WRF-Chem V3.4.1: Nested Simulation Considerations

Steven Peckham

# Nested Chemistry Simulation: Best practices

- Be familiar with running a nested WRF simulation
  - Namelist settings
  - Methodology

- Start by making a nested run following NDOWN methodology for meteorology only

- Move on to 2-way interactive nested simulations using meteorology only
  - Considerations:
    - time step for each domain,
    - namelist settings – set for each nest or once for all domains,
    - domain sizes large enough for study of item of interest

- When a nested meteorology simulation works as expected, then move on to adding chemistry.

Nested Chemistry Simulation: Best Practices

- Start a nested chemistry run by using NDOWN
  - Need to generate emissions for nested domain
    - Use nested domain map information in prep_chem_sources
    - Can not simply interpolate emissions from mother domain to nest
      - Mass conservation issues
      - Emissions source issues (land/water location, point emissions shifted to wrong location, etc.)

- Confirm that the nested domain with chemistry produces the correct results

- If 1-way nested run is correct, then advance to 2-way interactive nested run.
  - No moving nests possible when using chemistry!
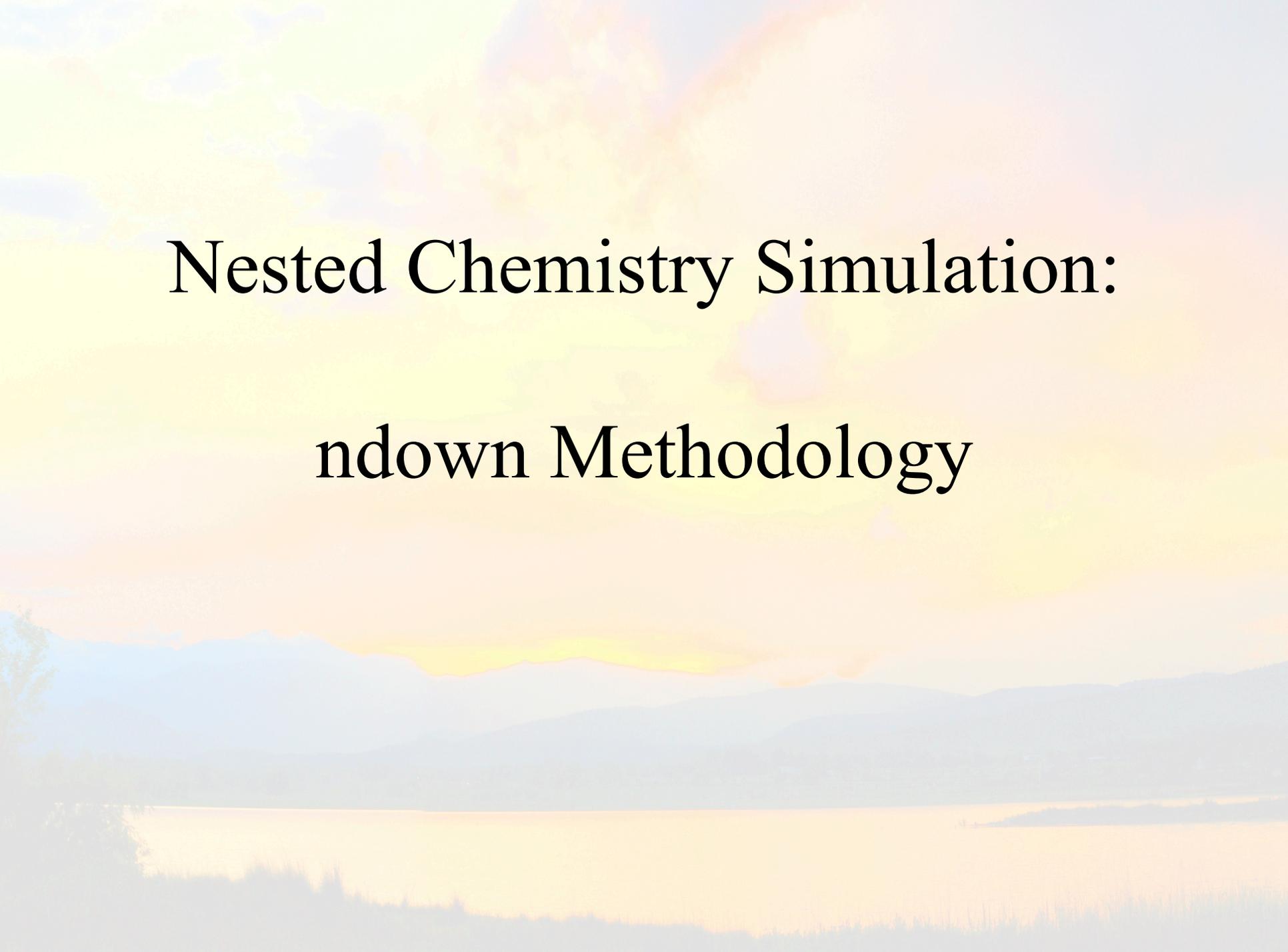
Nested Chemistry Simulation:

ndown Methodology

ndown without chemistry

- Save wrf output files for coarse domain
- Get met files for domain and rename them to domain 1 files (met_em.d01....)
- Run real for domain 2 with all settings in the domain 1 column
- Rename files generated by real.exe
- Get wrfout files for coarse domain
- Set namelist.input for nested domain run.
  - Make sure that inverval_seconds is set for the update interval of the wrfout files
- Run ndown.exe
- Rename files input files for domain 2 to domain 1 and clean-up directory.
- Verify that wrfinput and wrfbdy are correct.
- Run domain 2 now as as if you are running a single domain.

ndown with chemistry

- Save wrf output files for coarse domain
- Get met files for domain and rename them to domain 1 files (met_em.d01....)
- Run real for domain 2 with all settings in the domain 1 column
- Rename files generated by real.exe
- Get wrfout files for coarse domain
- Set namelist.input for nested domain run.
  - Make sure that inverval_seconds is set for the update interval of the wrfout files
- Build emissions for nested domain
- Run ndown.exe with namelist.input settings for chemistry turned on
- Rename files input files for domain 2 to domain 1 and clean-up directory.
- Verify that wrfinput and wrfbdy are correct.
- Run domain 2 now as as if you are running a single domain.

Nested Chemistry Simulation: prep_chem_sources Settings

- Building emissions with prep_chem_sources
  - Prep_chem_sources has nested domain settings in map projection calculation

- Grid mapping routines not as flexible as WRF mapping routine

- Make sure emissions map onto the nested domain

prep_chem_sources Settings for Nest

```
grid_type= 'lambert',

 NGRIDS   = 2,                              ! Number of grids to run

NNXP     = 41, 61,86,46,                   ! Number of x grid points
NNYP     = 41, 61,74,46,                   ! Number of y grid points
NXTNEST  = 0,1,2,3,                         ! Grid number which is the next coarser grid
DELTAX   = 100000.,
DELTAY   = 100000.,                         ! X and Y grid spacing

! Nest ratios between this grid and the next coarser grid.
NSTRATX  = 1, 5, 3, 4,                       ! x-direction
NSTRATY  = 1, 5, 3, 4,                        ! y-direction

NINEST = 1, 10,0,0,                          ! Grid point on the next coarser
NJNEST = 1, 10,0,0,                          !  nest where the lower southwest
                                             !  corner of this nest will start.
                                   !  If NINEST or NJNEST = 0, use CENTLAT/LON
POLELAT  = 35.,          ! If polar, latitude/longitude of pole point
POLELON  = 25.,           ! If lambert/mercator, lat/lon of grid origin (x=y=0.) (ref_lat /ref_lon from namelist.wps)

CENTLAT  = 35.0,  35.0,   27.5,  27.5,   ! (ref_lat/ref_lon from namelist.wps)
CENTLON  = 25.0,  25.0,    -80.5, -80.5,
```

Convert Emissions For Nest

- Link grid 2 output and grid 2 wrfinput to run convert_emiss (nested domain only)

- Set namelist.input for nested domain

```
max_dom                   = 1,
e_we                      = 61,   112,   94,
e_sn                      = 61,   97,   91,
e_vert                     = 35,   28,   28,
p_top_requested           = 5000,
num_metgrid_levels        = 27,
num_metgrid_soil_levels    = 4,
dx                        =  20000, 10000,  3333.33,
dy                        =  20000, 10000,  3333.33,
```

- Run convert_emiss.exe for one domain – not capable of doing nested domains

- Verify the emissions are correct for the nested domain (land vs sea, cities, roads, etc.)

Nested Chemistry Simulation: Methodology

- Save wrf output files for coarse domain
- Get met files for domain and rename them to domain 1 files (met_em.d01....)
- Run real for domain 2 with all settings in the domain 1 column
- Rename files generated by real.exe
- Get wrfout files for coarse domain
- Set namelist.input for nested domain run.
  - Make sure that inverval_seconds is set for the update interval of the wrfout files
- Build emissions for nested domain
- Run ndown.exe with namelist.input settings for chemistry turned on
- Rename files input files for domain 2 to domain 1 and clean-up directory.
- Verify that wrfinput and wrfbdy are correct.
- Run domain 2 now as as if you are running a single domain.

Ndown namelist.input

- Namelist.input settings for ndown with chemistry

```
&domains
 max_dom            = 2
```

With or without chem ←

```
&chem
 kemit                      = 1,
 chem_opt                   = 11,      11,
…
…
…
 bio_emiss_opt              = 2,      2,
…
…
…
 biomass_burn_opt           = 1,      1,
…
```

Needed for chem input ←

Emissions Part of ndown_em.F

```fortran
 IF( nested_grid%chem_opt .NE. 0 ) then
! Read the chemistry data from a previous wrf forecast (wrfout file)
      ! Generate chemistry data from a idealized vertical profile
      if(nested_grid%biomass_burn_opt == BIOMASSB) THEN
        message = 'READING BIOMASS BURNING EMISSIONS DATA '
        CALL  wrf_message ( message )
        CALL med_read_wrf_chem_emissopt3 ( nested_grid , config_flags)
      end if

      if(nested_grid%dust_opt == 1 .or. nested_grid%dmsemis_opt == 1
&
         .or. nested_grid%chem_opt == 300  .or. nested_grid%chem_opt ==
301) then
         message = 'READING GOCART BG AND/OR DUST and DMS
REF FIELDS'
         CALL  wrf_message ( message )
         CALL med_read_wrf_chem_gocart_bg ( nested_grid , config_flags)
      end if

      if( nested_grid%bio_emiss_opt .eq. 2 )then
        message = 'READING BEIS3.11 EMISSIONS DATA'
        CALL  wrf_message ( message )
        CALL med_read_wrf_chem_bioemiss ( nested_grid , config_flags)
      else if( nested_grid%bio_emiss_opt == 3 ) THEN
        message = 'READING MEGAN 2 EMISSIONS DATA'
        CALL  wrf_message ( message )
        CALL med_read_wrf_chem_bioemiss ( nested_grid , config_flags)
      endif
ENDIF
```

Biomass burning

GOCART background

Biogenic emissions
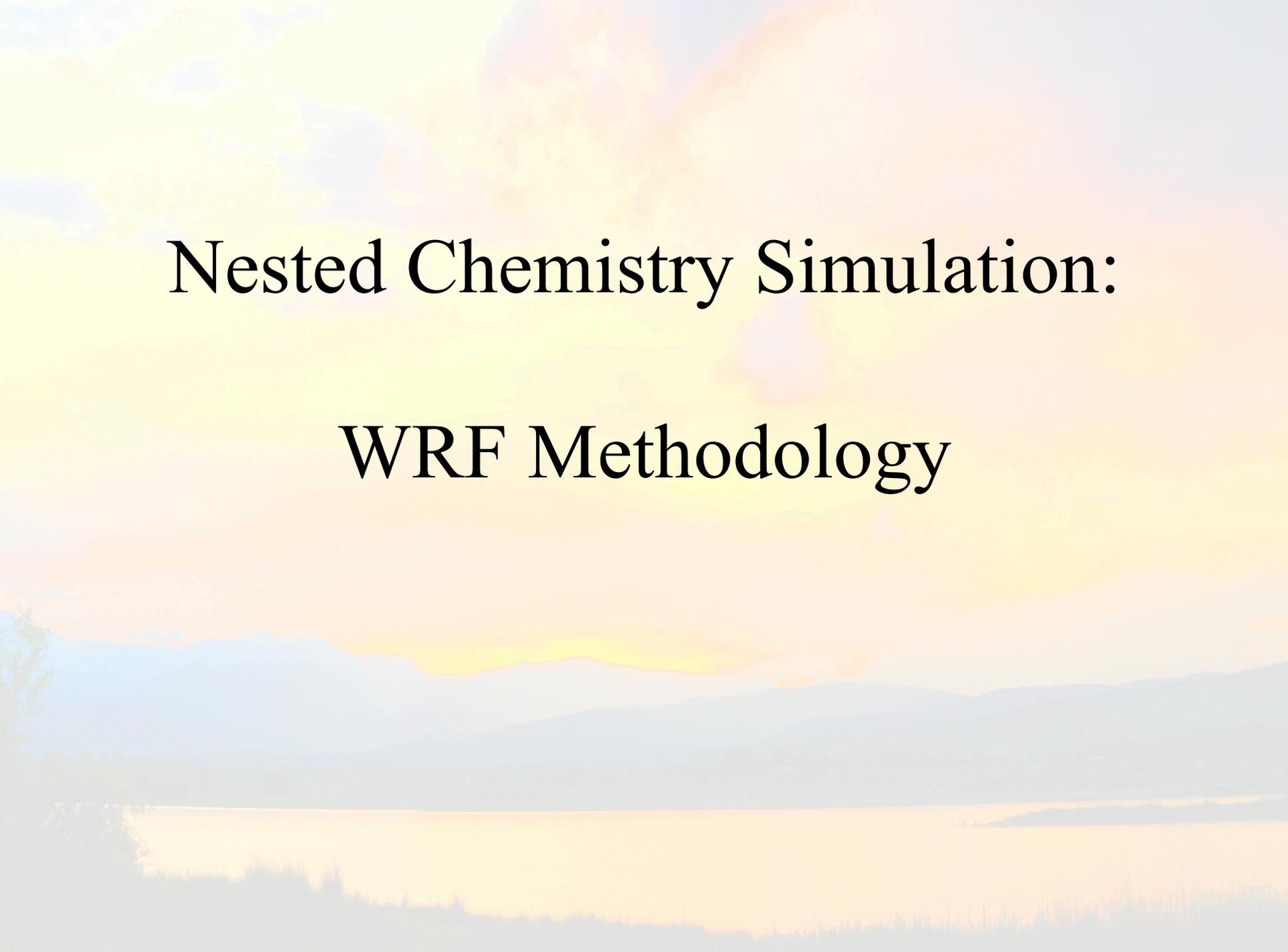
Nested Chemistry Simulation:

WRF Methodology

Nested Chemistry Simulation: namelist.input settings

- Registry provides information as to possible nested run settings

```
rconfig   real    BIOEMDT              namelist,chem      max_domains   0     h      "BIOEMDT"            ""  ""
rconfig   real    PHOTDT               namelist,chem      max_domains   0     h      "PHOTDT"            ""  ""
rconfig   real    CHEMDT               namelist,chem      max_domains   0     h      "CHEMDT"            ""  " »
rconfig   real    BIOEMDT              namelist,chem      max_domains   0     h      "BIOEMDT"            ""  ""
rconfig   real    PHOTDT               namelist,chem      max_domains   0     h      "PHOTDT"            ""  ""
rconfig   real    CHEMDT               namelist,chem      max_domains   0     h      "CHEMDT"            ""  " »
rconfig   integer ne_area             namelist,chem      1                    41    irh    "ne_area"            ""      ""
rconfig   integer kemit               namelist,chem      1                    9     irh    "kemit"              ""      ""
rconfig   integer nmegan              namelist,chem      1                    138   irh    "nmegan"             ""      "»
rconfig   integer kemit_aircraft      namelist,chem      1                    1     -      "kemit_aircraft"         ""      "»
rconfig   integer biomass_emiss_opt   namelist,chem      max_domains   0     rh     "biomass_emiss_opt"             ""    »»"
```


- Examine column 5 in registry.chem to determine which options are set for each domain

# Nested Chemistry Simulation: namelist.input

- Namelist.input settings for chemistry

```
kemit                     = 1,
chem_opt                   = 11,      6,       0,
chemdt                    = 1.50, 0.66666,
phot_opt                  = 2,        3,
emiss_opt                  = 5,        3,
chem_in_opt                = 0,        0,
gas_drydep_opt              = 1,        1,
aer_drydep_opt              = 1,        1,
bio_emiss_opt              = 1,        2,
gaschem_onoff               = 1,        0,
aerchem_onoff               = 1,        0,
chem_conv_tr               = 1,        1,
seas_opt                  = 1,
…
```

- Can one change chemistry options between domains?
    – Will the namelist above work?
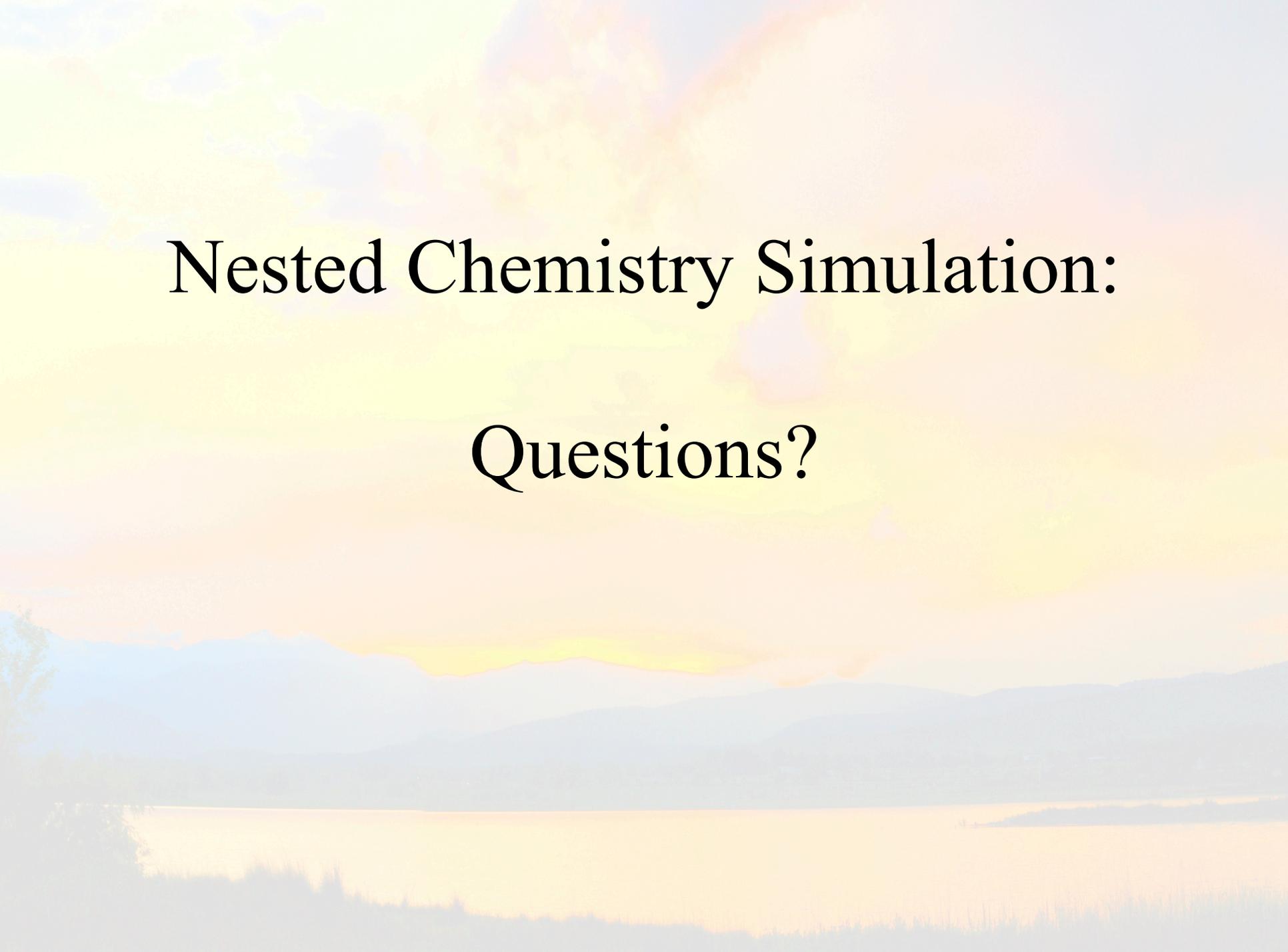
Nested Chemistry Simulation:

Questions?

Discussion

How large should mother domain (domain 1) be for a nested simulation? Nest likewise?

Need to consider:

- U~O[10 m/s] -> ~ 40 km/h ~ 500 km/d
- Mountain locations in domain, flow across mountains/gravity waves and reflection off top
- Recirculation of pollutants
- Available computing resources