Building Atmospheric Composition Modules for UFS: Different Strategies for Development and Coupling with Global and Regional NWP Models

Georg A. Grell, Raffaele Montuoro, Li Zhang, Stuart McKeen,
Dom Heinzeller, Ravan Ahmadov, Mark Govett

Overview

- A little bit of history:
  - Offline, online, inline
  - From barely coupled to much more complex coupling
- The future as we see it:
  - Merging with physics as much as possible and feasible
  - Recoding for exascale computing?

Offline, online, inline

Offline: Chemical Transport Models (CTM's) run independent of NWP models, using hourly or 3-hourly output values for wind and temperature, interpolate to their own grids and times

Online: Couple a CTM to an NWP model through a coupler. Could include CTM's advection, or may use CTM without advection

Inline: No coupler used, everything running in lockstep

Why inline/online? Atmospheric Composition (AC) impacts weather and climate, offline can cause significant errors for air quality forecasting (Grell and Baklanov 2011, Baklanov et al. 2014)

Because of time limits in this talk we will focus on NWP models used for weather forecasting, online/inline approaches also were developed in parallel from the climate community (GFDL: CM3 (Donner et al. 2011), AM4.1 (Zhao et al. 2018, Horowitz et al. 2020)

The beginnings (OAR labs were involved in these approaches unless otherwise stated)

- Early 1-way online coupling
  - Atmospheric composition required significantly more from numerics than your everyday regional weather forecast models (like LFM, MM5,…) in those days
  - Simple way to fix this: Use a complete Chemical Transport Model (CTM) and couple it inline with an NWP model
  - Example would be MM5-Chem (Grell et al. 2000). A coupled version of the Regional Atmospheric Deposition Model (RADM2, used offline for AQ forecasting in Germany) and MM5.
    - Well known and robust RADM chemistry and modal aerosol model
    - Used it's own advection algorithm which was mass conserving, but included the non-hydrostatic equations from MM5
    - Used this model at first at GSL and CSL (back then it was FSL and AL)

Still many inconsistencies with this approach, which would weigh in heavily especially for cloud resolving aqueous phase applications

WRF-CMAQ (Wong et al. 2012) was somewhat similar, but intentionally so

WRF-Chem, the next step up

1-way inline coupling

- Atmospheric composition suite (the “chem_driver”) from MM5-Chem was plugged into WRF (Grell et al. 2005), advection was taken out (WRF numerics was much improved over MM5)
- Physics was somewhat more consistent, still done in atmospheric composition suite, but used the same exchange coefficients passed from the physics as well as mass fluxes and precipitation rates for sub-grid scale transport
- The use of the Kinetic PreProcessor (KPP) quickly replaced the chemical mechanism in the chem_driver, which then allowed many modeling communities to start adding their own chemical mechanisms and aerosol approaches
- DOE/PNNL joined our effort early on, included radiative feedback (complex MIE calculations, a flexible routine with different approximation options, Fast et al. 2006)
- DOE/PNNL also added microphysics interaction processes (Gustafson et al. 2007) to look at cloud aerosol interactions

Improving the community model WRF-Chem

The additional complexities introduced early on were of great importance to make WRF-Chem a very successful community model

- Opening up the possibility to study cloud aerosol interaction processes in great detail with non-hydrostatic cloud resolving or even large eddy simulation approaches
- Making this modeling system much more interesting for many scientists leading to improvements also in the simple schemes
  - NASA's simple GOCART aerosol modules were added in collaboration with Mian Chin, Thomas Diehl, Rainer Schmitz (work was done in Chile)
- NCAR added MOZART mechanisms, coupled them both to GOCART modules (MOZCART) and bin aerosol schemes from the PNNL group

All still using the same chem_driver

WRF-Chem maintained at GSL with **almost no funding**

Further advancing the coupling in WRF-Chem

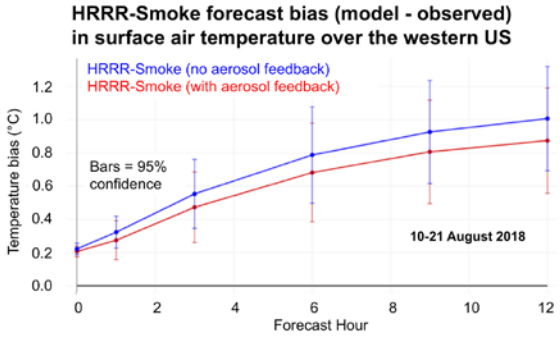
- The chem_driver now has 63 options (!!!) from very simple tracer transport/dispersion applications (1 variable) to very complex chemistry and/or weather interaction processes (several 100)
- Started merging more with the physics
  - Sub-grid scale tracer transport for some turbulent transport schemes
  - Sub-grid scale tracer transport for some convective parameterizations
  - Wet-scavenging for some sub-grid and grid-scale approaches
- Tried using GPU's for the chemical mechanism, but at that point, without major recoding, this was not successful.
- RAP-Chem was run in real-time for air quality forecasting at GSL for many years till May of 2019 – included assimilation of surface PM data

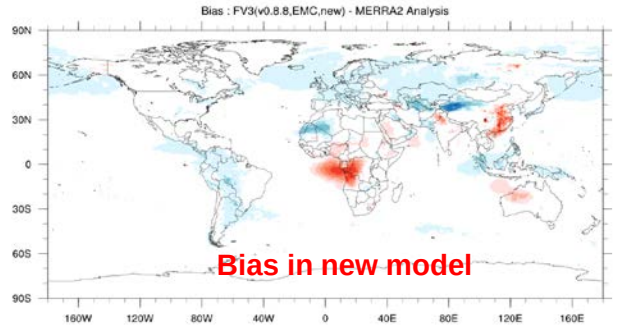
Original publication (Grell et al. 2005) has more than 1400 citations and received the Haagen-Smit prize in 2016, with co-authors from GSL, CSL, and ARL

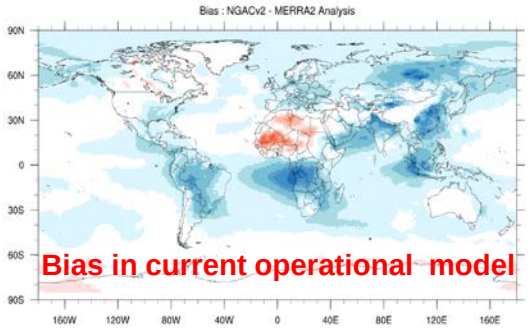
MPAS coupled with CMAQ is another inlined version

Towards operational applications

- Moving the chem_driver to FV3 (as an AC component and as a CCPP component in an inlined approach)
- Next a NUOPC component was created for use with FV3, slated to be operational later in September (GEFS-aerosols) to replace the current NGACv2
- This AC component in FV3 was only tested with GOCART routines, biomass burning and wildfire plumerise, and MIE calculations for aerosol optical properties
- Merging with physics: sub-grid scale transport and sub-grid wet-scavenging is treated in the physics, everything else still in the chem_driver
- Chem_driver is still used inline in RAP-Smoke and HRRR-Smoke – possibly making NWS the first major operational center that includes impact of wildfires on weather prediction and actually improves a world class storm scale prediction system







Three options for coupling: Inline, NUOPC (ESMF approach)，CCPP framework

1. Inline: the old-fashioned way.
   - Might be easiest to start with for us older science guys
   - Once created it is more difficult to move to a different model

2. NUOPC:
   - Much tougher to work with for the older science guys
   - Once created it may be much easier to move to a different modeling system, as long as the modeling system to be moved to has a NUOPC cap - NUOPC provides interoperability for model components among different coupled systems
   - Maybe the only way for alien models (different grids, resolutions,…)

3. CCPP:
   - Most of the older scientists will still find it a little harder to work with, but less so than NUOPC
   - CCPP appears to be the only way to make it easy to use any or all of the chemistry routines inside the physics – for the column modules, the atmosphere becomes more “united”, the reason is that CCPP is used for the physics for every single routine (NASA does that with ESMF)
   - Any routine in the CCPP framework can be mixed and matched with any other routine in the CCPP framework, almost no effort in moving to a different model, or different physics package

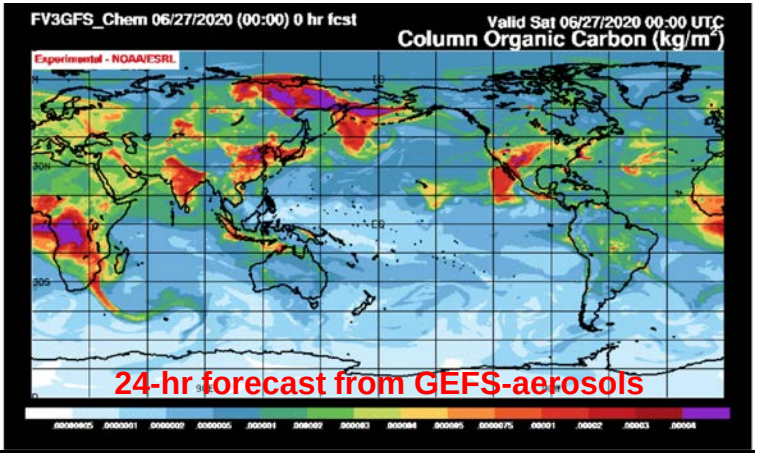
No matter which option to take, the lower level routines should and can be written independent of either approach and/or model

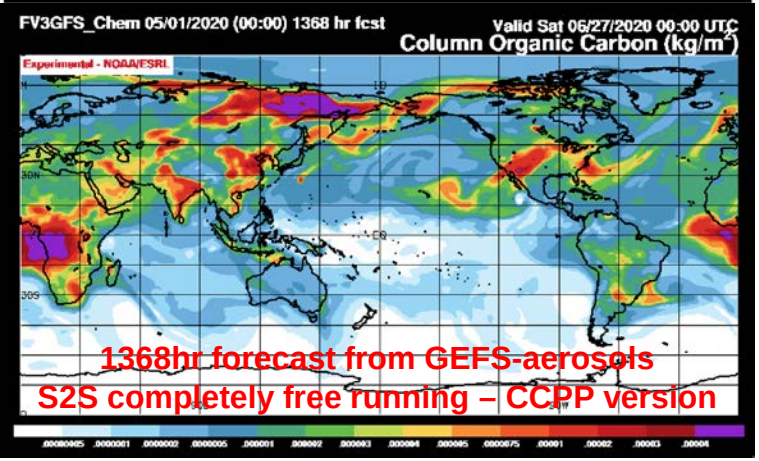
The optimal future as we see it – not everything is clearer than mud yet!

1. We are using CCPP for physics, let's use CCPP for at least some of the chemical modules
   - Lower level routines should be independent of CCPP and/or NUOPC (this is also planned for the shared NASA repository)
   - For our wildfire project: extremely simple routines, and only 2-3 aerosol variables, this is the easiest and fastest and most consistent way to success (it is already working in the global model, will be tested in the regional model)
   - Example of an advantage: The plume rise in CCPP will work for GEFS-aerosols, HRRR-Smoke, and CMAQ if it is used in the physics. No need to reimplement into a complex chemical component.
2. Let's hold onto NUOPC too
   - For complex setups, one of the most expensive routines is the chemical mechanism. This could be split off as a NUOPC component. It is a box approach (not column), massively parallel in all directions, and could be run on a different set of processors
   - If it is separate from all the other chemistry modules it can also easily be mixed and matched (just not inside the physics, since physics uses CCPP)
   - Another aspect may be anthropogenic emissions programs (we are currently discussing this), which can be very complex depending on the application
   - On the other hand biogenic emissions, sea salt, and dust emissions may be different again. Biogenic emission for example may find their most natural place in the Land Surface Model (LSM)

Mix and match, possible having the option of a NUOPC cap on top of CCPP may be the best approach. How about use of GPUs? Could the chemical mechanism be split off with NUOPC, recoded, and effectively use GPUs? What would a machine learning module look like that replaces the chemical mechanism?

One fun slide at the end





Air Quality forecast for today using RAPid refresh (RAP) coupled inline with gas-phase and aerosol chemistry