Results of Integrating the Models-3 I/O API and SMOKE emissions models into WRF-Chem

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Talk Outline

- Introduction
- WRF-Chem-SMOKE design concept
- Implementation of M3IO and SMOKE: from SMOKE to SMOKE-RT
- Case Study and Results
- Science Implications and Code Status
- Conclusions and Acknowledgments
Introduction

The WRF - Chemistry Model (2.1)

Calls to the chemistry driver are in-lined within the WRF meteorological driver (using the ARW core)

- Multiple choices in “legacy” chemical mechanisms:
  - RADM2, RACM [with or without aerosols (MADE - SORGAM) ], others

- Photolysis is represented by the Madronich model

- Convective transport is accounted for by a generalized Grell approach

- Dry deposition is accounted for (Wesley)

- Does not (yet) contain aqueous chemistry
Introduction

The WRF - Chemistry Model (2.1)

- Emissions Approach
  - Online biogenic emissions:
    - BEIS 3.11 or Guenther
  - All other emissions offline
    - “single representative day” for point, area, and mobile sources combined in one 24 hour file
    - July 15, 2004 used for all applications

Thus, the need for a more state-of-science emissions “module”: SMOKE
WRF-CHEM SMOKE DESIGN
CONCEPT: Coupled Cooperating Models

- Use WRF “external package” facility to put USEPA Models-3 I/O API (“M3IO”) into WRF
  - Fits in with official “layered-model” architecture
  - Use external-package approach to implement additional i/o choice compatible with EPA regulatory and operational models like CMAQ and SMOKE

- Use M3IO Coupling Mode for “cooperating process” WRF-Chem/SMOKE implementation
  - Met part of WRF-Chem provides met data to SMOKE
  - SMOKE provides meteorology-modulated emissions data to chemistry part of WRF-Chem
  - “Just works” for both on-line and off-line modeling
WRF-CHEM SMOKE DESIGN
CONCEPT: Coupled Cooperating Models
SMOKE-WRF-Chem Implementation: M3IO Challenges and Implementation

- Project began with early versions of WRF framework and API:
  - Moving target
  - Little documentation
  - Model-3 API was "more mature:" 10 years of thorough development/testing/use

- M3IO was more than just an external i/o package fully dependent on the WRF API interface: rather, it was a full API in and of itself

- Thus, two API’s had to be “taught” to talk to each other and maintain independent but cooperating “state.”

- After some thrashing, final result is easy to build and include in WRF as IOFORM=9

- Works with either the vanilla WRF, or with WRF-Chem

- For user’s familiar with the PAVE vis tool, files come out in PAVE compatible format!
SMOKE-WRF-Chem Implementation: SMOKE Challenges and Implementation

- Code was tangled, not parallelizable
- Existing regulatory-style programs did not work in coupled modeling systems
  - Not a “time stepped model” within the EPA Models-3 architecture definition
  - Example: made incorrect scenario start, duration assumptions
- Did not support sub-hourly time steps
- Did not easily support multi-inventory merges
- Inadequate computational performance
  - Inefficient algorithms
  - Keep up with operational AQM on hundreds of processors?!

- How resolve?? Turned out to be more involved than first thought
SMOKE-WRF-Chem Implementation: From SMOKE to SMOKE-RT

- **New** LAYPOINT, TMPBEIS, TMPMOBIL, EMISMRG
- Uses rest of (non-met-modulated) SMOKE
- 4x scalar performance improvement
- OpenMP Parallel
- User selectable time step (down to met time step)
- Time-stepped models, for model coupling.
- High performance merge processor
- M3IO-compliant *make* system
- (Optional sub-grid scale terrain parameterization)

MORE DETAILS ON NEXT 4 SLIDES
**Mobile Time-Step Sub-Model**

- Completely new code
  - New driver, UI, computational layers
  - Prototype uses Mobile-5b emissions factors; update to Mobile-6 planned
  - File-compatible with EPA regulatory version
  - Uses $TA$, $TAMAX_{24}$, $TAMIN_{24}$ from WRF meteorology
  - Includes lapse corrections for met-model terrain height error
Biogenics Time-Step Sub-Model

- New implementation of driver, UI code (much simpler task than the other three)
  - Arbitrary user-selected time step
  - Uses $TA$, $QV$, $GSW$ from WRF with lapse corrections for WRF terrain height error
- BEIS3.12 biogenics modeling code
- Can work in either gridded mode or in landuse-tract mode
- Now OpenMP parallel
Plume Rise Time-Step Sub-Model

- New driver, UI layers
  - Arbitrary user-selected time step
  - Does not override user’s run-specifications
  - Uses $TA, QV, P, Z, U, V$ from met model
- Same Briggs-algorithm plume-rise module
- Stack height re-adjustment on basis of sub-grid scale terrain is optional

SMOKE-WRF-Chem Implementation:
- What about SMOKE??
Forecasting a Better Future

SMOKE-WRF-Chem Implementation: What about SMOKE??

Merge Sub-Model

- Single-Stage merge program
  - Supports *multi-inventory merge*
  - Reads and combines *sparse-matrix files* for gridding, speciation, control, future/past projection
  - Optionally reads layer fractions files
  - Reads *time stepped source level* emissions files for area, point, mobile, biogenics, and *plume rise* files
  - Applies matrices, layer fractions, plume rise to emissions, to produce *time stepped model ready emissions for aerosol and chemical species*
  - Open-MP parallel for performance
Late July-early August 2004 featured a modest ozone air quality event over much of the mid- and deep south:

This day chosen for comparison
WRF-Chem Namelist settings were configured as recommended by the WRF-Chem FAQ web-page; aerosols were turned off.

Utilized standard WRF-Chem 27km “real-time” domain in use at FSL.

Meteorological initial and boundary conditions were supplied by the WRF SI.

WRF-Chem was cold started on July 28 using background chemical profiles.

WRF-Chem was spun-up for five days using “vanilla” emissions only.

Spin-up was accomplished by self-cycling with the WRF-Chem version of “real.exe” after fixing an internal time stamp problem.
Forecasting a Better Future

CASE Study and Results

Example “initial condition” SO2 concentrations after 5 day spin-up showing identical IC’s for SMOKE and “vanilla” runs

WRF-SMOKE

WRF-Vanilla

Integrating M3IO and SMOKE-RT into WRF-Chem: 8th WRF User’s Workshop, June, 2007
WRF-Chem Results for Aug 2, 2004:
- SO2
- SULF
- NO2
- ISO
- PAN
- O3

WRF-Chem initialized at 00z, run for 24 hours with “vanilla” emissions; then same period again with “SMOKE” emissions
CASE Study and Results: SO2 at 18z

WRF-SMOKE

WRF-Vanilla

Integrating M3IO and SMOKE-RT into WRF-Chem: 8th WRF User's Workshop, June, 2007
CASE Study and Results:
SO2:

* difference field at 18z (left);
* difference time series for Ohio Valley (right)
CASE Study and Results:
Sulfate at 18z

WRF-SMOKE                       WRF-Vanilla

Integrating M3IO and SMOKE-RT into WRF-Chem: 8th WRF User’s Workshop, June, 2007
CASE Study and Results: Sulfate (SMOKE) minus Sulfate (VANILLA) at 18z

Layer 1 SULFb−SULFa

August 2, 2004 18:00:00
Min= -0.001 at (84,74), Max= 0.002 at (72,58)

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CASE Study and Results:
NO2 at 18z

Layer 1 NO2b

Layer 1 NO2a

WRF-SMOKE

WRF-Vanilla

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CASE Study and Results:

NO2:

* difference field at 18z (left);
* difference time series for Houston metro (right)
CASE Study and Results: Isoprene at “24z”

Layer 1 ISOb

Layer 1 ISOa

WRF-SMOKE

WRF-Vanilla
CASE Study and Results: Isoprene Difference Field after 24 hours (left): Isoprene (SMOKE) minus Isoprene (VANILLA); Difference time series (right)
CASE Study and Results: PAN at 18z

WRF-SMOKE

WRF-Vanilla
CASE Study and Results: PAN difference field (SMOKE minus VANILLA) at 18z
CASE Study and Results: O3 at 18z

WRF-SMOKE vs WRF-Vanilla

Integrating M3IO and SMOKE-RT into WRF-Chem: 8th WRF User’s Workshop, June, 2007
CASE Study and Results: O3 difference field at 18z

Layer 1 O3b–O3a

August 2, 2004 18:00:00
Min = -0.085 at (64, 69), Max = 0.052 at (99, 53)
CASE Study and Results: Regional O3 Difference fields at 18z

Integrating M3IO and SMOKE-RT into WRF-Chem: 8th WRF User's Workshop, June, 2007
CASE Study and Results: Regional O3 Difference fields at 18z [DFW and Ohio Valley]
CASE Study and Results: Regional O3 Difference fields at 18z [Houston]
CASE Study and Results: Regional O3 Difference Time Series near DFW: note difference of nearly 20PPB
Results of a 24-hour sensitivity run show modest-to-very-significant differences in all key primary and secondary species without aerosol consideration.

Results may have profound implications for the performance of WRF-Chem for both real-time forecast and case-study simulations in the future.
Code has been provided to Georg Grell/Steven Peckham for inclusion in WRF Repository:

- the community will be interested, at least, in the science upgrades that integration with SMOKE-RT provides.
- Further, this should be consistent with a wide-range of community work going on w/in the WRF-Chem working group and beyond, including the following activities:
  - High order positive definite advection
  - PBL schemes
  - Chemical mechanisms and solvers: gas, aerosol, aqueous
  - Interactions between chemistry and microphysics, clouds, radiation
  - Wet and Dry Deposition
  - Profiling and optimization
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