Implementation of CBM-Z, MOSAIC, and Aerosol-Radiation-Cloud-Chemistry Interactions in WRF-chem

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The Technical Details

The Nuts & Bolts of Using MOSAIC & Cloud-Aerosol Interactions

i.e. what you really need to know

to get your work done…

Namelist Variables for PNNL Modules

&time_control
auxinput5_interval_m
io_form_auxinput5

&physics
progn
mp_physics
ra_sw_physics

&chem
emiss_inpt_opt
frames_per_emissfile
io_style_emissions
kemit

chem_opt
phot_opt
drydep_opt
bio_emiss_opt
aer_ra_feedback

chem_in_opt
gas_bc_opt
gas_ic_opt
aer_bc_opt
aer_ic_opt
have_bcs_chem

gaschem_onoff
aerchem_onoff
wetscav_onoff
cldchem_onoff
vertmix_onoff

bioemdt
chemdt
photdt

Start with the basics… chem_opt

PNNL chem_opt additions

- 5 = CBMZ gas mechanism (w/ DMS)
- 6 = CBMZ gas mechanism (w/o DMS)
- 7 = CBMZ+MOSAIC (4 bins) sectional aerosol
- 8 = CBMZ+MOSAIC (8 bins) sectional aerosol
- 9 = CBMZ+MOSAIC (4 bins)+Aq. Chem.
- 10= CBMZ+MOSAIC (8 bins)+Aq. Chem.

Meteorology Feedback Settings

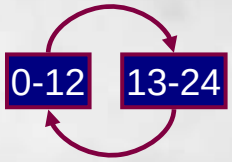
- Direct effect
  - aer_ra_feedback = 1
    - Turns on aerosol radiation feedback
  - ra_physics = 2 (GSFC) & phot_opt = 2 (FastJ)
    - Currently only GSFC is linked to the aerosols and FastJ is needed to get the Mie parameters
- Indirect effects
  - chem_opt = 9 or 10
    - Adds cloud-phase aerosol species to Registry
  - progn = 1
    - Turns on prognostic aerosols
  - mp_physics = 2 (Lin)
    - Currently only Lin is linked to cloud-phase aerosols

What are you trying to do?

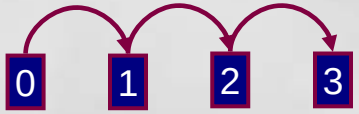
- Simplest MOSAIC run for aerosol chemistry w/o clouds & no affect on meteorology
  - chem_opt=8; aer_ra_feedback=0; progn=0
- Aerosol chemistry plus the direct effect
  - chem_opt=8; phot_opt=2; aer_ra_feedback=1; ra_sw_physics=2 (GSFC); progn=0
- Aerosol chemistry plus direct and indirect effects, wet scavenging, & aqueous chemistry, i.e. the whole shebang
  - chem_opt=10; phot_opt=2; aer_ra_feedback=1; ra_sw_physics=2; progn=1; mp_physics=2 (Lin)

Emissions Namelist Variables (1)

- Emissions are tied to auxinput5
  - File format (i.e. netCDF, Grib), frequency of reads, etc. controlled with auxinput5 controls
    - io_form_auxinput5=2 (netCFD)
    - auxinput5_interval_h=1 (hourly input)
- io_style_emissions chooses “dated” or “cyclical” files
  - Two 12-hr files that keep repeating



    - io_style_emissions=1
    - emi_inname=“wrfchemi_d<domain>”
    - frames_per_emissfile is ignored
  - Hour specific files (or daily, etc.)



    - io_style_emissions=2
    - emi_inname=“wrfchemi_d<domain>_<date>”
    - frames_per_emissfile=1 (for one file per hour)

Emissions Namelist Variables (2)

- Number of levels for emissions, kemit=8
- Speciation within the emissions file set with emiss_inpt_opt
  - emiss_inpt_opt=1, RADM2-SORGAM (RS)
  - emiss_inpt_opt=101, CBMZ-MOSAIC (CB)
  - emiss_inpt_opt=102, RS for use with CB

MOSAIC Emissions - Parsing Into Bins

- Breakdown from modes/size ranges to sectional size bins is done in module_mosaic_addemiss.F□□ by setting percentages applied to each bin
- Same percentage applied to all species
- If using an RS emissions file
  - fr8b_aem_sorgam_i (Aitken mode)
  - fr8b_aem_sorgam_j (accumulation mode)
  - fr8b_aem_sorgam_c (coarse mode)
- If using a CM emissions file
  - fr8b_aem_mosaic_f (fine, 0-2.5 μm)
    - (/ 0.060, 0.045, 0.245, 0.400, 0.100, 0.150, 0., 0./)
  - fr8_aem_mosaic_c (coarse, 2.5-10 μm)
    - (/ 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.300, 0.700 /)

CM Emission Files - Gas Species

Variable Redefinitions in CBMZ vs. RADM2

RADM2 Variable	CBMZ Variable	Species Name for CBMZ
E_ALD	ALD2	Aldehydes
E_CSL	CROS	Cresol
E_ETH	C2H6	Ethane
E_KET	AONE	Ketone
E_OL2	ETH	Ethene (C2H4)
E_OLI	OLEI	Internal Olefin
E_OLT	OLET	Terminal Olefin
E_HC5	PAR	Paraffin
E_NO2	NO2	NO_2 added in CBMZ

CM Emission Files - Aerosol Species

Differences from an RS Emissions File

Coarse species added	Fine species reinterpreted	e_XXi not used
e_so4c	e_so4j	
e_no3c	e_no3j	
e_orgc	e_orgj	
e_ecc	e_ecj	
	e_pm25j (OIN <2.5 μm)	
	e_pm10 (OIN >2.5 μm)	

Initial and Boundary Conditions (1)

- ICs method chosen with chem_in_opt
  - chem_in_opt = 1 uses previous gridded chem output in a file named wrf_chem_input_d<domain>_<date>
  - chem_in_opt = 0 uses fixed profiles (see below)
- Fixed MOSAIC aerosol profiles set in module_mosaic_initmixrats.F
  - We have predefined some aerosol profiles using CPP directives at the top of modules_mosaic_initmixrats.F
  - Fractional breakdowns by bin with fr8b_fine and fr8b_coar
  - Each aerosol species mass for “fine” and “coarse” is set with variables like qfine_so4 and qcoar_so4, etc.
  - Interpolation to a height profile is hacked in here
  - ICs and BCs are each set independently - MAKE SURE TO SET BOTH in the appropriate subroutines

Initial and Boundary Conditions (2)

- Fixed CBMZ gas profiles set in module_input_chem_data.F and module_cbmz_initmixrats.F
  - NALROM profiles in module_input_chem_data.F that are used by RADM are also used by CBMZ
  - The exception are any species that are overridden in module_cbmz_initmixrats.F (currently O3 and HCl)
- gas_ic_opt and aer_ic_opt can be used to toggle from RS (=1) to CM (=101) ICs
- gas_bc_opt and aer_bc_opt can be used to toggle from RS (=1) to CM (=101) BCs
- These IC and BC setups are clearly hacked
  - Make sure the values you are getting are what you want for your particular case - these are not necessarily “turn-key”
  - We would not be offended if a generous user sets up a better way to do this
  - A better way would be to use lookup tables that could be set at runtime

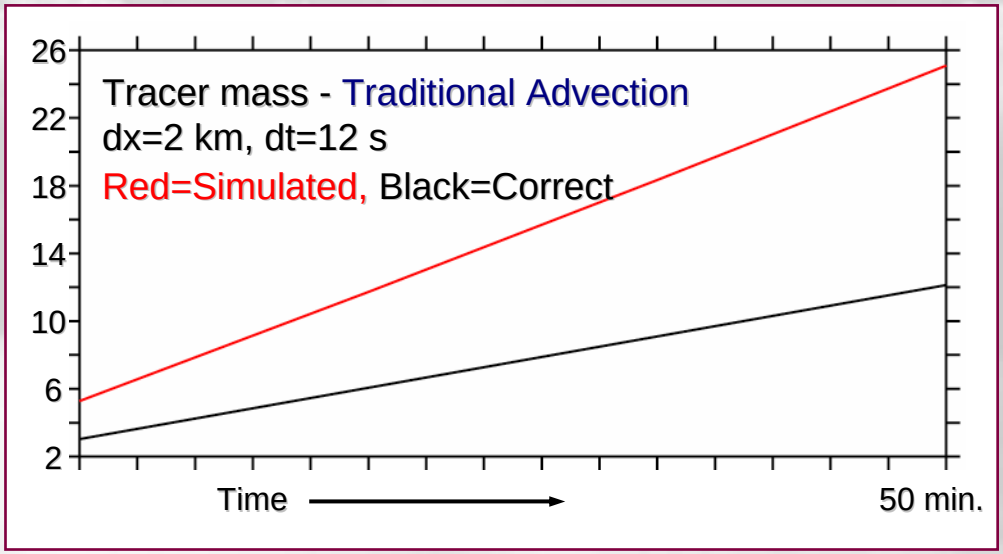
Debugging and Sensitivity Namelist Vars

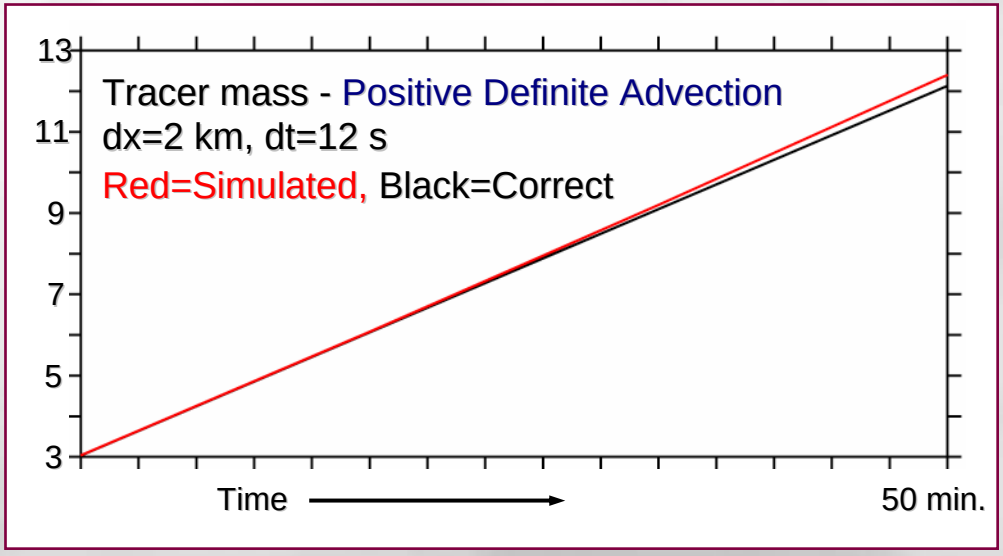
Processes can be turned on (1) or off (0) individually as needed using:

- vertmix_onoff (triggers dry dep. and vertical mixing)
- drydep_opt (0=no dry dep. if still want vertical mixing on)
- gaschem_onoff
- aerchem_onoff
- wetscav_onoff (must be off unless using cloud phase aer.)
- cldchem_onoff (must be off unless using cloud phase aer.)

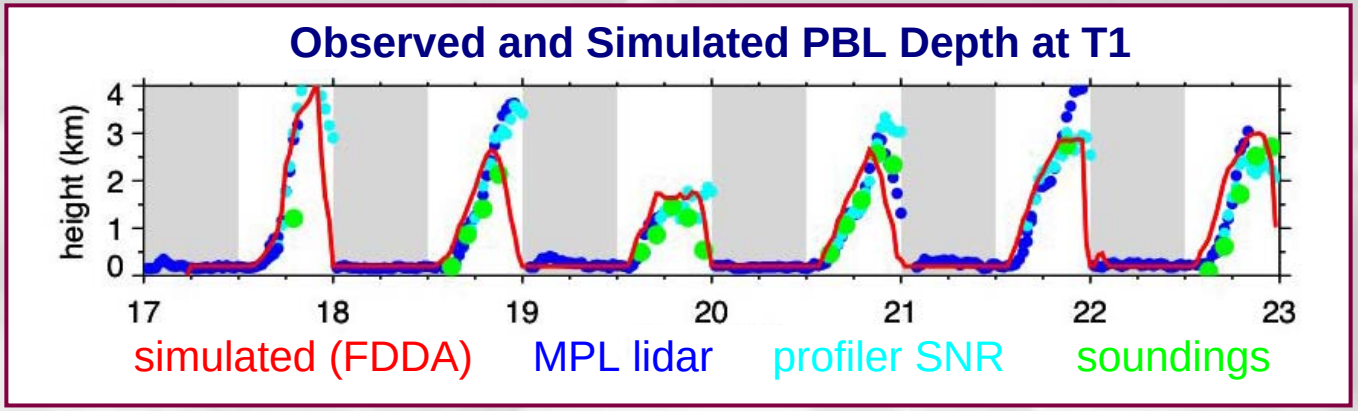
Positive Definite Advection

- Using positive definite advection for scalars reduces concentra-tions of plume-centric species noticeably
- Idealized tests with a point emission shows that the tracer mass in the domain is doubled due to erroneous mass production with “traditional” advection
- pd_chem = 1, pd_moist = 1, pd_scalar = 1





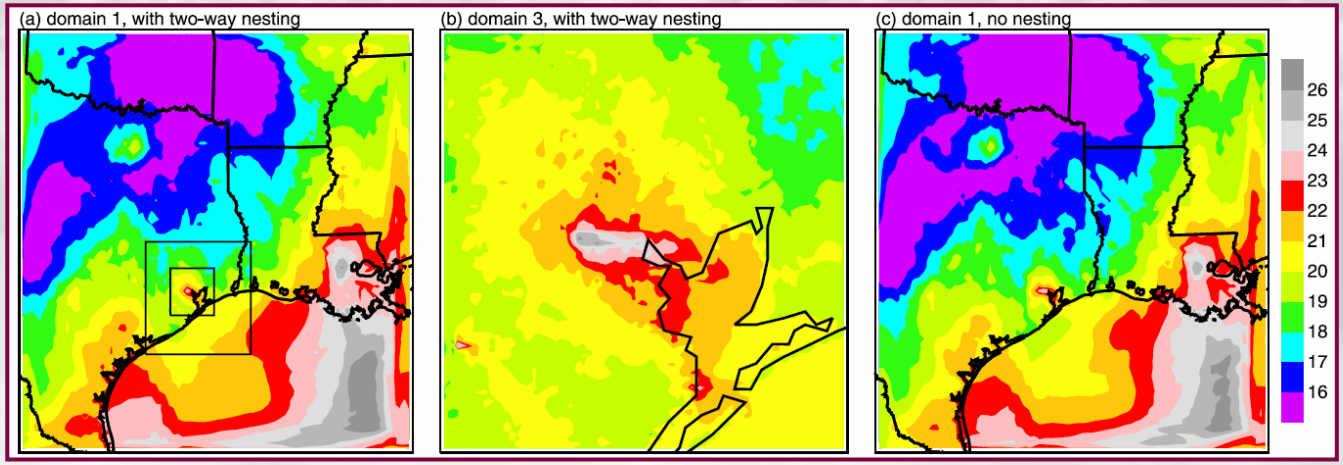
PBL Mixing



- YSU and MYJ PBL schemes both poorly simulate nighttime mixing
  - They typically only mix the bottom model level
  - This results in unrealistically high tracer concentrations at night near the surface
- We added hpblmin to YSU to prevent the PBL from dropping below a specified minimum, typically 150 or 200 m based on observations

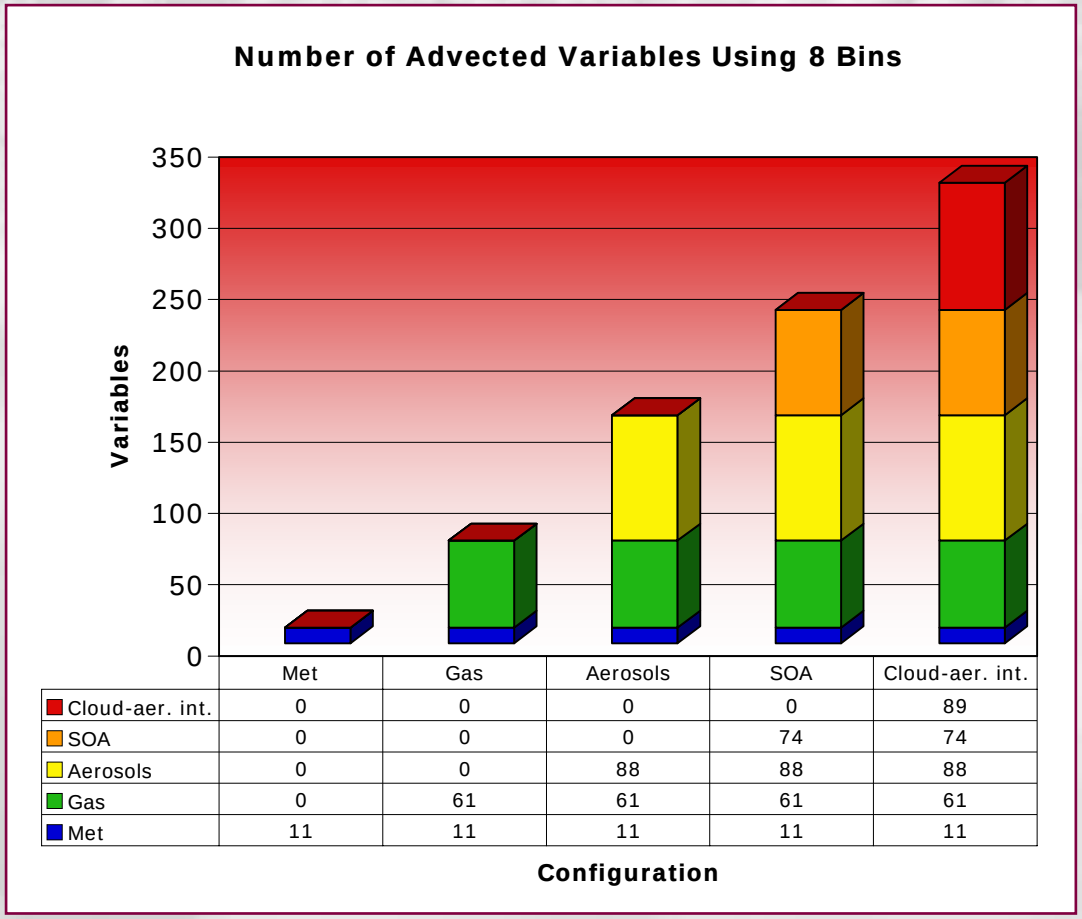
Comparing chem_opt Options

Changes in SW Due to Aerosols in Houston



- Direct effect
  - Run with aer_ra_feedback on vs. off
  - Output clean-sky and dirty-sky from the same run
- Indirect effects
  - Be careful that simulations are comparable
  - Cannot compare a chem_opt=8 w/ a chem_opt=10 run because the autoconversion scheme used in Lin et al. will be different
  - Have to determine a prescribed aerosol scenario to compare with chem_opt=10
  - An approach used with GCMs is to output dirty-cloudy, dirty-clear, clean-cloudy, and clean-cloudy radiation from the same run

Number of Advected Scalars



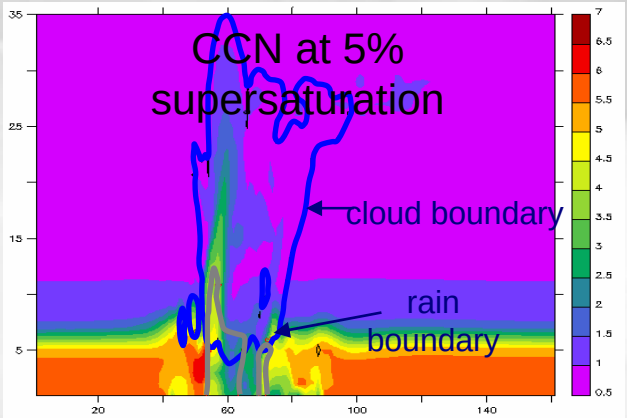
	Met	Gas	Aerosols	SOA	Cloud-aer. int.
Cloud-aer. int.	0	0	0	0	89
SOA	0	0	0	74	74
Aerosols	0	0	88	88	88
Gas	0	61	61	61	61
Met	11	11	11	11	11

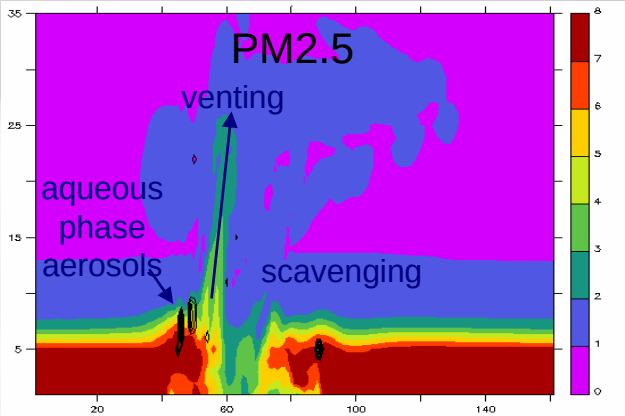
- Added complexity means added cost for advection and memory
- Sectional aerosols increases variables by an order of magnitude
- Adding cloud-phase doubles the number of aerosols
- SOA is on the way

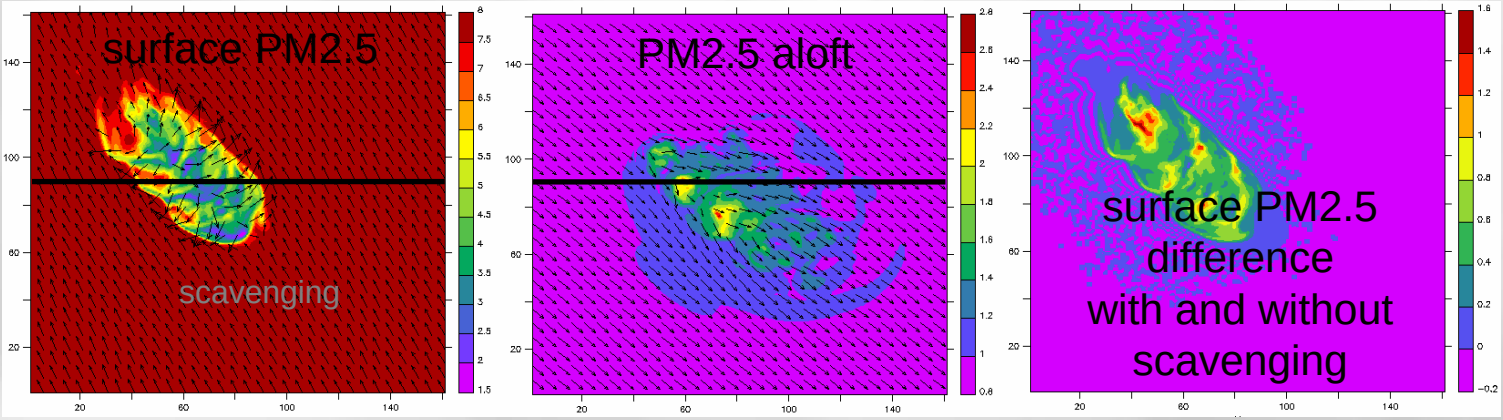
WRF-Chem in Idealized Mode

- If you want vertical mixing, need to add code for initializing the surface and boundary layer schemes

Explicit Convective Cloud Simulation







160 km

Generalized Aerosol Pointer Array

- The problem: As the complexity of the aerosol mechanisms increase, uniquely identifying each aerosol variable within the chem field array becomes cumbersome

- The solution: In addition to the p_XXX pointers established by the registry, add a pointer array that groups the aerosol variables by specific characteristics

massptr_aer(c,s,t,p)

Subset of chem array:

. . .	p_so4_a01	p_so4_a02	p_so4_a03	p_so4_ao4	p_so4_a05	p_so4_a06	p_so4_a07	p_so4_a08	p_so4_cw01	. . .	p_so4_cw08	p_so4_aged01	. . .	p_so4_aged08	p_so4_cwaged01	. . .	p_so4_cwaged08	. . .

Size Distribution Bins (8)

Multiple Phases (16 more for total of 24)

Different Mixtures (24 more for total of 48)

Generalized Aerosol Pointer Array

massptr_aer(c,s,t,p)

- The new pointer array groups aerosols by the following characteristics:
  - Composition, e.g. sulfate, black carbon, inorganic, etc.
  - Size bin, e.g. MOSAIC currently is configured with 8 bins
  - Type, for use with external mixtures, e.g. fresh primary OC/BC, freshly nucleated SO_4, aged BC/OC/SO_4
  - Phase, e.g. interstitial, cloud, ice, rain
- Looping over all species with a given set of characteristics is now simple

Compiling & Then The End!

- CBMZ and MOSAIC are not fully “WRF compliant.” They cannot be used with OpenMP
- With ifort I use “-O2”
  - “-O3” has trouble compiling
  - “-fpe0 -traceback” to force a model crash on floating point error and to get a full traceback to know where the error occurred
- Questions?