WRF-GC: an on-line coupling of WRF & GEOS-Chem model structure and preliminary results

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3:15-3:45 Model Clinic 2:
WRF-GC: GEOS-Chem in WRF (Haipeng LIN and Xu FENG, PKU)
Maxwell-Dworkin G115

Atmospheric Chemistry & Climate @ SUSTech
How can GC users benefit from a WRF-GC coupled model?

• Multi-scale meteorology / chemistry interactions

• Flexible grid systems, including nested grids and moving nest grids, at resolutions 100 km to 1 km

• Hindcast and forecast capabilities, driven by NCEP, EC, CESM, FGOALS-g2, etc

• WRF hindcasts can be nudged with observations to mimic assimilated meteorological fields at high resolution

• Atmosphere-land-water-ecosystem studies may be more achievable, because many other models are already coupled to WRF
What about current WRF / WRF-Chem / other model users?

- GEOS-Chem is a state-of-the-science, well-documented, traceable, benchmarked, GCST-supported chemical module for gases and aerosols, backed by a large atmospheric chemistry community

- GEOS-Chem provides a “standard” mechanism that is suitable for most applications, but still customizable

- GC as an abstraction layer can provide consistency when coupled to current and future NCAR models from global to local scales

- Adoption of WRF / WRF-GC by the large meteorology / AQ communities for AQ applications for both research and operation
Development guideline: coupling structure that is easy to use, massively parallel, and ready for the future

- Very specific goal: regional GEOS-Chem simulations with online meteorology

- A coupling structure with minimal changes to either model, such that *either parent model could be updated independently*

  → WRF-GC can stay state-of-the-science

- GEOS-Chem High Performance (GCHP) technology is used, allowing WRF-GC to run in *massively parallel architectures* for high performance

- We further “columnized” GC so that it can operate as a *stateless, grid-independent column model* that can be fully driven by external models, which will also ease the development of future coupling projects with GC

- WRF-GC is free and open-access ([wrf.geos-chem.org](http://wrf.geos-chem.org))
WRF-GC architectural overview

Input and IC/BC

WRF timestep loop

WRF-GC Model v0.1

WRF v3.9.1.1
(EM Core, Distributed Memory)

WRF grid and I/O

Physics

Dynamics
Including advection

WRF-to-chemistry Interface

WRF-GC v0.1 Coupler Component

GEOS-Chem v12.2.1
(Grid-Independent, MPI Enabled)

Deposition

Emissions (HEMCO)

Convection / PBL mixing

Chemistry

GEOS-Chem column interface

In distributed memory

State Conversion Module

State Management Module

Output

Released 2019-01-04
WRF-GC architectural overview

Both WRF and GEOS-Chem codes are off-the-shelf!
No modifications necessary!
Case: Chinese surface PM$_{2.5}$ Jan 21-28, 2015

**GEOS-Chem classic**
0.25° x 0.3125°

**WRF-GC (nudged)**
27 x 27 km

Slope = 1.33
R = 0.75

Slope = 1.20
R = 0.71
Better representation of PBL height Jan 21-28, 2015

PBLH observation data from Guo et al. (2016)

MYNN PBL scheme, nudged with sfc and upper level data
Performance comparison w/ GC-classic (China, 24-h, 32 cores)

Surprisingly, transporting chemicals using archived met data is no longer saving us time!

Coupler is extremely light-weight
Scalability of WRF-GC

- 48-h simulation on Tianhe-1A
- GEOS-Chem Column is perfectly scalable
- Coupler requires inter-processor communication, dependent on domain decomposition
- WRF handles I/O, overhead too high > 150 cores (dependent on domain size)
Future plans and challenges

- Alpha version release (Jan 4, 2019)

- **WRF-GC can already do what GC-classic can do!**

- Nested-grid capability (Haipeng Lin + GCST, on-going)

- Robust one-way coupling (static nested-grids, limited physical options) (Xu Feng, on-going)

- **Beta release with nested-grid capability (Late 2019)**

- Two-way coupling (aerosol feedback based on bulk aerosol mass) by late 2019 (Xu Feng, on-going)
  - Binding for aerosol feedbacks will be in the Coupler. Goal is to develop a more general binding for aerosol mass / size / number / composition to connect to WRF *(may need to involve WRF developers)*

- More complex two-way coupling? Size segregated aerosols with APM and TOMAS?

- Output / analyses: Python tools developed for WRF-GC (just started)

- Compatibility with NCAR model development efforts?
We welcome collaborations

- Research projects using WRF-GC
- Joint effort in model development:
  - Direct and indirect effect of aerosols
  - Chemical mechanisms for high-resolution simulations
  - Representation of small-/meso-scale/boundary layer meteorology
- Atmosphere-land-ecosystem studies may be more achievable
- We are hiring: 1-2 research scientists, 3-4 postdocs, 1 software engineer

Try WRF-GC!
Case: PM$_{2.5}$ during Jan 21-28, 2015

GEOS-Chem classic

0.25° x 0.3125°

Slope = 1.33
R = 0.75

WRF-GC (nudged)

27 x 27 km

Slope = 1.20
R = 0.71
Review of development efforts

• Creating a *chemistry abstraction layer* for the WRF Model

• Isolating the *GEOS-Chem Column Code* from GCHP:
  • Reduced ESMF/MAPL dependencies;
  • Stateless, grid-independent operation fully driven by external model;

• Conversion of meteorology & chemistry variables between WRF and GC

• Creation of a state management module further abstracting WRF and GC data structures into the coupler, allowing for easier development of multi-domain work & coupling of GC with other models

• Accepts IC/BC from previous WRF-GC run outputs and MOZART4-GEOS5 output files using the mozbc tool (BC from CESM-GC in the future?)

• **PBL mixing and vertical convective transport** in GC using meteorological data from WRF
WRF-GC Architectural Overview

- Data structures managed by the state management module and ingested by the respective parent models (WRF, GC) in their native format
- Conversion performed after each timestep loop by the state conversion module
- ESMF not used

- New bindings replace the “chem” part of WRF-Chem, which is isolated from the rest of WRF
- Chemistry output currently in WRF

“One-step” compilation of the coupled models
Comparison w/ GC-classic  (China domain, 24-h, 32 cores)

Surprisingly, transporting chemicals using archived met data is no longer saving us time!

Coupler is extremely light-weight!
Comparison w/ GC-classic, nested China 0.25x0.3125

WRF-GC vs. GC Classic

- **WRF-GC**
  - Emissions: 5087 s
  - Chemistry: 16790 s
  - Transport: 18192.453 s
  - Initialization: 39.162 s

- **GC Classic**
  - Coupler: 2625.358 s
  - GC Column: 2462.525 s
  - Transport: 2768.469 s
  - Chemistry: 3031.891 s
  - Emissions: 2231.594 s
  - I/O: 8192.453 s

**Timers/Cores**

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