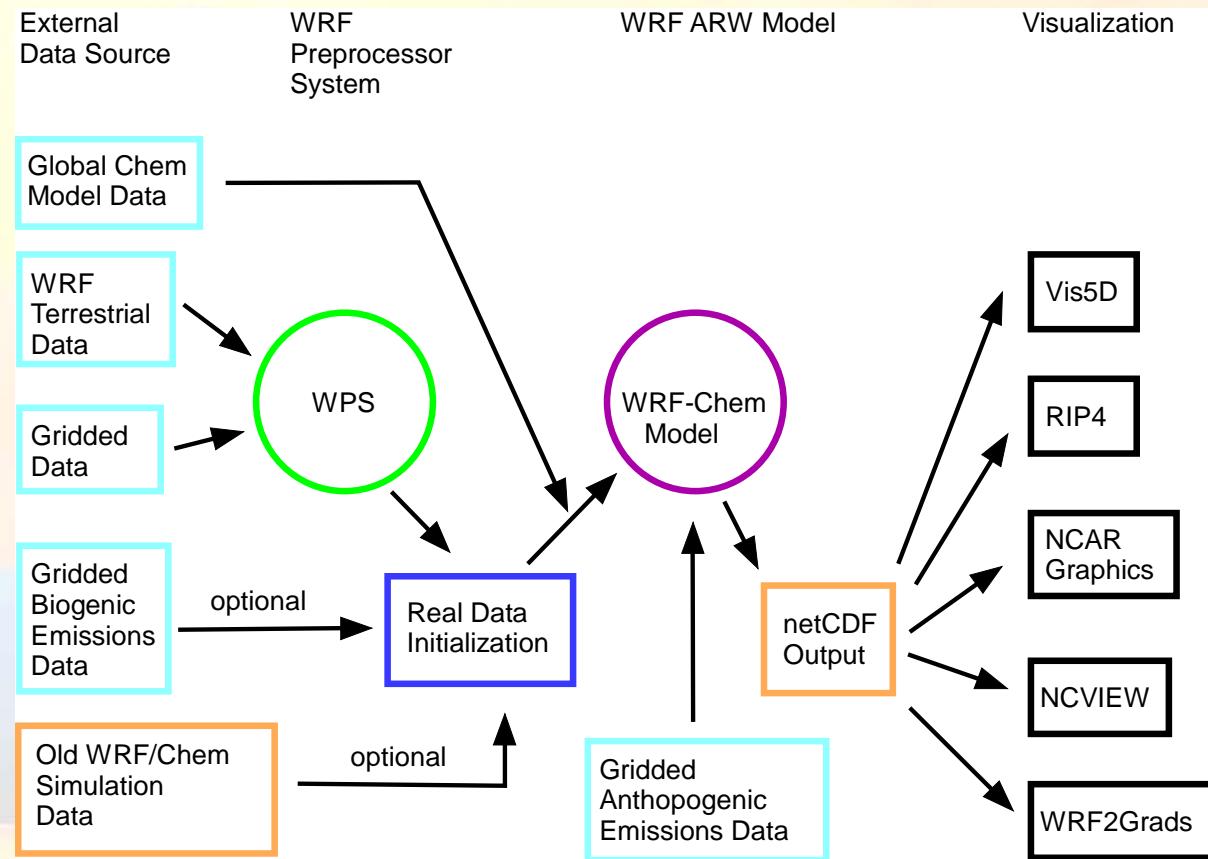


WRF/Chem: A Quick Review Of How To Set-Up & Run

Steven Peckham

WRF/Chem Model System



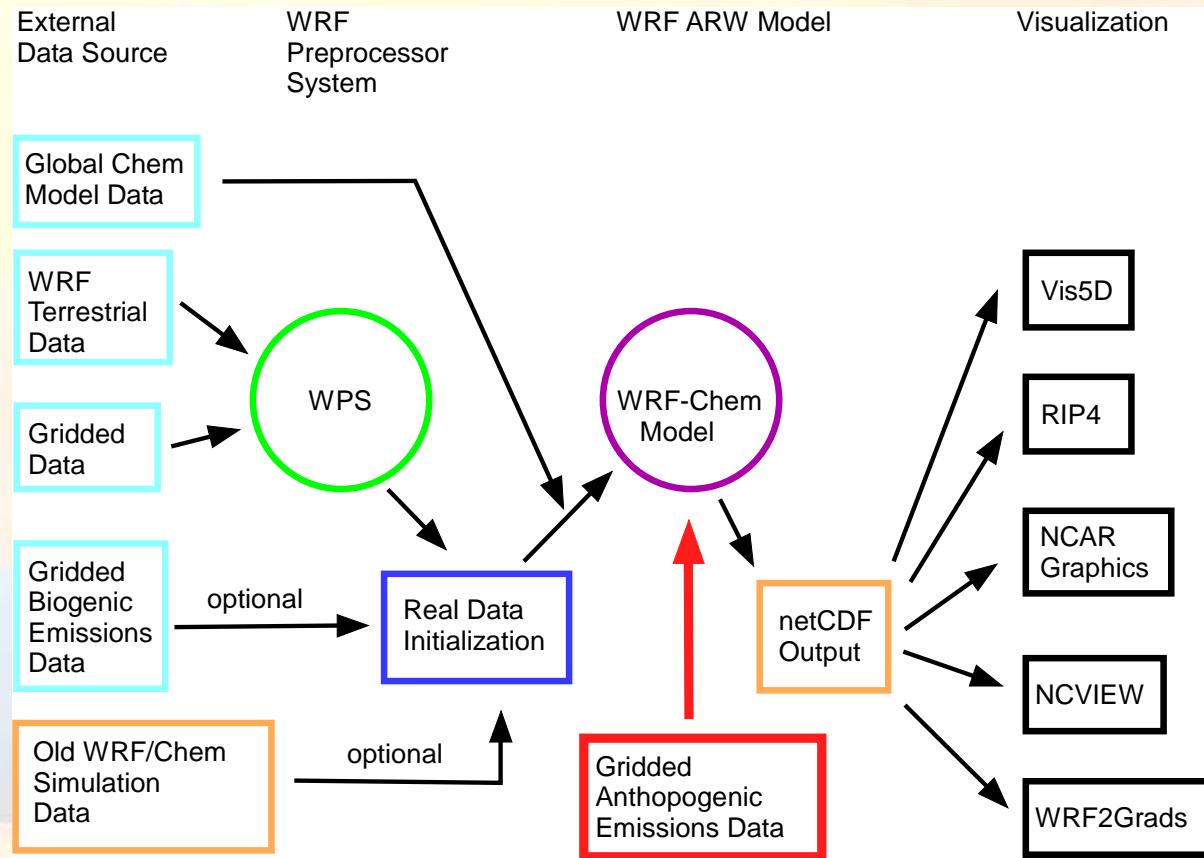
WRF/Chem

- It is assumed that the user of WRF/Chem :
 - is *very familiar* with the WRF model system
 - have run WPS/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 exclude(butanes)
! HC05	e_hc5	0.97	00	Alkane 5000< kOH <10000 exclude(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
! HC14	e_hcho	1.00	00	Formaldehyde exclude(xylenes)
! 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 ( bdynname , ' ../../run/wrfem12k_00to12z' , grid%id , 2 )
        IF (wrf_dm_on_monitor()) THEN
          open (91,file=bdynname,form='unformatted')
        ENDIf
        write(message, '(A,A)' ' OPENED FILE: ',bdynname
              call wrf_message( TRIM( message ) )
        ENDIF
        IF(intime == 12 ) THEN
          CALL construct_filename1 ( bdynname , ' ../../run/wrfem12k_12to24z' , grid%id , 2 )
          IF (wrf_dm_on_monitor()) THEN
            open (91,file=bdynname,form='unformatted')
          ENDIf
          write(message, '(A,A)' ' OPENED FILE: ',bdynname
                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

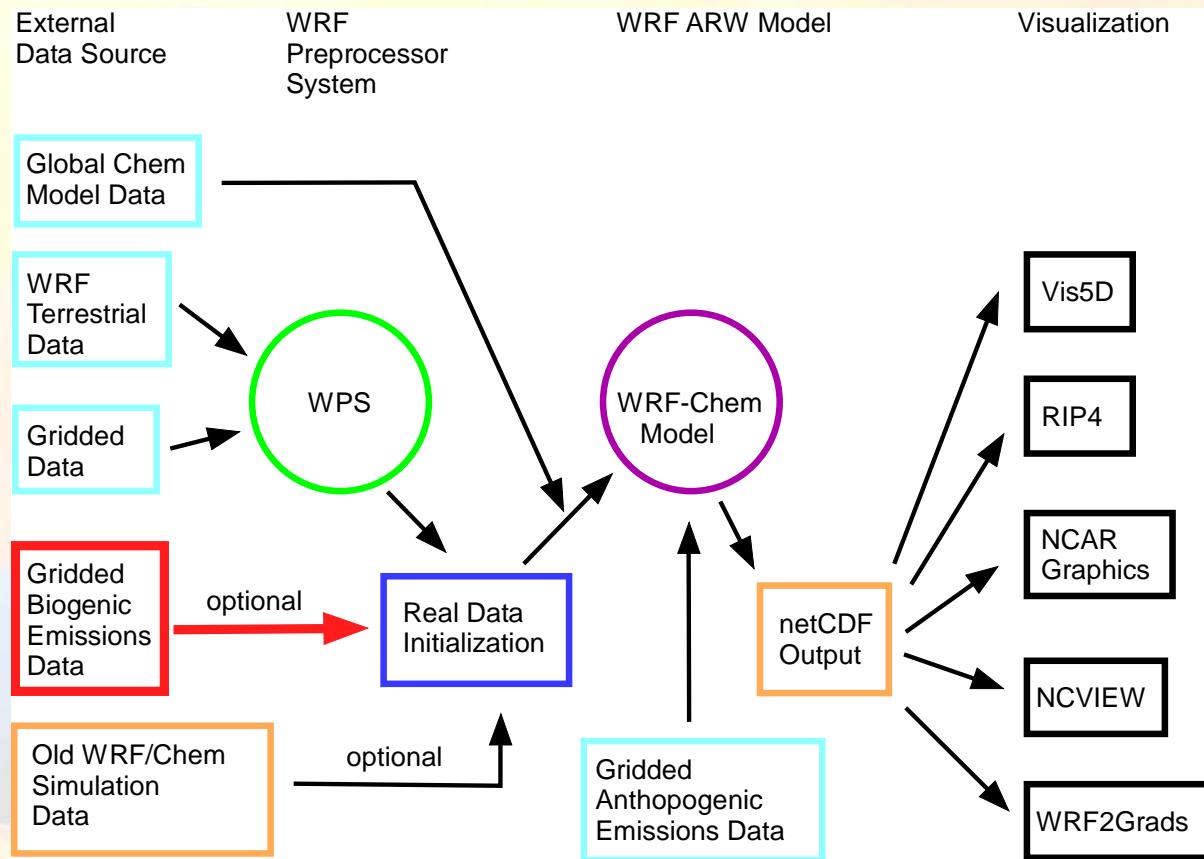
auxinput5_interval_m = 60 - Minutes between reading emissions (used with *io_style_emissions*=2)

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.

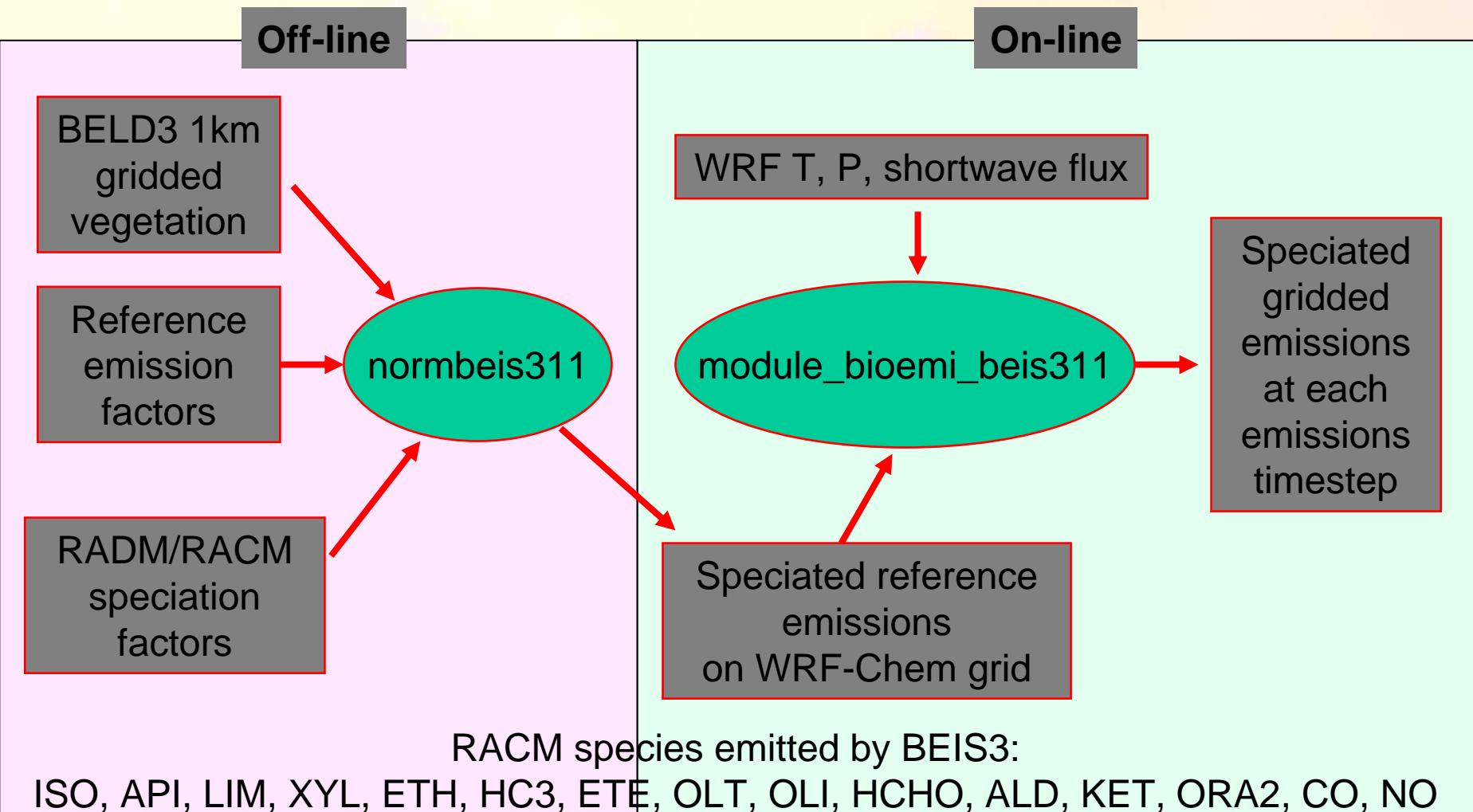
WRF/Chem

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



WRF/Chem Biogenic Emissions

Option 3 (cont.)

- If you decide to create your own biogenic emissions
 - Units are mole/km²/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.

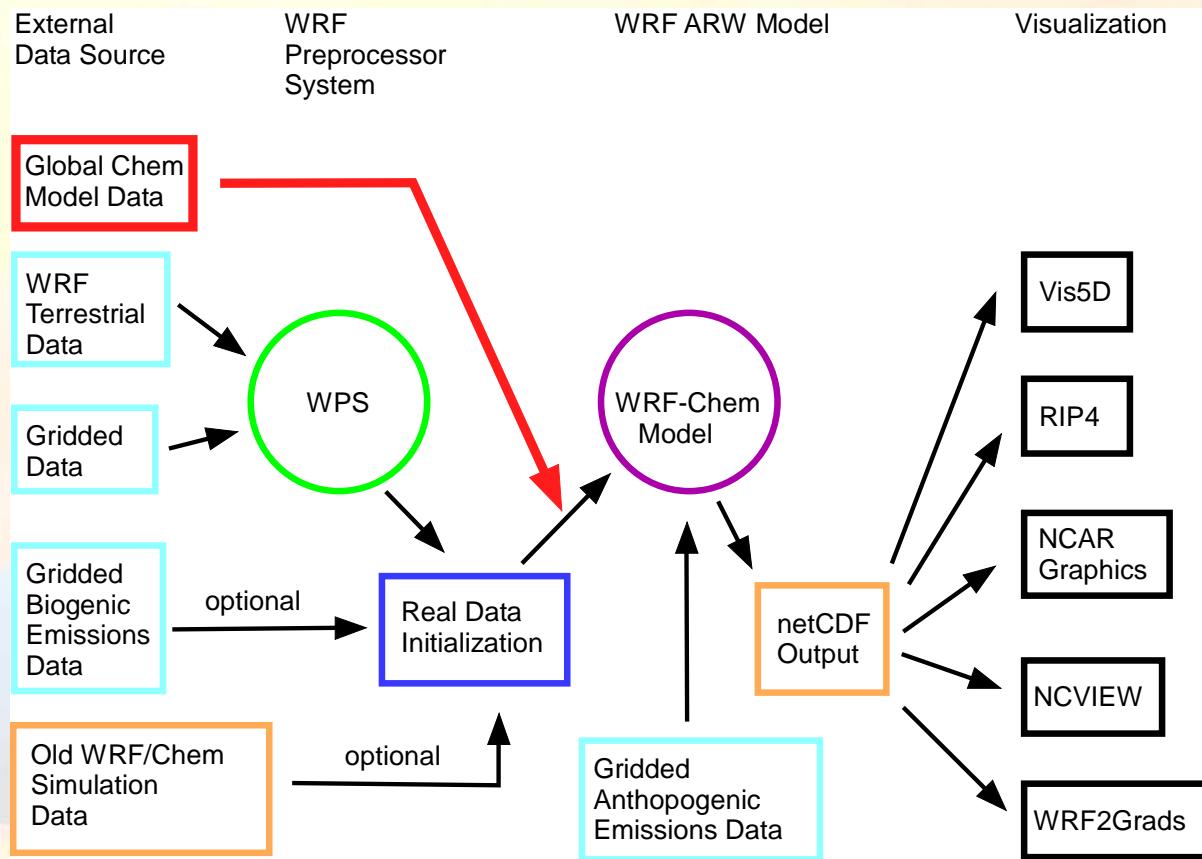
```
%> compile bio_conv
```

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



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

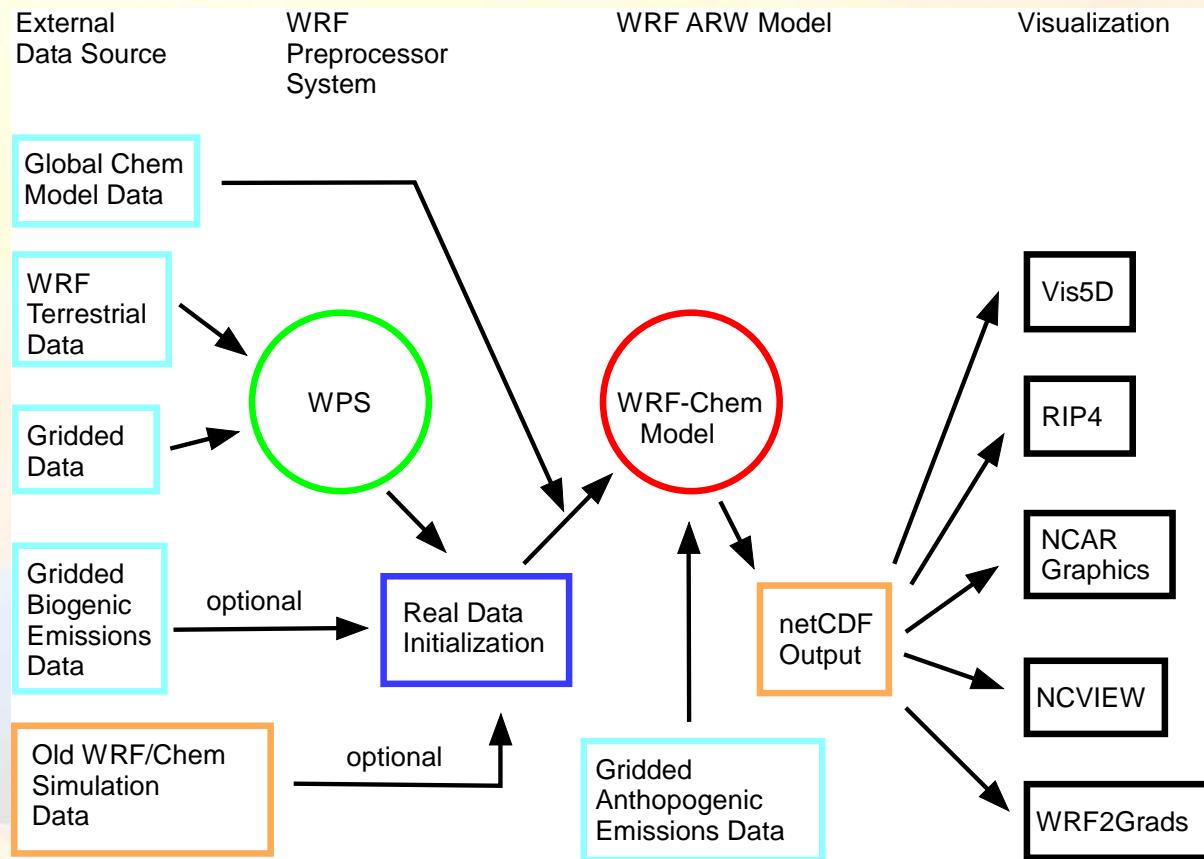
WRF/Chem Chemistry B.C.s

- 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, (SO ₂ 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
wetscov_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

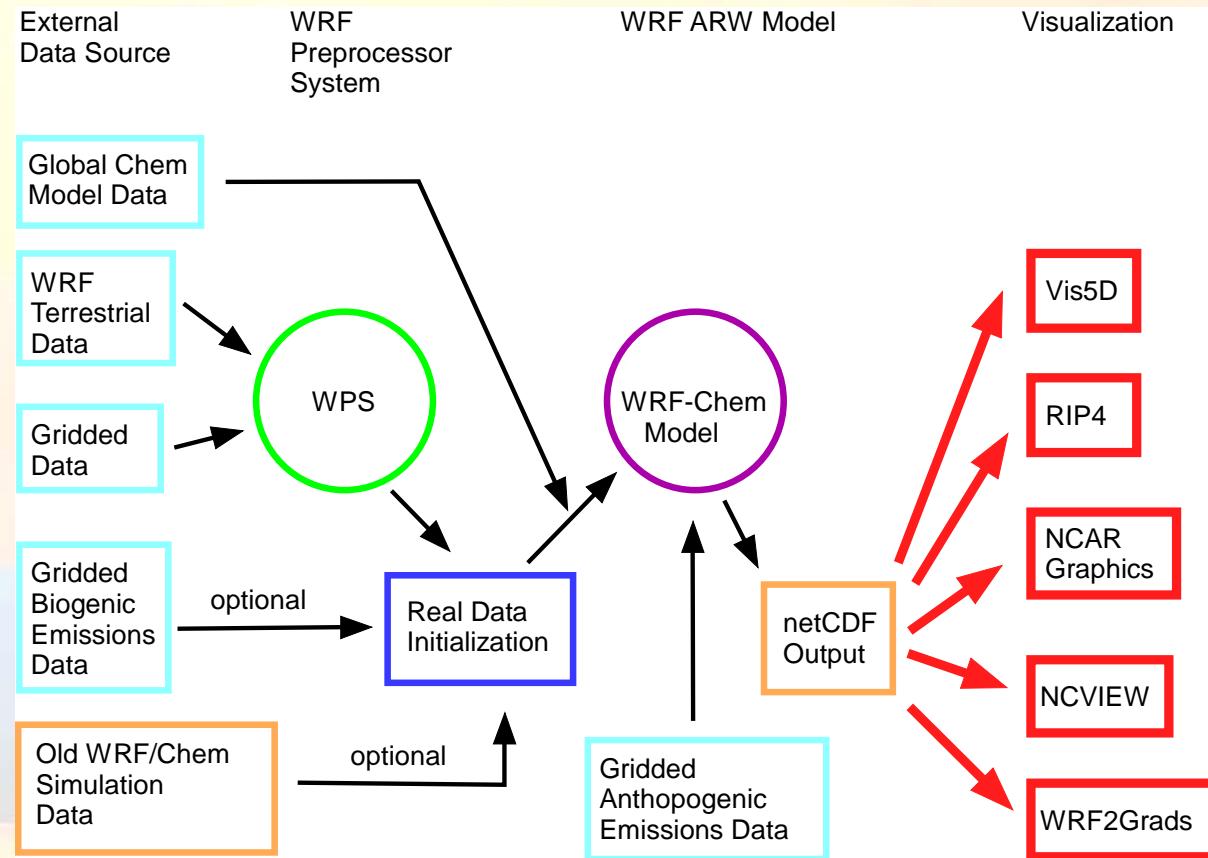
Running WRF/Chem

- After running real.exe, you have:
 - wrfout_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.