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

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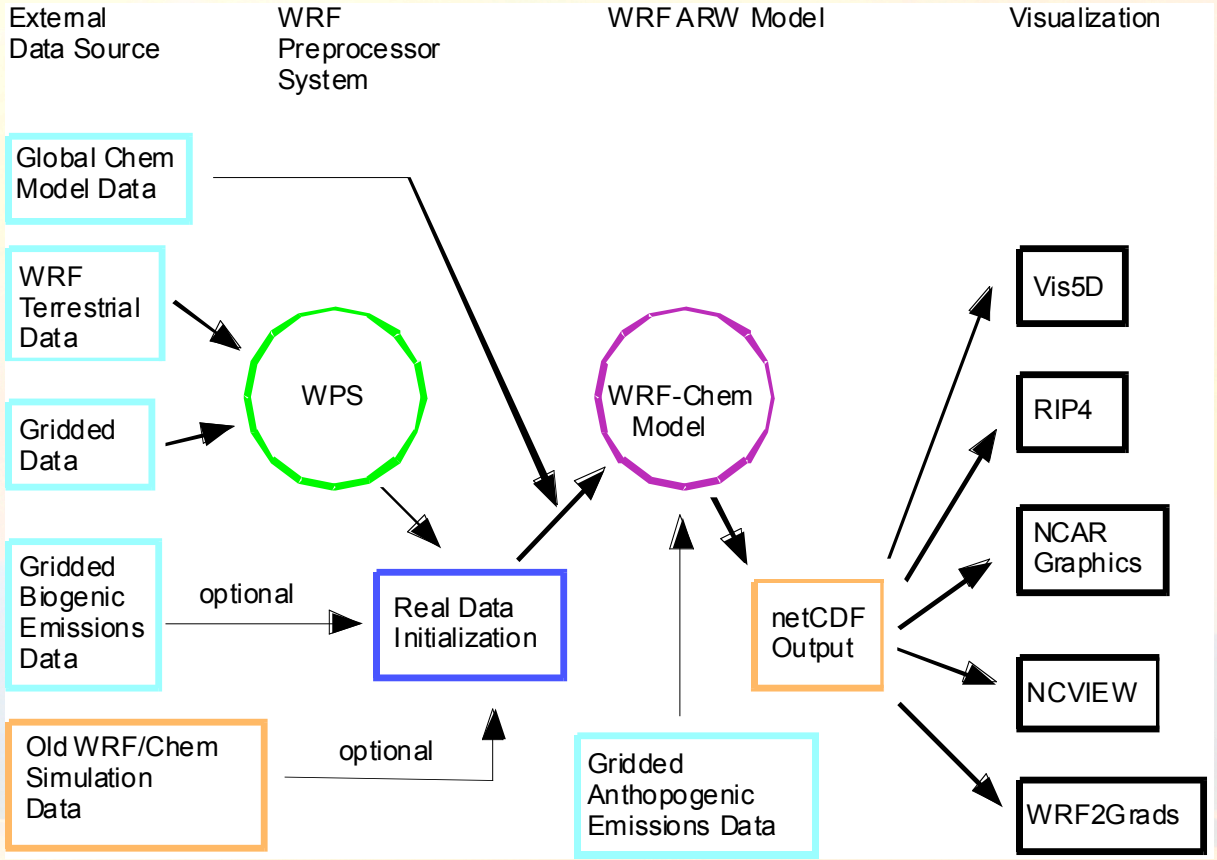
WRF/Chem Model System



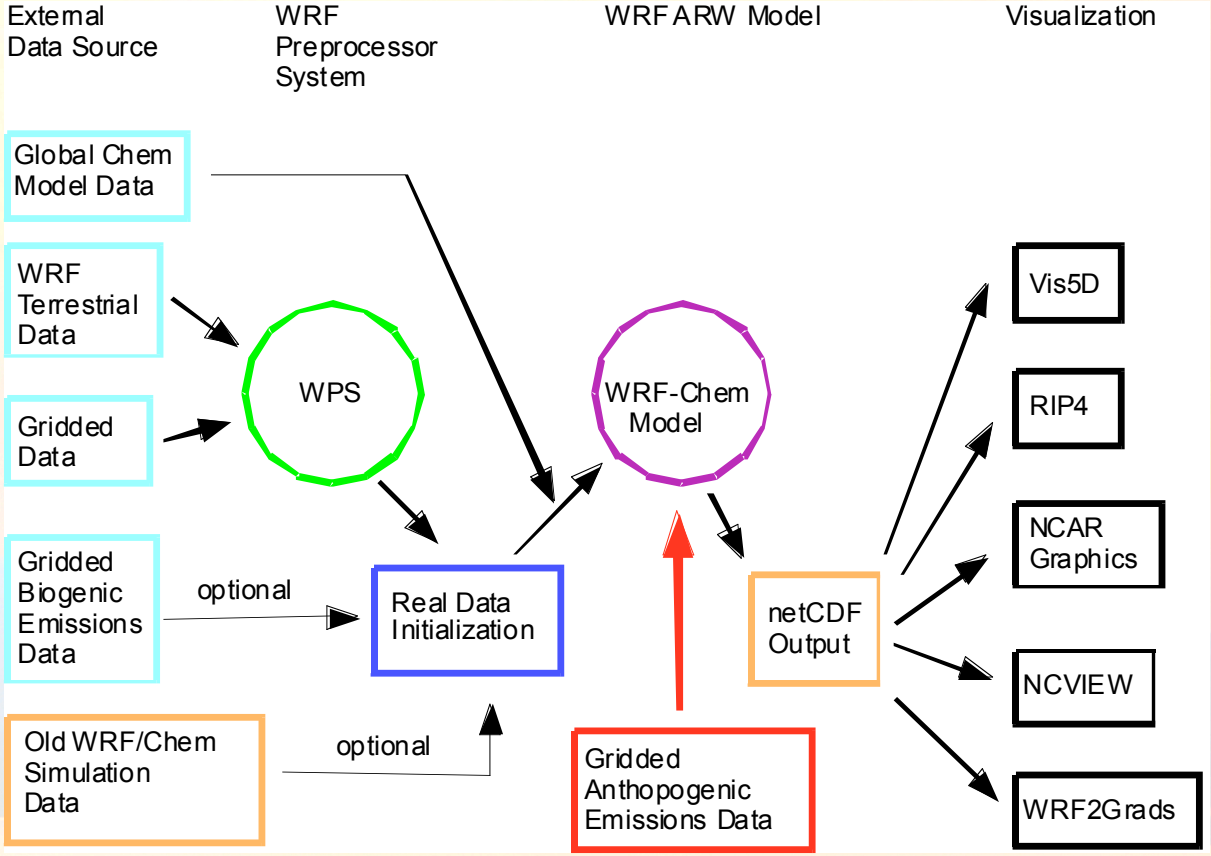
WRF/Chem

- It is assumed that the user of WRF/Chem :
  - is ***very familiar*** with the WRF model system
  - have run WPS/WRF-SI
  - and has made more than one weather simulation using WRFV2
- The chemistry code is not available with WRF V2.2.
  - Code is available upon request from wrfchemhelp
    - Send email to WRF/Chem help (wrfchemhelp.gsd@noaa.gov)
    - www.wrf-model.org/WG11
  - Chemistry & full tutorials to be available with WRFV3.0
- Test data is available as well
  - Small domain (40x40x35 grid points, 60 km horiz. spacing)
  - Run with single processor (compile option 1)
  - Need to have WRF/Chem compiled “single processor” for emissions conversion (don’t remove executables!)

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

- Emissions data methodology
  - Start with "raw" emissions data (could be your own data)
    - Provided 4-km emissions data set (area and point source)
  - Specify the speciation for the desired chemical mechanism
    - Provided routines assume RADM2
  - Prepared the 3-D (or 2-D) anthropogenic emissions data set
    - Map data onto your WRF-Chem simulation domain
    - Account for stack plume rise
    - Output data in proper format
      - User can change format to match their needs
    - We have made a program available, but user can develop other routines
  - Convert the emissions data to a WRF netCDF data file
    - Match emissions names in model
    - Format matches the format specified in conversion routine
    - Map data (in wrfinput_d01 header) needed for some plotting routines to function properly

WRF/Chem Emissions

- For the U.S. – A tool is already built. (Stu McKeen, ESRL/CSD)

- Gridded anthropogenic emissions data is available for the US.
  - Considered as “interim' inventory” until updates to WRF and emissions inventory are made available.
  - Based upon the U.S. EPA's 1999 National Emissions Inventory version 3
    - Gridded 4 km data
  - Canada area and mobile source emissions for south of ~52 deg. N
  - Mexico emissions from the BRAVO study (north of ~24 deg N latitude).
  - Representative of a typical summer day (average of weekday and weekend days)
  - No biogenic sources of VOC, NOx, nor fire-related emissions

WRF/Chem Emissions

- (gridded U.S. emissions, cont.)

- Designed for regional scale photochemical models of North America
  - 24 average hourly emissions for NOx, VOC, CO, SO2, NH3, PM2.5 & PM10
  - 41 speciated VOC compounds, 5 PM2.5 aerosol species, 7 primary species

- The intent of this inventory:
  - Use as a reference for air quality model development and research
  - Provide the necessary information in a convenient format
  - Continental scale coverage so that regional to global scale run can use data
  - Sufficient detail so to work with several lumped photochemical mechanisms.
  - Not a substitute for more detailed emissions processing
    - (e.g. the Sparse Matrix Operational Kernel Emissions (SMOKE) model)

http://ruc.fsl.noaa.gov/wrf/WG11/anthropogneic.htm

WRF/Chem Emissions

- (gridded U.S. emissions, cont.)

"sample_anthropogenic_emissions_input_code.F"

nradm	-> number of emission arrays
ename	-> name of the emission arrays (character) ***
ihour	-> integer specifying emissions hour
e_so2	-> 3D emissions for so2
…	
…	
e_pm10	-> 3D emissions for coarse particulates (PM10)
ihour	-> integer specifying emissions hour
e_so2	-> 3D emissions for so2
…	
…	
e_pm10	-> 3D emissions for coarse particulates (PM10)
…	

*** e_[name] are the names of the species used in the WRF-Chem chemical mechanism. You may need to introduce/remove more species for your particular chemical mechanism.

Anthropogenic emissions dimensions are (nx-1, nz-1, ny-1).

The units are mol km^{-2} h^{-1} for the gaseous constituents and μg m^{-3} s^{-1} for the aerosol constituents.

WRF/Chem Emissions

- If not using the available emissions data – you need to construct your own emissions!
- Need to know how to group the chemical compounds and by what factor.
- Need to know which chemistry option is to be used in WRF/Chem
- See **emiss_v01.F** for full table (code is available w/ emissions data).

```
!  Conversion table.  Table lists the field, the emissions name, the weight factor
to apply, the molecular weight (not used) and the emissions name  - some with
units.  The fields are basically SAPRC emissions that are being converted to
RADM2 emissions input.
!
! CO       e_co              1.00        28       1
! NOX      e_no              1.00        46       1
! SO2      e_so2             1.00        64       1
! NH3      e_nh3             1.00        17       1
! HC02     e_eth             1.00        00       Ethane  kOH<500 /ppm/min
! HC03     e_hc3             1.00        00       Alkane 500<kOH<2500
exclude(C3H8, C2H2,
                                                        organic acids)
! HC04     e_hc3             1.11        00       Alkane 2500<kOH<5000
exlude(butanes)
! HC05     e_hc5             0.97        00       Alkane 5000<kOH<10000
exlude(pentanes)
! HC06     e_hc8             1.00        00       Alkane kOH>10000
! HC07     e_ol2             1.00        00       Ethylene
! HC08     e_olt             1.00        00       Alkene kOH <20000 /ppm/min
! HC09     e_oli             1.00        00       Alkene kOH >20000 /ppm/min
! HC10     e_iso             1.00        00       Isoprene
! HC12     e_tol             1.00        00       Aromatic kOH <20000
/ppm/min exclude(benzene
                                                        and toluene)
! HC13     e_xyl             1.00        00       Aromatic kOH >20000
/ppm/min
                                                        exclude(xylenes)
! HC14     e_hcho            1.00        00       Formaldehyde
! HC15     e_ald             1.00        00       Acetaldehyde
! HC16     e_ald             1.00        00       Higher aldehydes
! HC17     e_ald             1.00        00       Benzaldehyde
! HC18     e_ket             0.33        00       Acetone
! HC19     e_ket             1.61        00       Methylethyl ketone
! HC20     e_ket             1.61        00       PRD2 SAPRAC species
(ketone)
! HC21     e_hc3             0.40        00       Methanol
! HC22     e_ald             1.00        00       Glyoxal
! HC23     e_ald             1.00        00       Methylglyoxal
! HC24     e_ald             1.00        00       Biacetyl
```

WRF/Chem Emissions

- Code from chem/module_input_chem_data.F
- May modify the med_read_bin_chem_emiss routine to fit your needs.
- Can change output file name (wrfem12k….d01), number of species, etc.

…

…

```
write(message, '(A,A)') 'call read emissions', intime
call wrf_message( TRIM( message ) )

IF(intime == 0 ) THEN CALL construct_filename1 ( bdyname , '../../run/wrfem12k_00to12z' ,
    grid% id , 2 )
IF (wrf_dm_on_monitor()) THEN
open (91,file=bdyname,form='unformatted')
ENDIf
write(message, '(A,A)') ' OPENED FILE: ',bdyname
call wrf_message( TRIM( message ) )
ENDIF
IF(intime == 12 ) THEN
CALL construct_filename1 ( bdyname , '../../run/wrfem12k_12to24z' , grid% id , 2 )
IF (wrf_dm_on_monitor()) THEN
open (91,file=bdyname,form='unformatted')
ENDIf
write(message, '(A,A)') ' OPENED FILE: ',bdyname
call wrf_message( TRIM( message ) )
```

…

…

WRF/Chem Emissions

- chem/module_input_chem_data.F continued

. . .

. . .

```
ALLOCATE (dumc0(ids:ide-1,kds:config_flags% kemit,jds:jde-1))

write(message, '(7A)') ' I am reading emissions, dims: =',ids, ide-1, jds, jde-1, kds, config_flags% kemit
call wrf_message( TRIM( message ) )
IF(intime == 0 .or. intime == 12) then
read(91)nv
read(91)ename
write(message, '(2A)') ' Number of emissions: ',nv
call wrf_message( TRIM( message ) )
write(message, '(2A)') ' Array names : ',ename
call wrf_message( TRIM( message ) )
ENDIF

read(91)itime
write(message, '(4A)') ' EMISSIONS INPUT FILE TIME PERIOD (GMT): ',itime-1,' TO ',itime
call wrf_message( TRIM( message ) )

read(91)dumc0
grid% e_so2(ids:ide-1,kds:config_flags% kemit,jds:jde-1)=dumc0
read(91)dumc0
grid% e_no(ids:ide-1,kds:config_flags% kemit,jds:jde-1)=dumc0
read(91)dumc0
grid% e_ald(ids:ide-1,kds:config_flags% kemit,jds:jde-1)=dumc0
read(91)dumc0
grid% e_hcho(ids:ide-1,kds:config_flags% kemit,jds:jde-1)=dumc0
read(91)dumc0
grid% e_ora2(ids:ide-1,kds:config_flags% kemit,jds:jde-1)=dumc0
```

WRF/Chem Emissions

- Building the WRF/Chem emissions conversion
  - Compile WRF/Chem for single processor (no multi-tasking)
  - Compile the emissions conversion code

```
%>      setenv  WRF_CHEM 1
%>      ./configure  (option 1)

%>      ./compile em_real
%>      ./compile emi_conv
```

  - Should have convert_emiss.exe in chem directory

WRF/Chem Emissions

Important namelist choices for building emissions:

io_style_emissions = 0 - No emissions files are read
1 - Two 12 hour long emission files are cycled throughout the run
2 - Date/time specific emission files are read

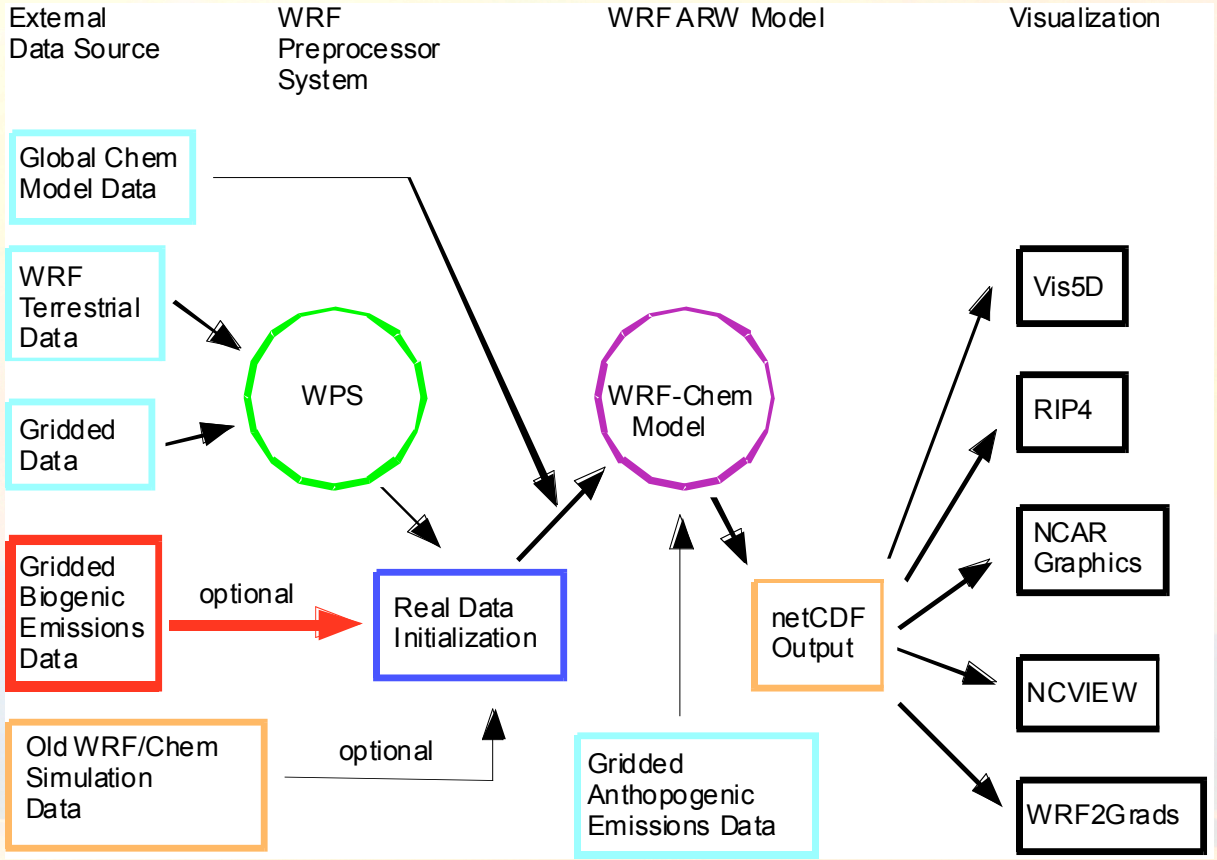
auxinput5_interval_m = 60 - Minutes between reading emissions (used with io_style_emissions=2)

interval_seconds = 3600 - seconds between emission times (important for convert_emiss.exe)

frames_per_emissfile = Number of times in each wrfchemi file
12 for io_style_emissions=1
arbitrary for io_style_emissions=2, we set to 1 for hourly files

kemit = Number of vertical levels in the emissions file.

WRF/Chem Biogenic Emissions



WRF/Chem
Biogenic Emissions

- 3 choices for Biogenic emissions

- Option 1 (bio_emi_opt = 0):
  - Provide biogenic emissions through anthropogenic input.
  - No additional input data files.

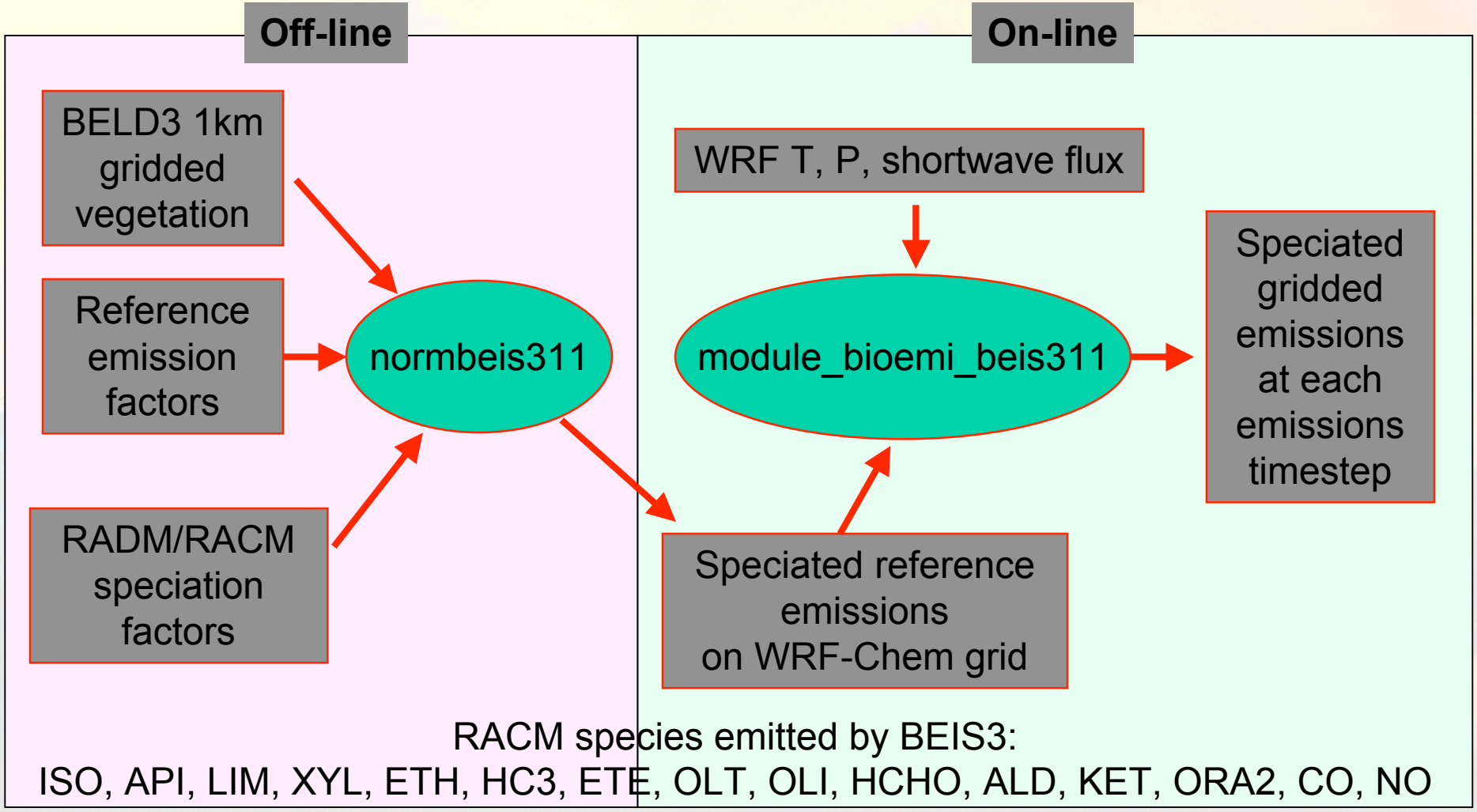
- Option 2 (bio_emi_opt = 1):
  - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
  - No additional input data files.

WRF/Chem
Biogenic Emissions

- Option 3 (bio_emi_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 (wrfbiochemi_d01)
  - Static biogenic fields are modified according to the meteorological conditions

Implementation of BEIS3 in WRF/Chem

Based on EPA BEIS3 v11 for SMOKE processor



RACM species emitted by BEIS3:

ISO, API, LIM, XYL, ETH, HC3, ETE, OLT, OLI, HCHO, ALD, KET, ORA2, CO, NO

WRF/Chem Biogenic Emissions

Option 3 (cont.)

- If you decide to create your own biogenic emissions
  - Units are mole/km^2/hr
  - Formatted for conversion program is 12E9.2
  - Dimensions (nx-1,ny-1)
    - surface data only
  - Still use bio_emiss_opt = 2 in namelist.input
  - Need data for only one (1) time
    - start of simulation

- The emissions order is:
  - iso, oli, api, lim, xyl, hc3, ete, olt, ket, ald, hcho, ethora2, co, nr, noag_grow, nononag, lai

WRF/Chem Biogenic Emissions

Edit **namelist.input** file in the WRFV2/test/em_real directory:

- chem_opt=1, (need to turn on chemistry)
- bio_emiss_opt=2.

If necessary, modify the med_read_bio_chem_emiss routine in WRFV2/chem/module_input_chem_bioemiss.F to read your data set.

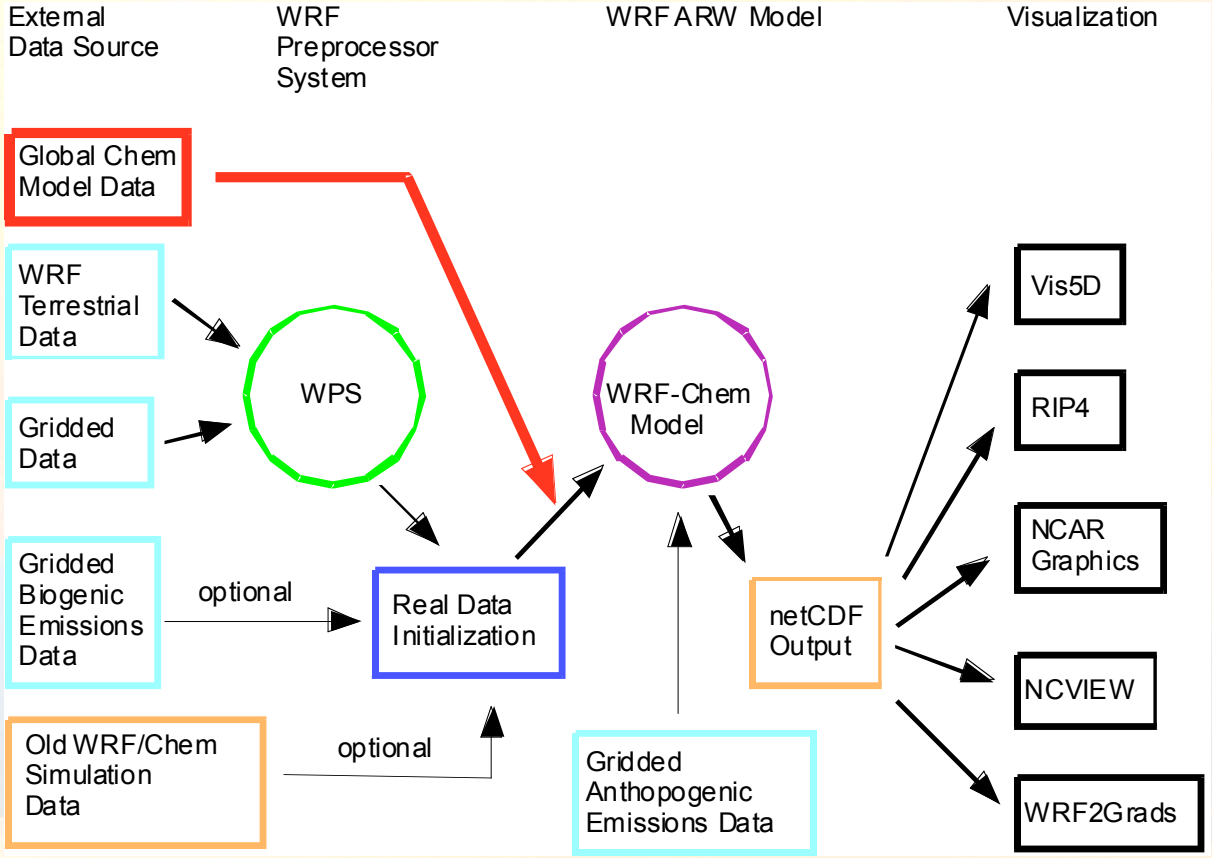
%> compile bio_conv

convert_bioemiss.exe placed in chem directory

Run convert_bioemiss.exe to make wrfbiochemi_d01 data file.

Run real.exe to create wrfinput data file - the biogenic emissions should now be included in the wrfinput data file.

WRF/Chem B.C.s


External Data Source
WRF Preprocessor System
WRF ARW Model
Visualization
Global Chem Model Data
WRF Terrestrial Data
Gridded Data
Gridded Biogenic Emissions Data
Old WRF/Chem Simulation Data
WPS
optional
Real Data Initialization
optional
WRF-Chem Model
Gridded Anthopogenic Emissions Data
netCDF Output
Vis5D
RIP4
NCAR Graphics
NCVIEW
WRF2Grads

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 MOZART & 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

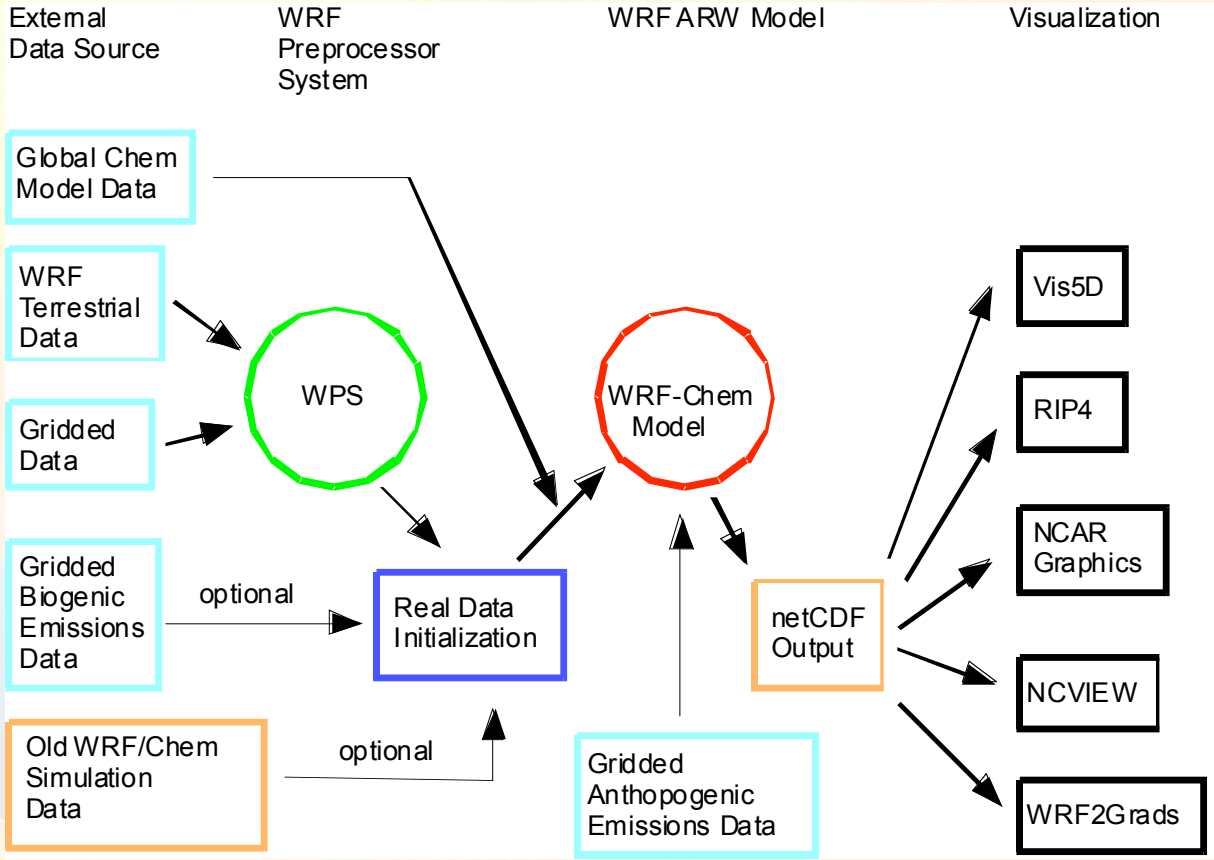
- wrfchembc methodology
  - Read global model chemistry data
  - Skip over if not a desired chemistry species
  - Determine grid point location on WRF/Chem grid
  - If at boundary, interpolate data to WRF/Chem grid
  - Once completed reading/interpolating global data:
    - Open wrfbdy_d01 data file
    - Write boundary data to wrfbdy_d01

WRF/Chem Chemistry B.C.s

- Other groups are exploring other possible ways to generate input/B.C. data for WRF/Chem
  - New stand alone code?
  - Possible use of WPS and real.exe?
    - How to generate input and boundary files given 50 to 100 chemical species?

- No code provided at this time

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)
- Boundary conditions currently assumed constant, except during outflow
  - May be problematic depending upon the simulation
  - User could change chemistry profile in chem/module_input_chem_data.F,
  - Or make changes similar to chem/module_init_mixrats_cbmz.F

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

WRF/Chem namelist options

Namelist options available online on the WRF/Chem FAQ web page:

http://ruc.fsl.noaa.gov/wrf/WG11/FAQ.htm

&time_control

auxinput5_interval_m = 60 anthropogenic emissions update interval (minutes)
io_form_auxinput4 = 2 neCDF data file format

io_form_auxinput5 = 2 netCDF data file format

&physics

cu_rad_feedback = .true. Feedback from parameterized convection to radiation
= .false. No feedback from parameterized convection to radiation

WRF/Chem namelist options

```
&chem
kemit =                    number of vertical levels in each emissions data file

chem_opt =                 0 no chemistry
                           1 RADM2 - no aerosols
                           2 RADM2 and MADE/SORGAM
                           5 CBM-Z with DMS added
                           6 CBM-Z w/o DMS (the version used with MOSAIC)
                           7 CBM-Z+MOSAIC using 4 aerosol size bins
                           8 CBM-Z+MOSAIC using 8 aerosol size bins
                           9 CBM-Z+MOSAIC using 4 aerosol size bins + aqueous chemistry
                                  and cloud-aerosol interactions
                           10 CBM-Z+MOSAIC using 8 aerosol size bins + with aqueous chemistry
                                  and cloud-aerosol interaction
                           11 RADM + SORGAM + aqueous chemistry (place holder)
                           12 RACM + SORGAM + aqueous chemistry (place holder)
                           13 Tracers with emissions but no chemical transformations, (SO2 and CO)
                           101 (RADM2 Chemistry using KPP library)
                           102 (RACM-MIN Chemistry using KPP library)
                           103 (RACM Chemistry using KPP library)
                           104 (RACM Chemistry and MADE/SORGAM aerosols using KPP library)

bioemdt = 30,              update time interval used by biogenic emissions (minutes)
photdt = 30,               photolysis time step (minutes)
chemdt = 4.0               Chemical mechanism time step (minutes)
frames_per_emissfile = 36          (number of times in each emissions data file,
                                   set to 12 for io_style_emissions=1)
```

WRF/Chem namelist options

&chem (cont.)

io_style_emissions = 0 (no emissions data read)
1 (two 12-h emissions data files used)*
* remove aux_model_input5_only from case statement in input_wrf.F
2 (Date/time specific emissions data files used)

emi_inname = wrfchemi_12z_d<domain> for io_style_emissions=1
wrfchemi_d<domain>_<date> for io_style_emissions=2

emiss_inpt_opt = 1 - The species breakdown for RADM/SORGAM.
101 - The species breakdown for CBM-Z/MOSAIC.
102 – Same as 101, but for RADM/SORGAM, isoprene is included.

chem_in_opt = 0 use idealized profile to initialize chemistry
1 use previous simulation data to initialize chemistry

phot_opt = 0 no photolysis
1 use madronich photolysis

drydep_opt = 0 no dry deposition
1 include dry deposition

bio_emiss_opt = 0 no biogenic emissions
1 calculate biogenic emissions online using the Gunther scheme
2 include biogenic emissions in wrfinput data file and modify values online

WRF/Chem additional namelist options

gas_bc_opt:
gas_ic_opt: 1 - Default values as specified in chem/module_input_chem_data
aer_bc_opt: 101 - PNNL values used for the Houston test case
aer_ic_opt:

gaschem_onoff = 0 chemical mechanism off
1 chemical mechanism on

aerchem_onoff = 0 aerosol scheme off
1 aerosol scheme on

wetscav_onoff = 0 wet scavenging turned off
1 wet scavenging turned on

vertmix_onoff = 0 vertical mixing turned off
1 vertical mixing turned on

aer_ra_feedback = 0 No aerosol – radiation feedback in simulation
1 vertical mixing turned on

have_bcs_chem = .false. Use idealized profile for lateral boundary conditions
.true. Use global model data for lateral boundary conditions
(data needs to be added to wrfbdy_d01 file)
1-way nested boundary conditions data
* need to have every chemical species defined or defaults to 1.E-16

WRF/Chem Registry

registry.chem

```
state integer emissframes - - - - - "emissframes" "" ""
#-----------------------------------------------------------------------------------------------------------------------------------------------
# Chemistry Variables (all shared at this point)
# emissions first
state   real   e_iso    i+j   misc     1    Z    i5h   "E_ISO"    "Isoprene EMISSIONS (Anth. for RADM/RACM,…"
                                                                                                  "mol km^-2 hr^-1"
state   real   e_so2    i+j   misc     1    Z    i5h   "E_SO2"    "EMISSIONS"                     "mol km^-2 hr^-1"
state   real   e_no     i+j   misc     1    Z    i5    "E_NO"     “EMISSIONS"                      "mol km^-2 hr^-1"
state   real   e_co     i+j   misc     1    Z    i5h   "E_CO"     "EMISSIONS"                      "mol km^-2 hr^-1"
…
…

# Chem Scalars
state    real     -       ikjftb   chem   1   - - -
state    real    so2      ikjftb   chem   1   -   irhusdf=(bdy_interp:dt)   "so2"   "SO2 concentration"     "ppmv"
state    real    sulf     ikjftb   chem   1   -   irhusdf=(bdy_interp:dt)   "sulf"  "SULF concentration"   "ppmv"
state    real    no2      ikjftb   chem   1   -   irhusdf=(bdy_interp:dt)   "no2"   "NO2 concentration"    "ppmv"
state    real    no       ikjftb   chem   1   -   irhusdf=(bdy_interp:dt)   "no"    "NO concentration"     "ppmv"
state    real    o3       ikjftb   chem   1   -   irhusdf=(bdy_interp:dt)   "o3"    "O3 concentration"     "ppmv"
…
…
```

Running WRF/Chem

- Now that you have:
  - WRF/SI or WPS data (need the “wrf_real_input”, or “met_em” files to make wrfinput_d01 and wrfbdy files)
  - Optional biogenic emissions data for the domain (wrfbiochemi_d01)
  - Optional wrf_chem_input_data_d01_<date>.<time> data file from previous simulation

- Set the namelist.input options

- Run real.exe to produce wrfinput and wrfbdy data files
  - Use multi-processor compiled code
  - Should get messages regarding the reading of
    - biogenic emissions
    - chemistry data used to initialize model run
    - If you do not get these messages, an error is likely

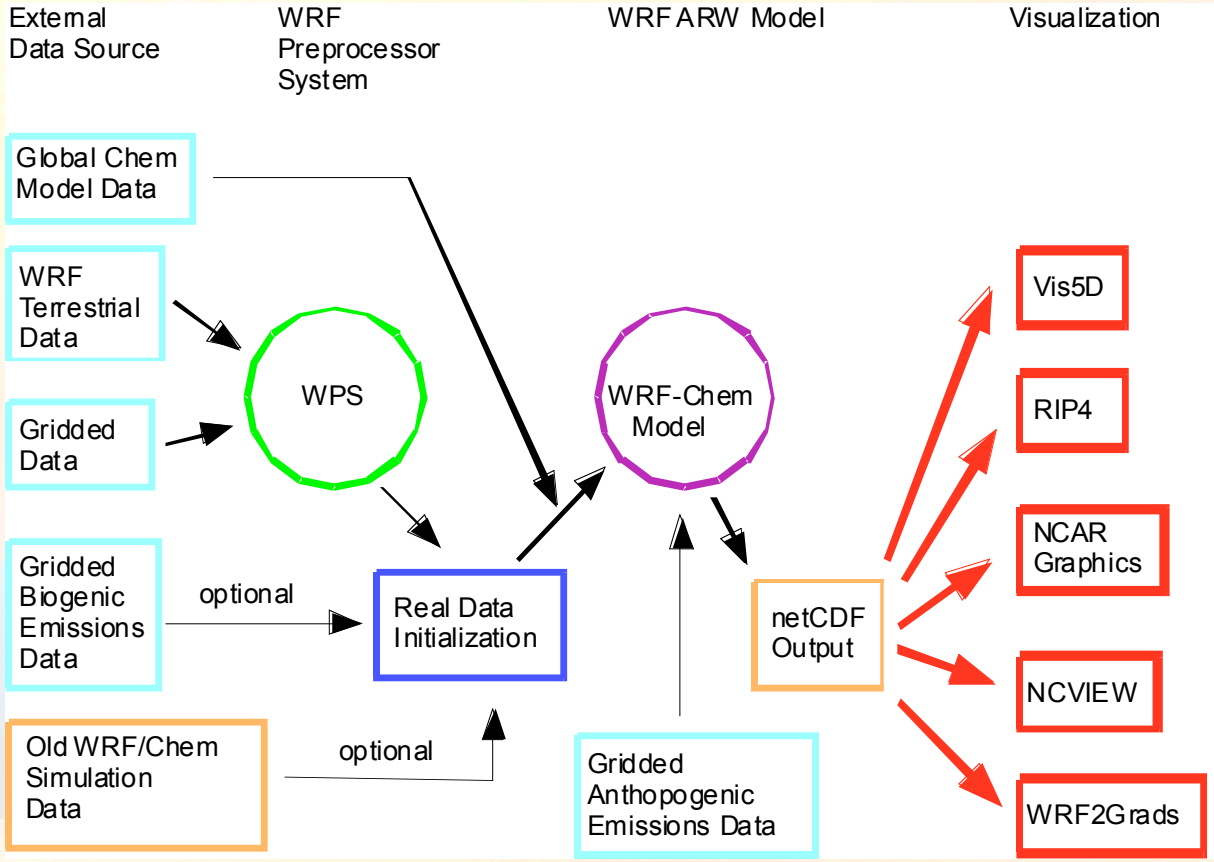
Running WRF/Chem

- 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, etc.
- Other standard WRF visualization tools work with the chemistry variables as well as the meteorology
  - VIS5D
  - Grads
  - Etc.