home directory, compile (w/o chem)
- Get WPS into your home directory, compile
- Get initialization data (e.g., global model data)
- Build ”met_em” input data files using WPS
- Set options in namelist.input
- Run real.exe
- Run wrf.exe
- Check results

Running WRF-Chem

Option 2: Run with dust only (tutorial exercise 1)

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

  cp -R /wrfhelp/SOURCE_CODE/WRF-CHEM/WRFV3   WRFV3

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

- Set WPS links to include dust
  - link GEOGRID.TBL.ARW_CHEM to GEOGRID.TBL
  - Should have EROD data

- Build ”met_em” input data files (include dust (EROD) fields)

- Set options in namelist.input

- Run real.exe with the dust only chemistry option turned on.
  (Save the wrfinput_d01 data file for use later on.)

- Run wrf.exe and check results

Running WRF-Chem

Option 3: Run with chemistry/aerosols (exercises 2 & 3)

- Start with WPS output and wrfinput file from option 2 then…
- Compile the prep_chem_sources program
- Set namelist input options (directories, on/off switches)
- Run the prep_chem_sources program
- Link output files to your meteorology run directory
- Retrieve the wrfinput file from your meteorology or dust only run

Running WRF-Chem

Option 3: Run with chemistry/aerosols (cont.)

- Set namelist options
  - Auxiliary input stream 5 for anthropogenic emissions
    - auxinput5_interval = 60
    - io_form_auxinput5 = 2
    - chem_opt = 301
    - emiss_opt=5
    - kemit=1
    - dust_opt=1
    - biomass_burn_opt=1
- Run convert_emiss.exe
  - Produces wrfchemi_d01, wrfchemi_gocart_backg_d01, wrffirechemi_d01 input data files.
  - No volcanic ash emissions as chem_opt and emiss_opt_vol not set.
- Copy emissions files to WRFV3/test/em_real run directory

Running WRF-Chem

Option 3: Run with chemistry/aerosols (cont.)

- 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
- After running real.exe
  - Have wrfinput_d01 and wrfbdy files with chemistry fields
  - Should get messages showing chemistry is in run.
  - Verify data

Running WRF-Chem

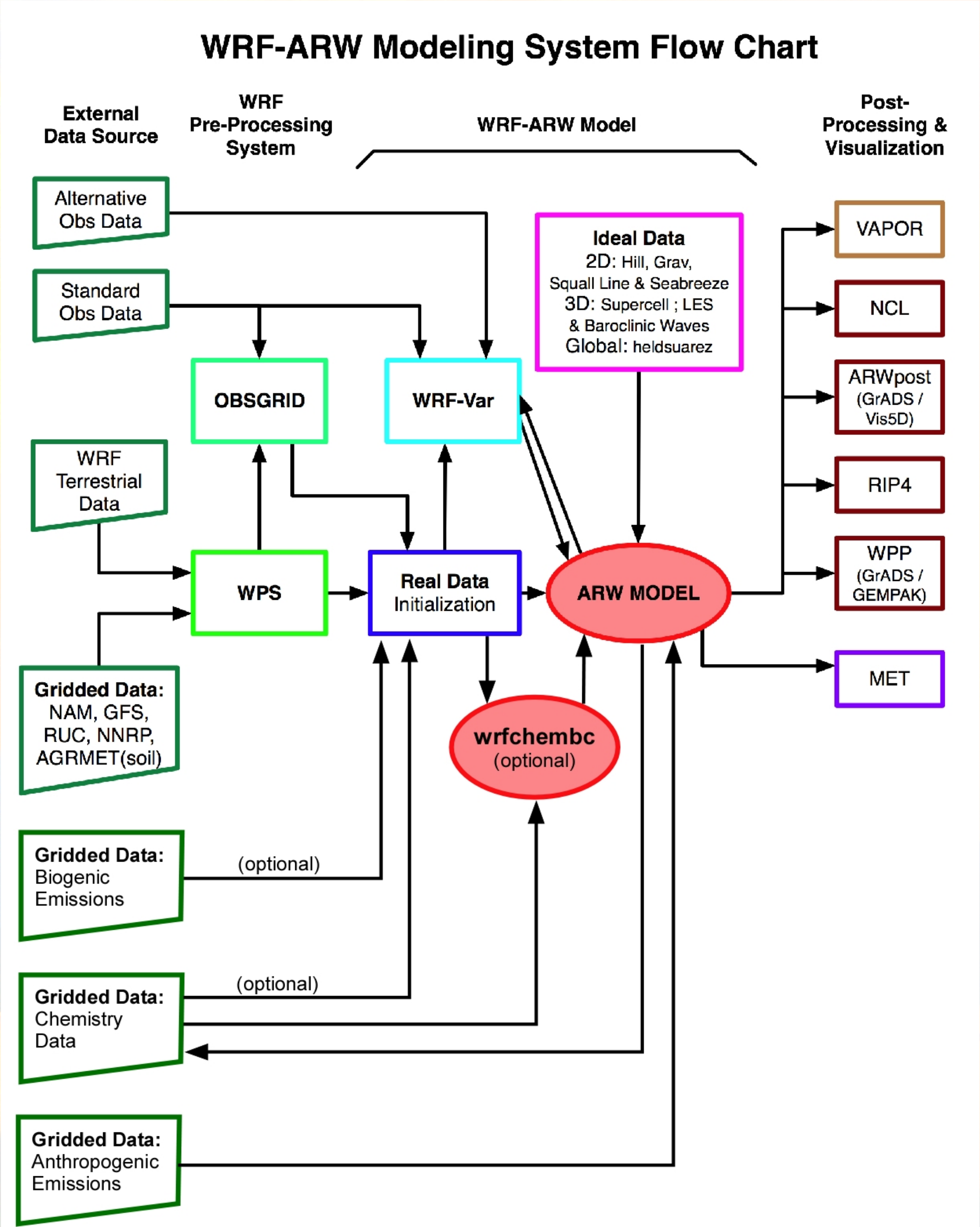
Option 3: Run with chemistry/aerosols (cont.)

- Run wrf.exe to produce wrfout data files
  - Set namelist options to include additional inputs
    - Auxinput5 – anthropogenic emissions
  - Turn off namelist options that are included in wrfinput file
    - 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

- And still other options (tracer, volcano, etc.)
- For any of the run time options
  - 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 correct so you have data?
        - » Max<some array> = 1.e-16 is not data. It is noise.
  - 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 on tutorial web page).

  Exercises start simple and build on complexity in each subsequent exercises (add in anthropogenic emissions, biogenic emissions, etc.) so do each one in order.

- 1 – Dust only simulation
  – Use global dust erosion data set
  – July 2010 dust transport event
  – Mediterranean basin domain location

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

WRF-Chem Exercises

- 3 – RADM2 chemistry with MEGAN
  biogenic emissions

- 4 – Full interactive physics
  - Understand namelist.input choices as domain too coarse to get significant impact

- 5 – Cycle (recycle?) chemistry
  - Understand methodology
    to obtain “best” chemical initial conditions

WRF-Chem Exercises

- 6 – Volcanic emissions

- 7 – Using NEI emissions over United States
  - Methodology applies to using other emissions data
- Use the User's Guide (and ask for help) during practice
- Work tutorial problems
  - No time/resources to conduct your own research project
  - 99% of time question can be answered just by tutorial exercises

WRF-Chem Exercises

- Start now!
  - Work at your own pace
  - During practice remember to use
    - Notes, lecture information
    - Tutorial exercise page
    - User's Guide
    - And ask for help if you get stuck
  - Work tutorial problems only
    - No time to conduct your own research project
    - Most questions will be answered by doing the tutorial exercises