

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

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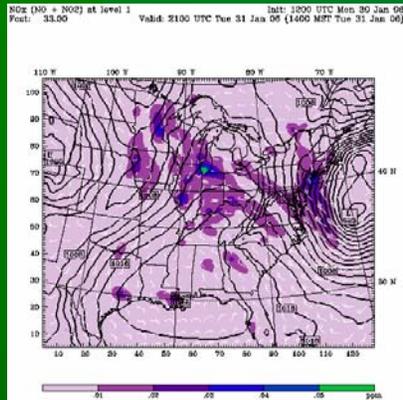
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Talk Outline

- 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

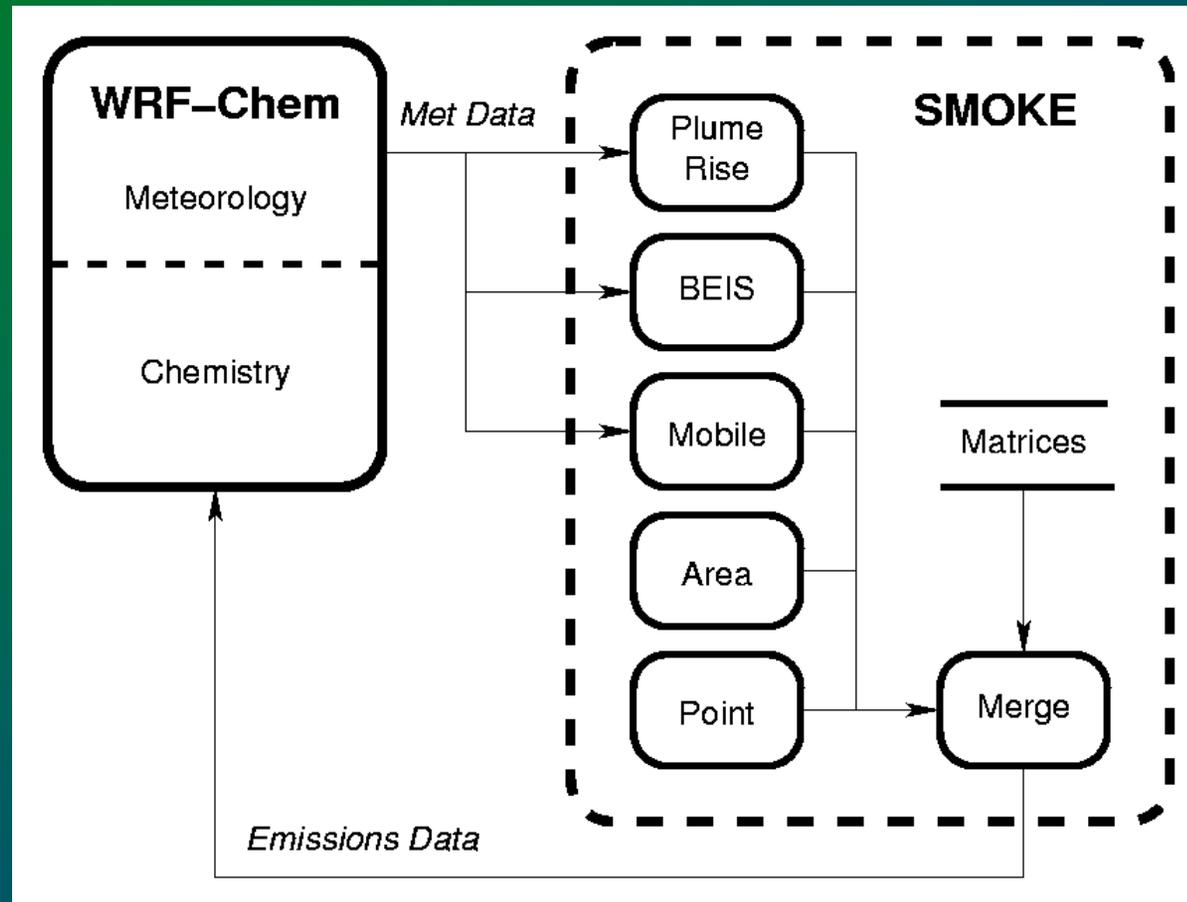
Thus, the need for a more state-of-science emissions “module”: SMOKE

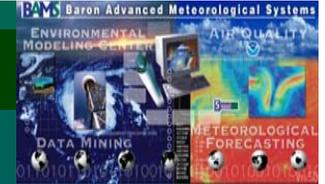


**WRF-CHEM SMOKE DESIGN
CONCEPT: Coupled
Cooperating Models**

- 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**





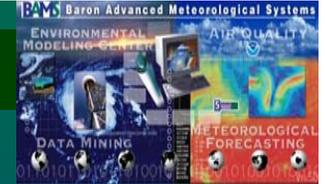
SMOKE-WRF-Chem Implementation: M3IO Challenges and Implementation

- Project began w/ 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**

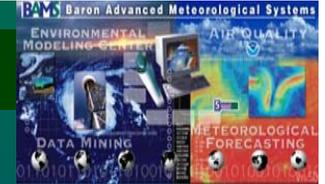
- **Code was tangled, not parallelizable**
- **Existing regulatory-style programs did not work in coupled modeling systems**
 - Not a “time stepped model” within the EPA Models-3 architecture definition
 - Example: made incorrect scenario start, duration assumptions
- **Did not support sub-hourly time 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



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

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

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

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**

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

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**



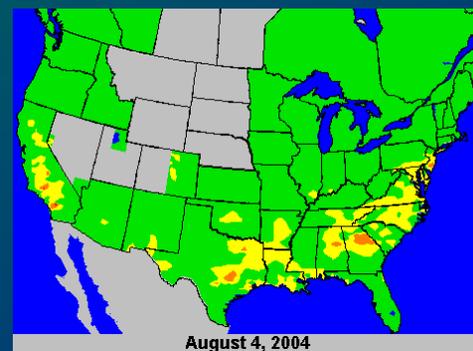
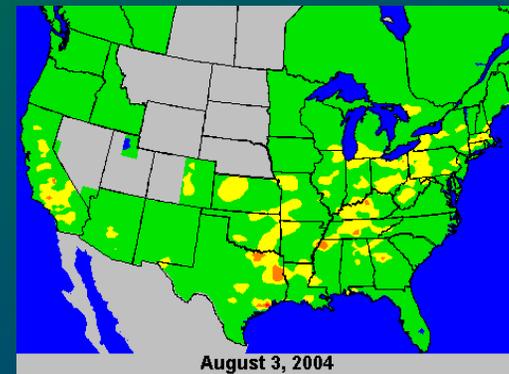
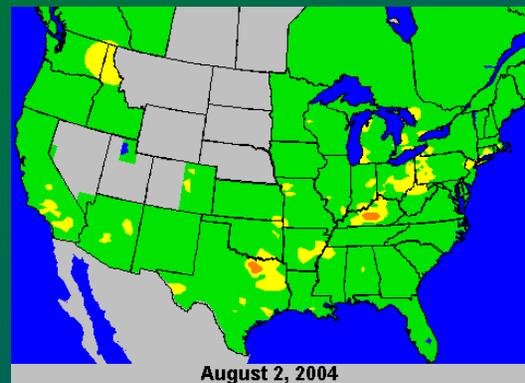
SMOKE-WRF-Chem Implementation: What about SMOKE??

Merge Sub-Model

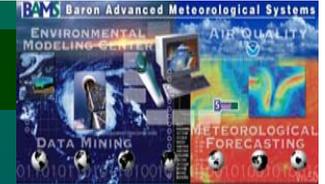
- **Single-Stage merge program**
 - Supports *multi-inventory merge*
 - Reads and combines *sparse-matrix files* for gridding, speciation, control, future/past projection
 - Optionally reads layer fractions files
 - Reads *time stepped source level* emissions files for area, point, mobile, biogenics, 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

CASE Study and Results

- Late July-early August 2004 featured a modest ozone air quality event over much of the mid- and deep south:

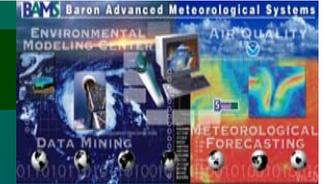


This day chosen for comparison



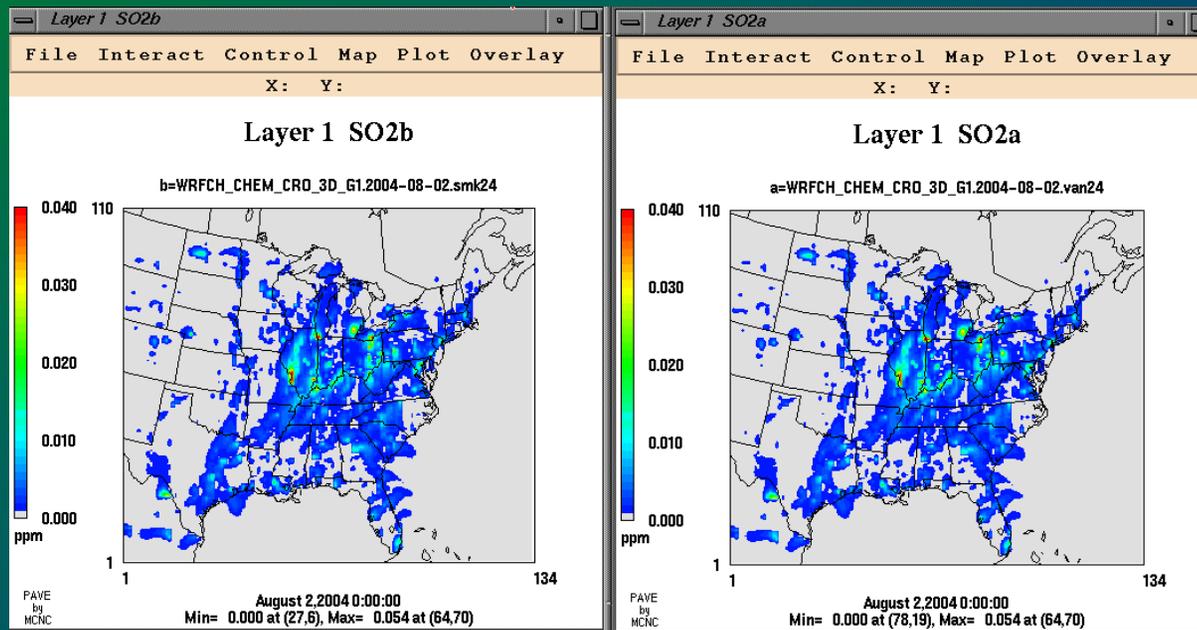
CASE Study and Results

- 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



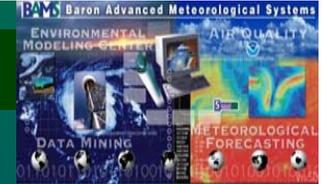
CASE Study and Results

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



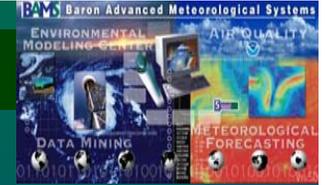
WRF-SMOKE

WRF-Vanilla

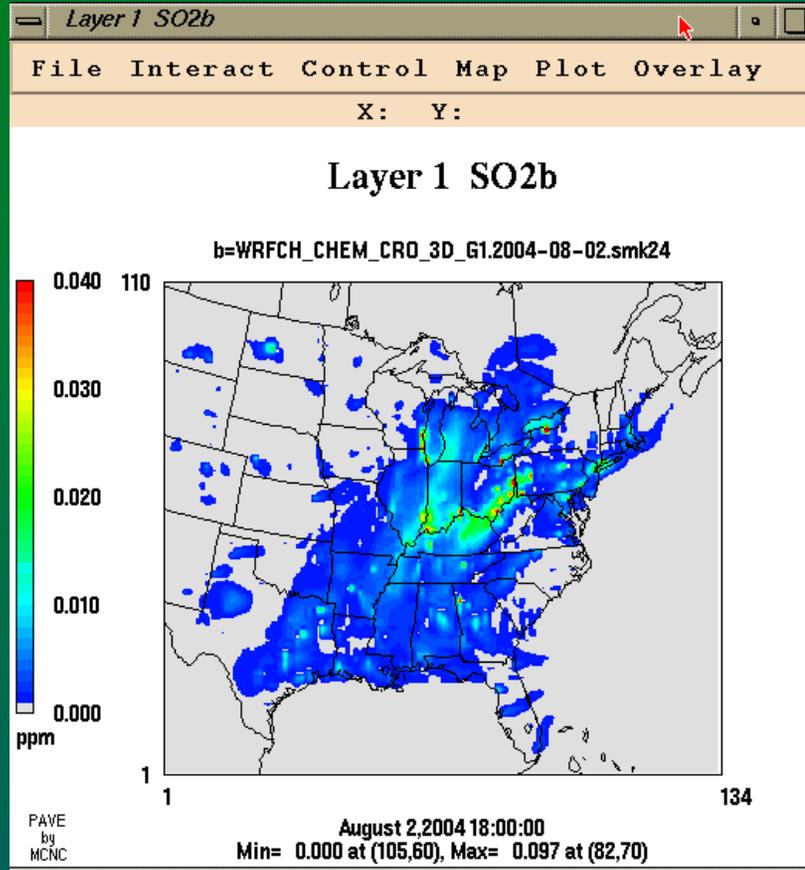


CASE Study and Results

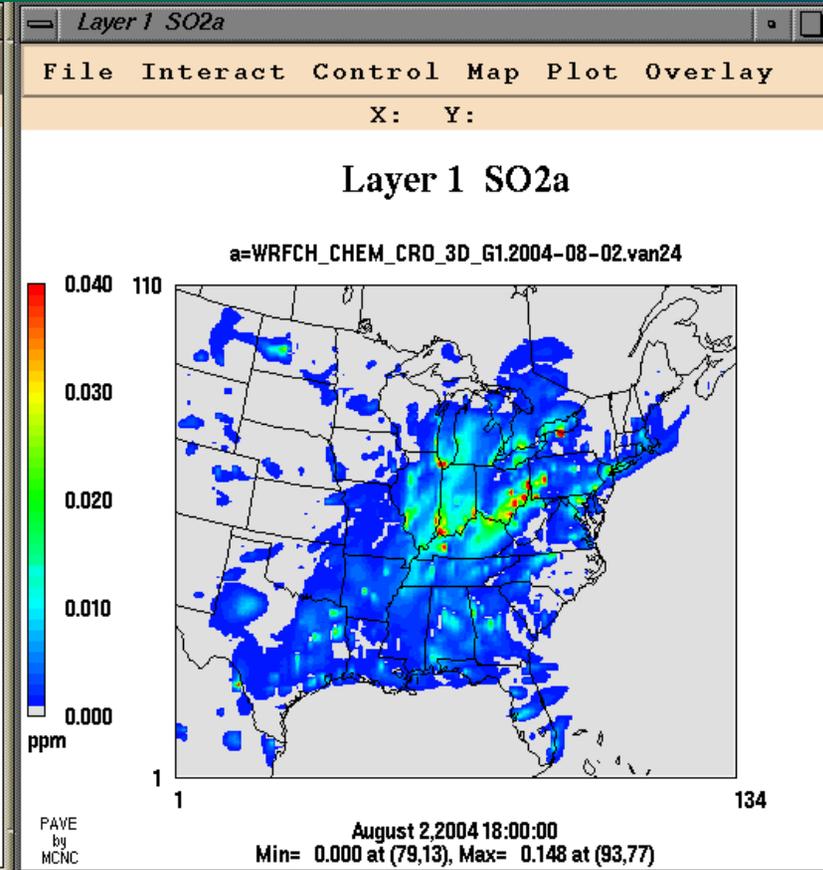
- **WRF-Chem Results for Aug 2, 2004:**
 - SO₂
 - SULF
 - NO₂
 - ISO
 - PAN
 - O₃
- **WRF-Chem initialized at 00z, run for 24 hours with “vanilla” emissions; then same period again with “SMOKE” emissions**



**CASE Study and Results:
SO₂ at 18z**

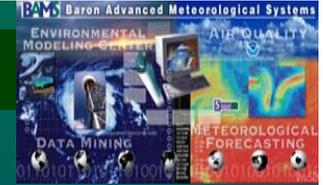


WRF-SMOKE



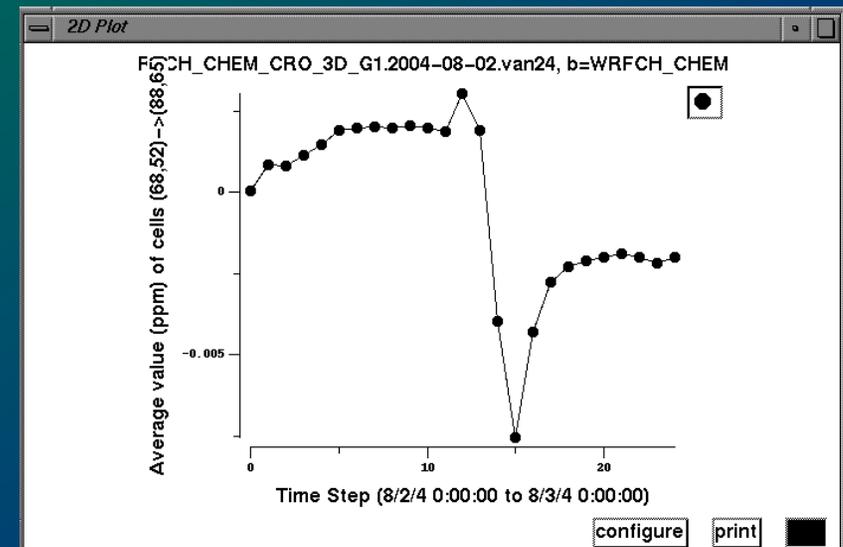
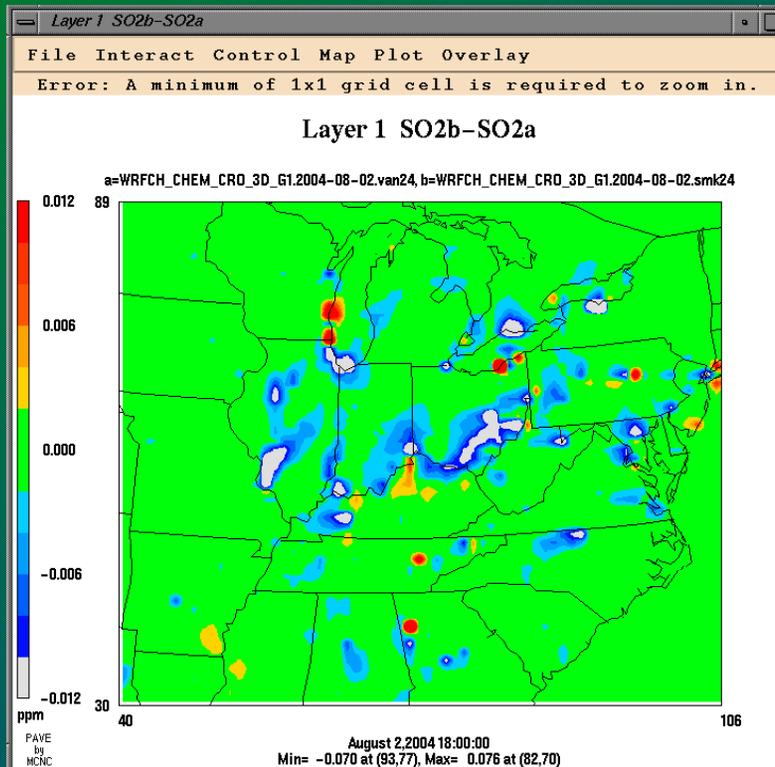
WRF-Vanilla

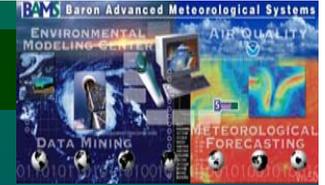
Forecasting a Better Future



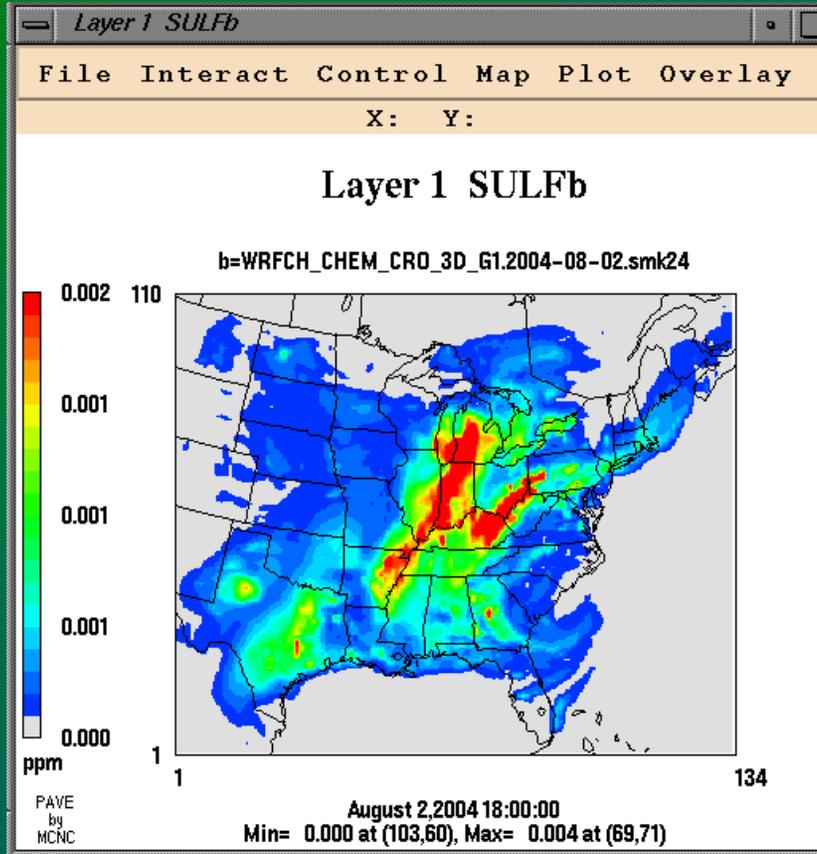
CASE Study and Results: SO₂:

- *difference field at 18z (left);
- *difference time series for Ohio Valley (right)

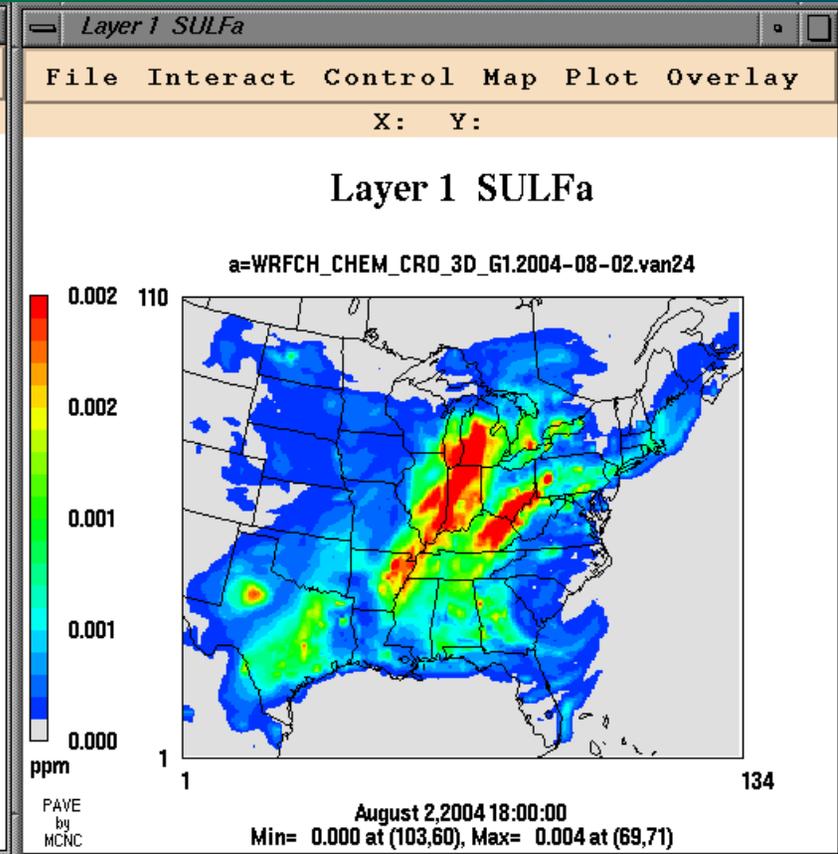




**CASE Study and Results:
Sulfate at 18z**

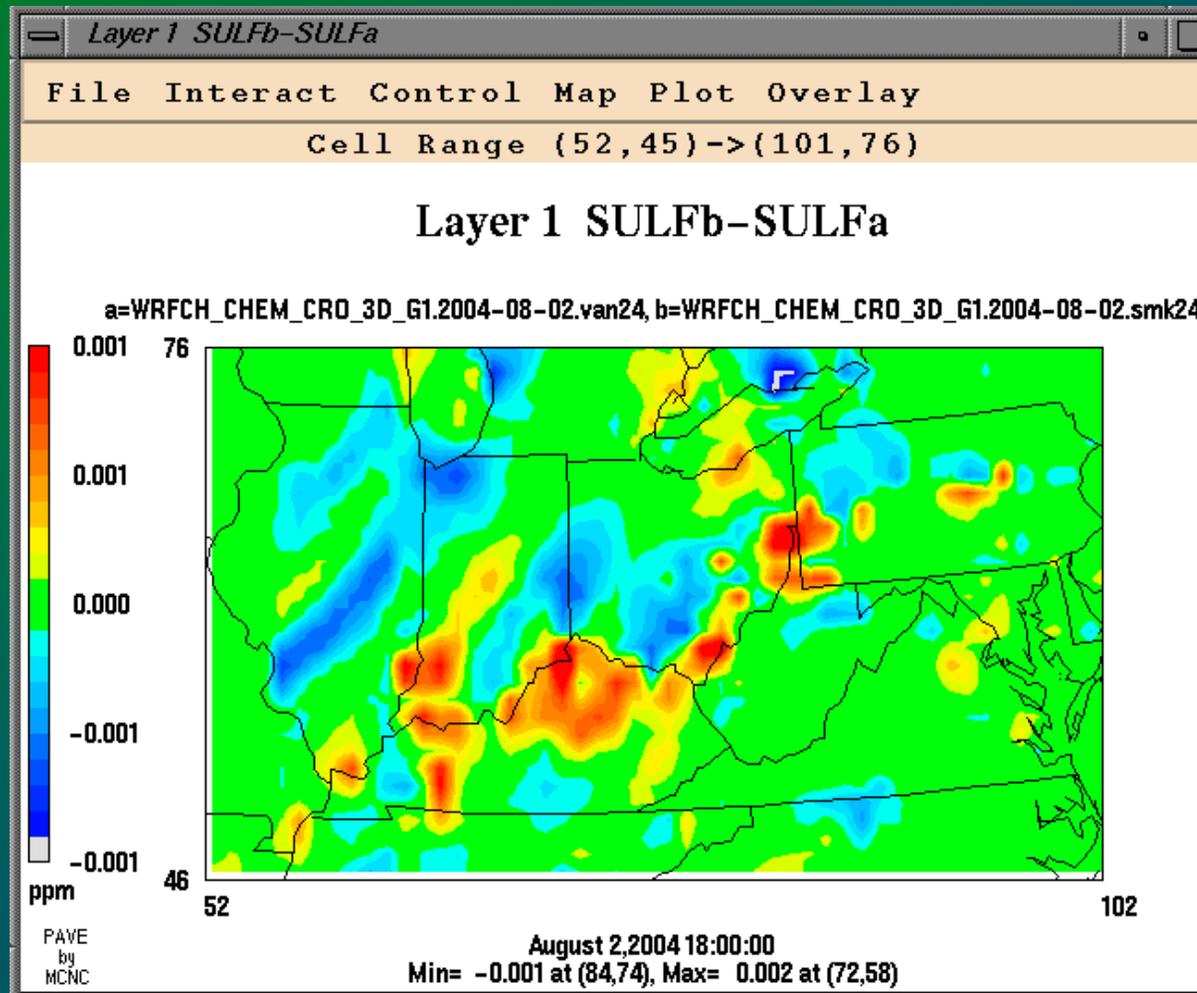


WRF-SMOKE



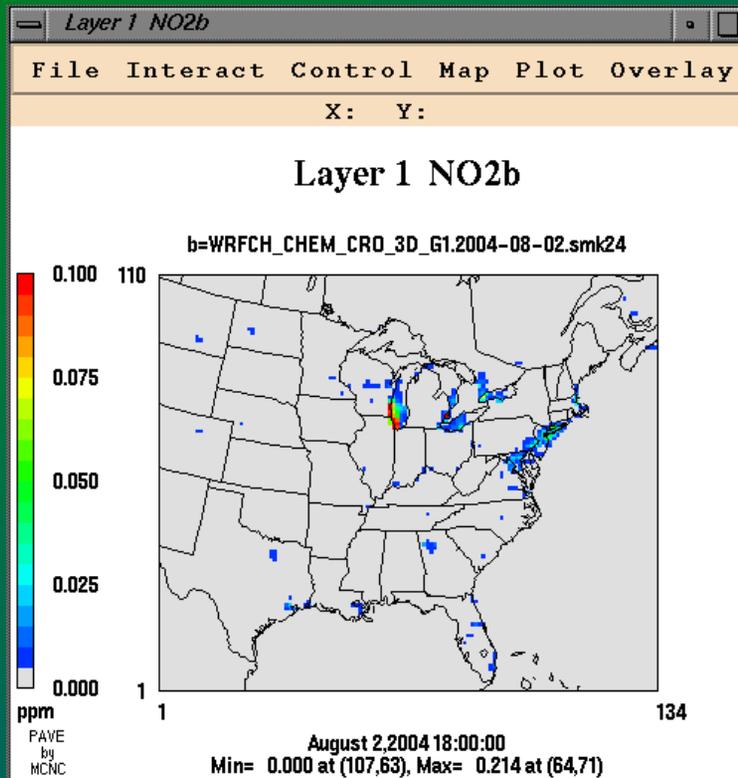
WRF-Vanilla

**CASE Study and Results:
Sulfate (SMOKE) minus
Sulfate (VANILLA) at 18z**

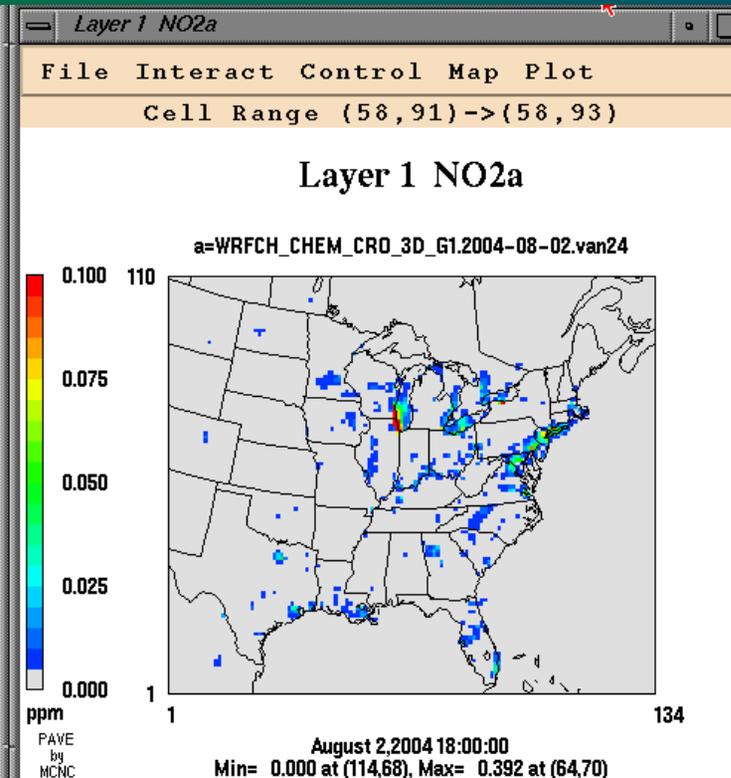




**CASE Study and Results:
NO₂ at 18z**



WRF-SMOKE

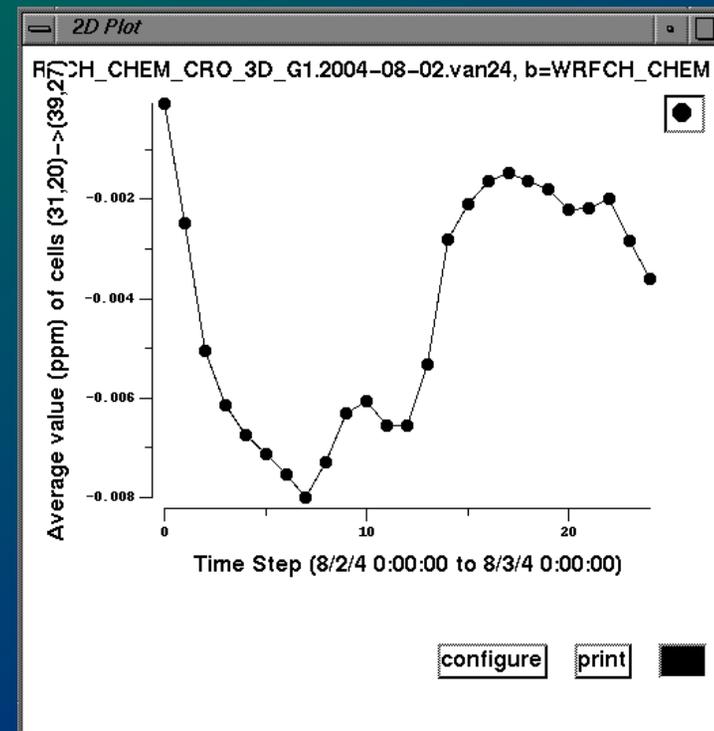
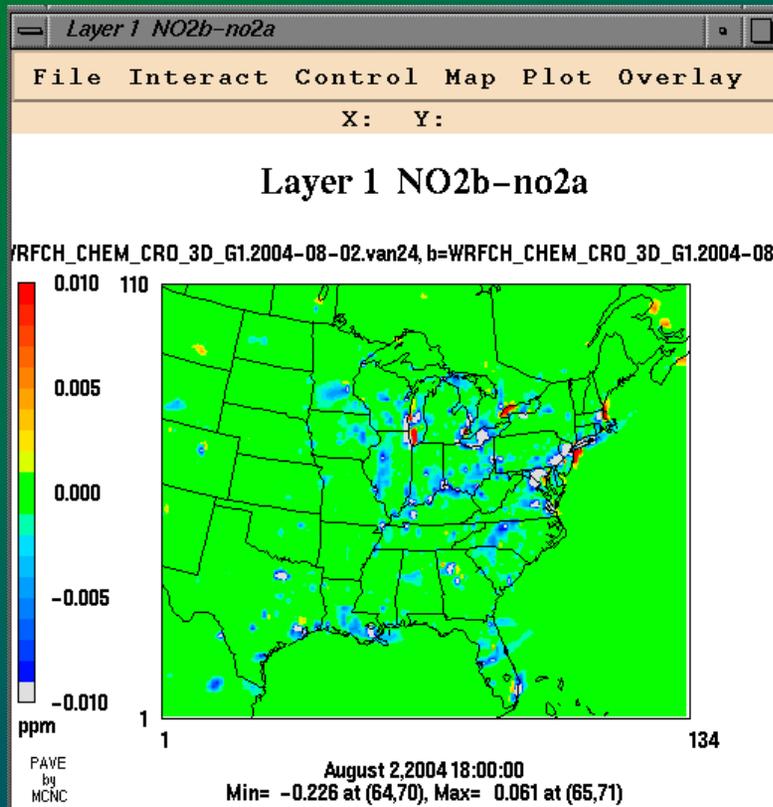


WRF-Vanilla



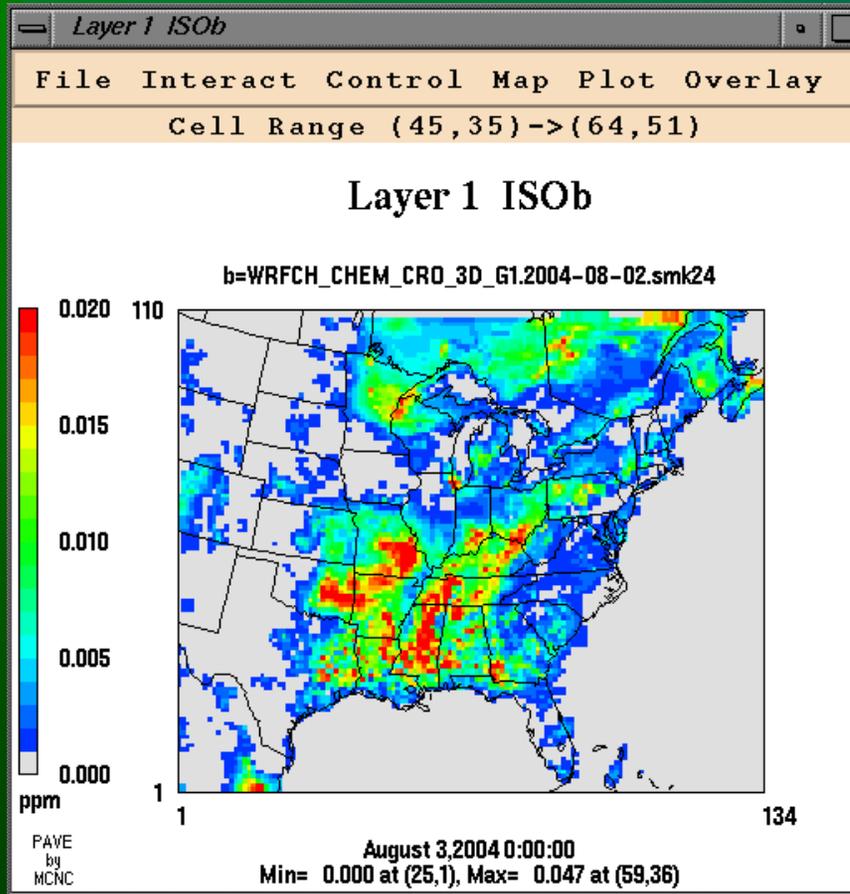
CASE Study and Results: NO₂:

- *difference field at 18z (left);
- *difference time series for Houston metro (right)

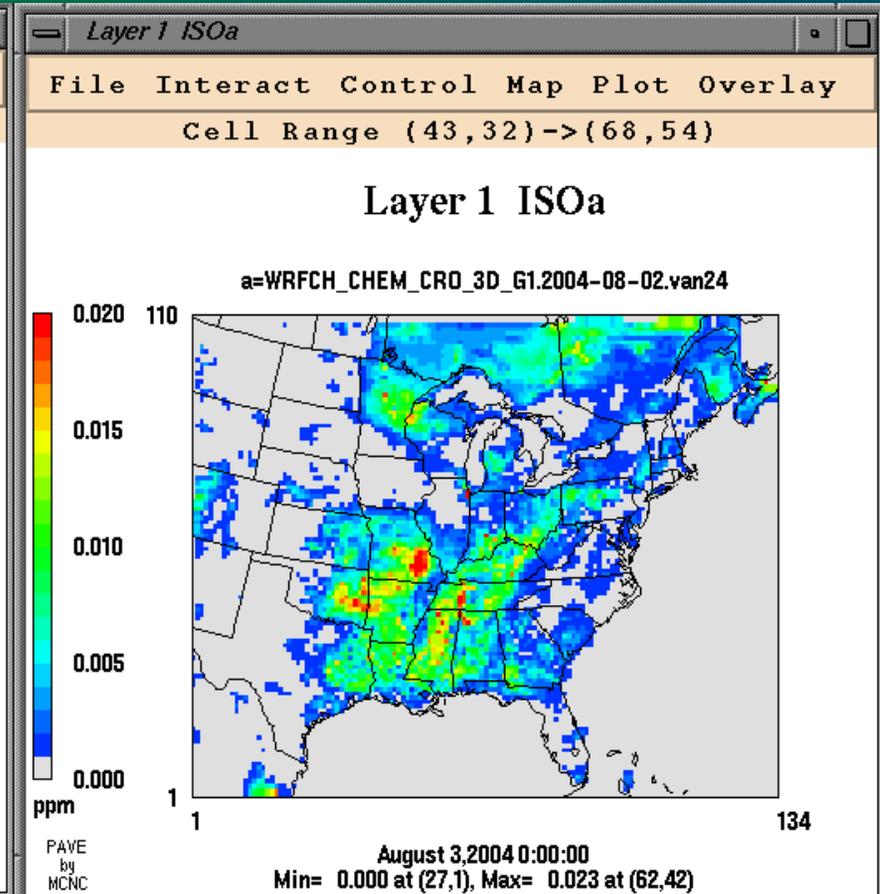




**CASE Study and Results:
Isoprene at "24z"**



WRF-SMOKE

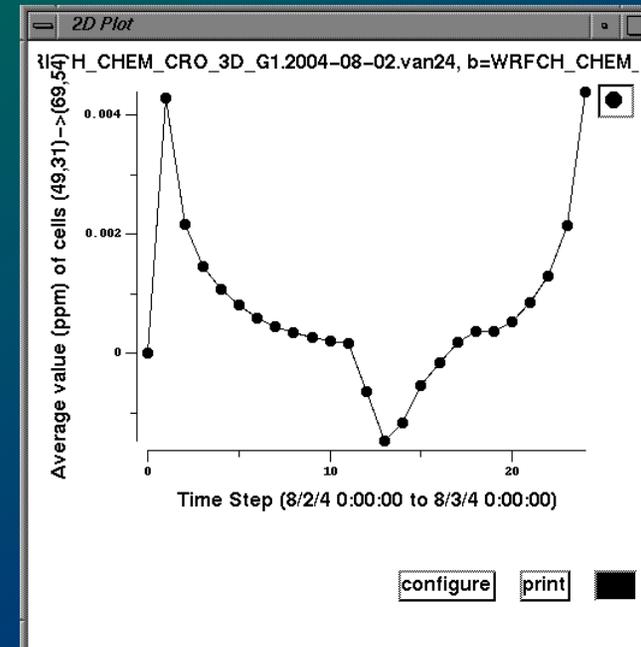
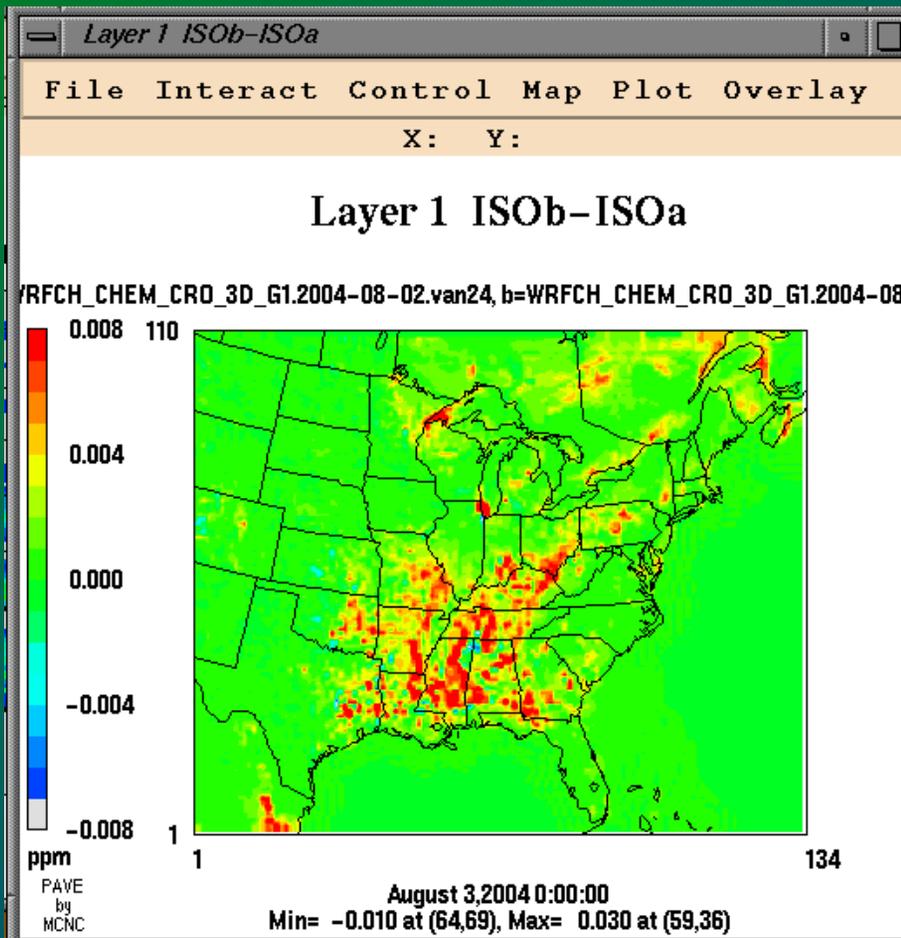


WRF-Vanilla

Forecasting a Better Future

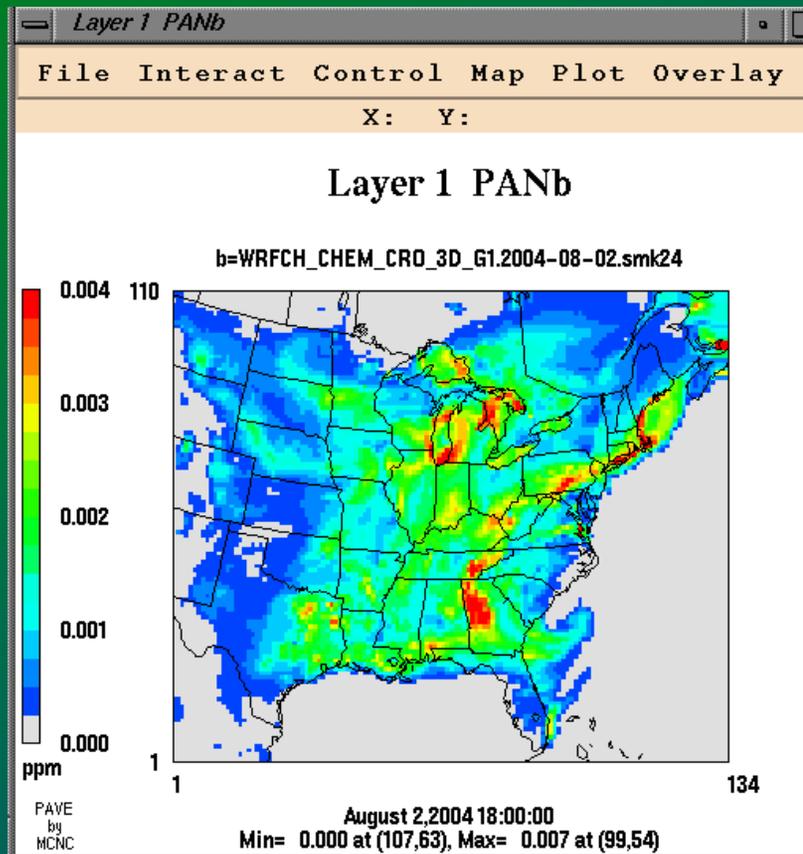


**CASE Study and Results: Isoprene
Difference Field after 24 hours (left):
Isoprene (SMOKE) minus
Isoprene (VANILLA);
Difference time series (right)**

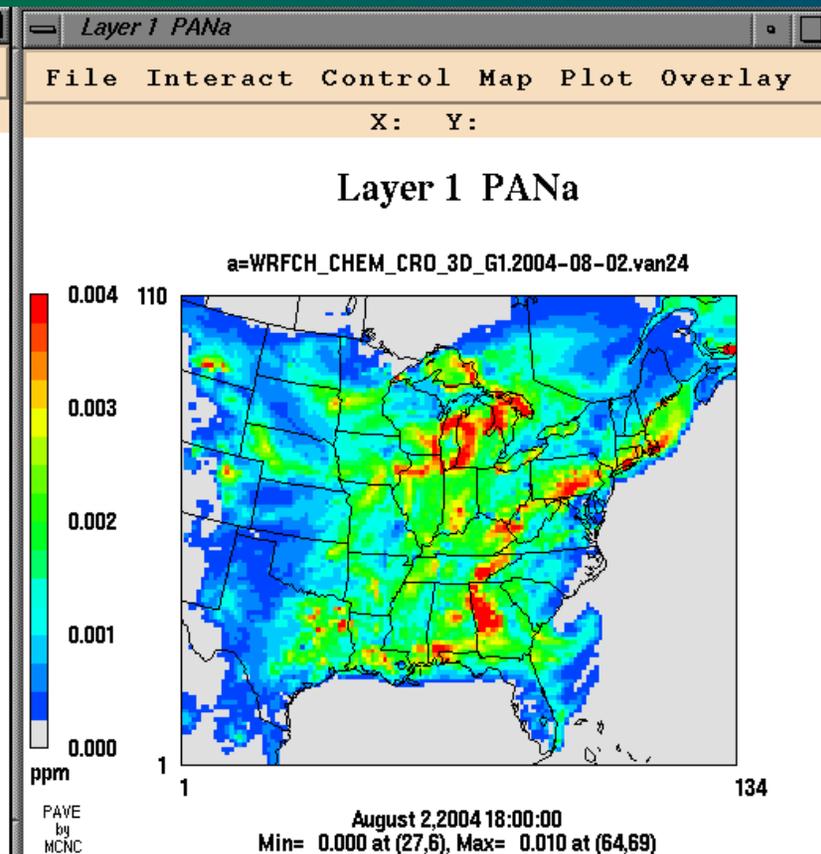




CASE Study and Results: PAN at 18z

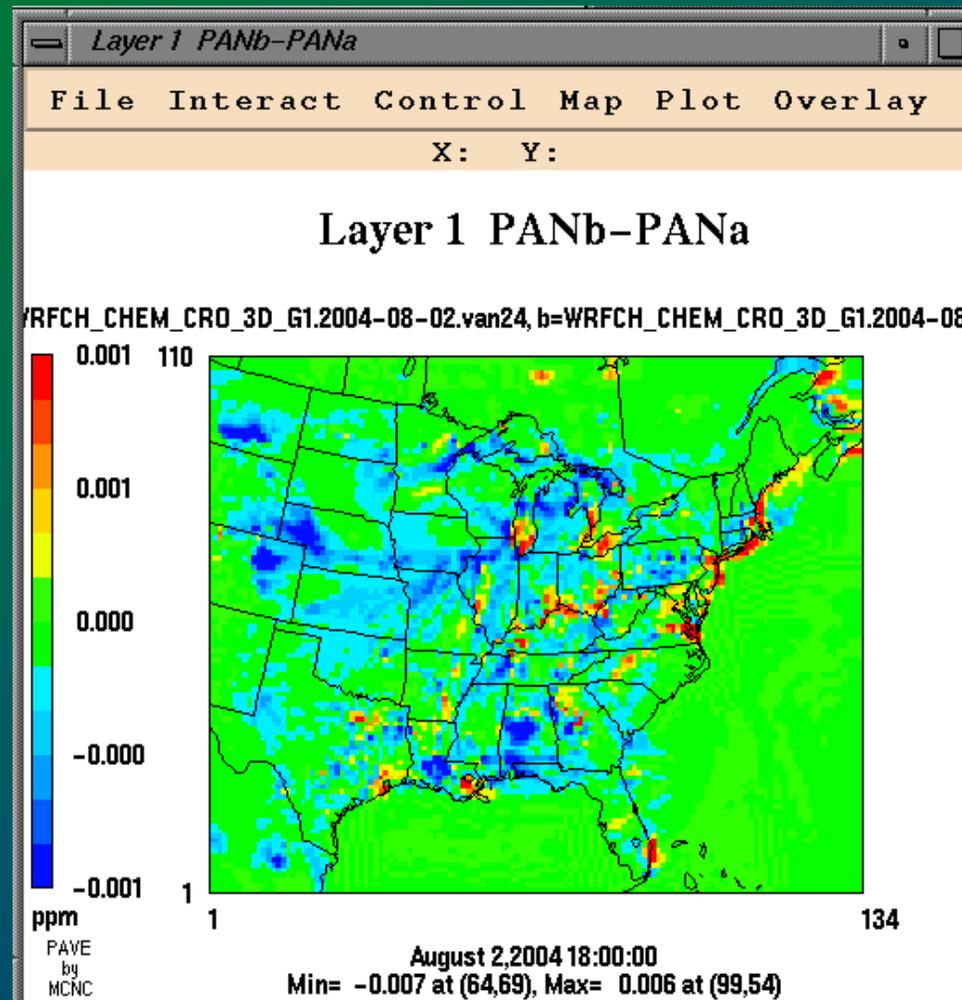


WRF-SMOKE

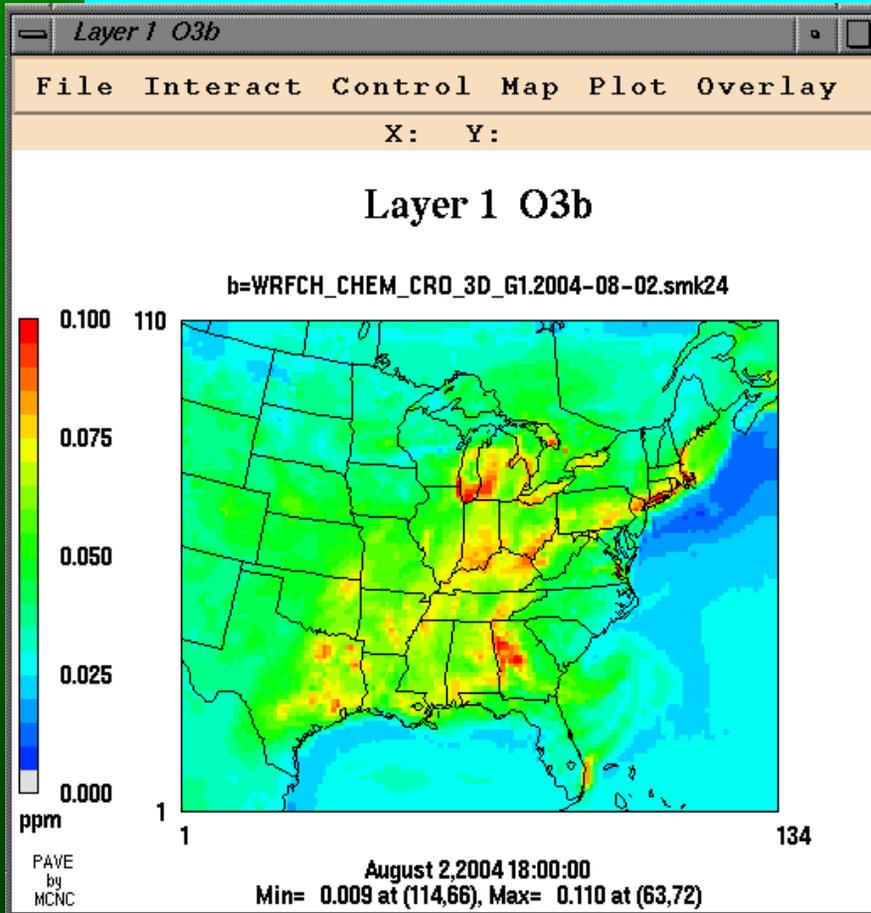


WRF-Vanilla

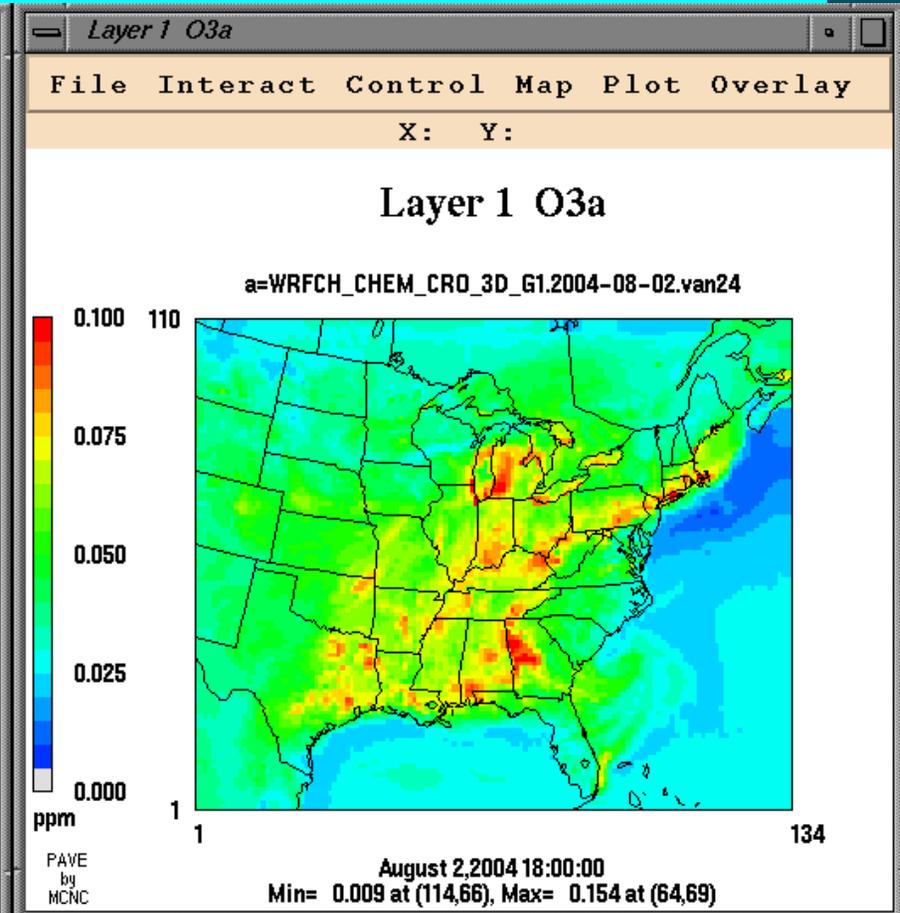
CASE Study and Results: PAN difference field (SMOKE minus VANILLA) at 18z



CASE Study and Results:O3 at 18z



WRF-SMOKE

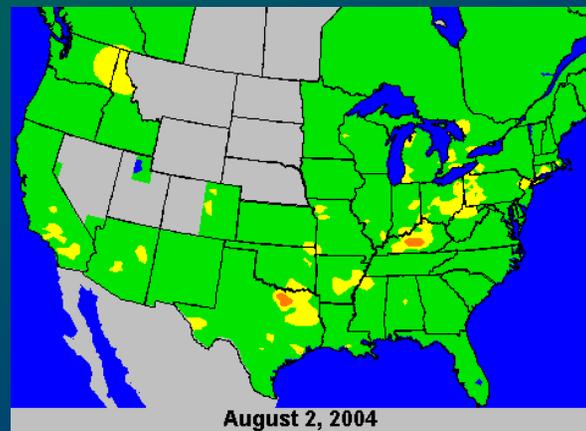
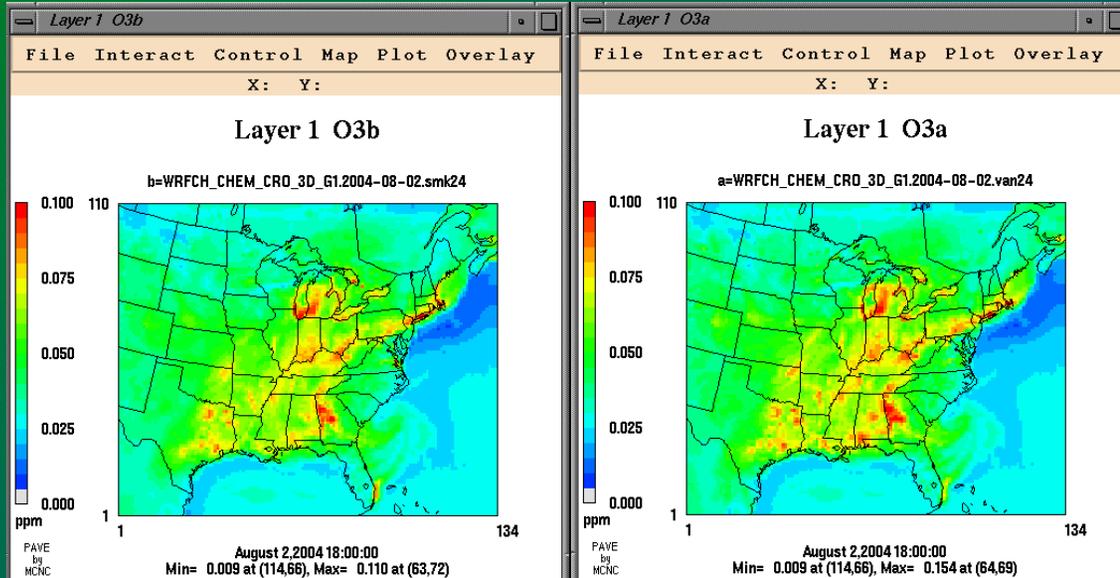


WRF-Vanilla

CASE Study and Results:O3 at 18z

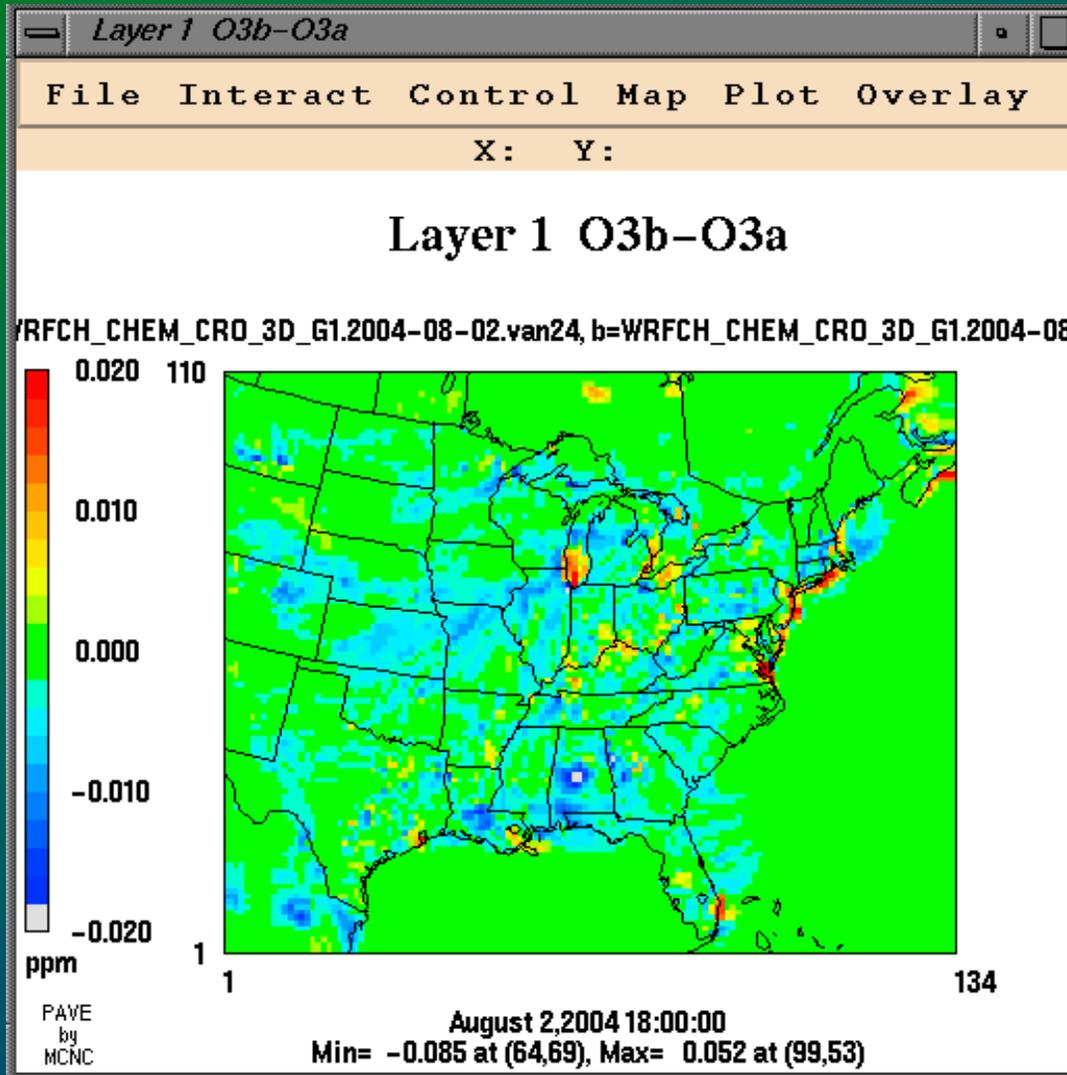
WRF-SMOKE

WRF-Vanilla



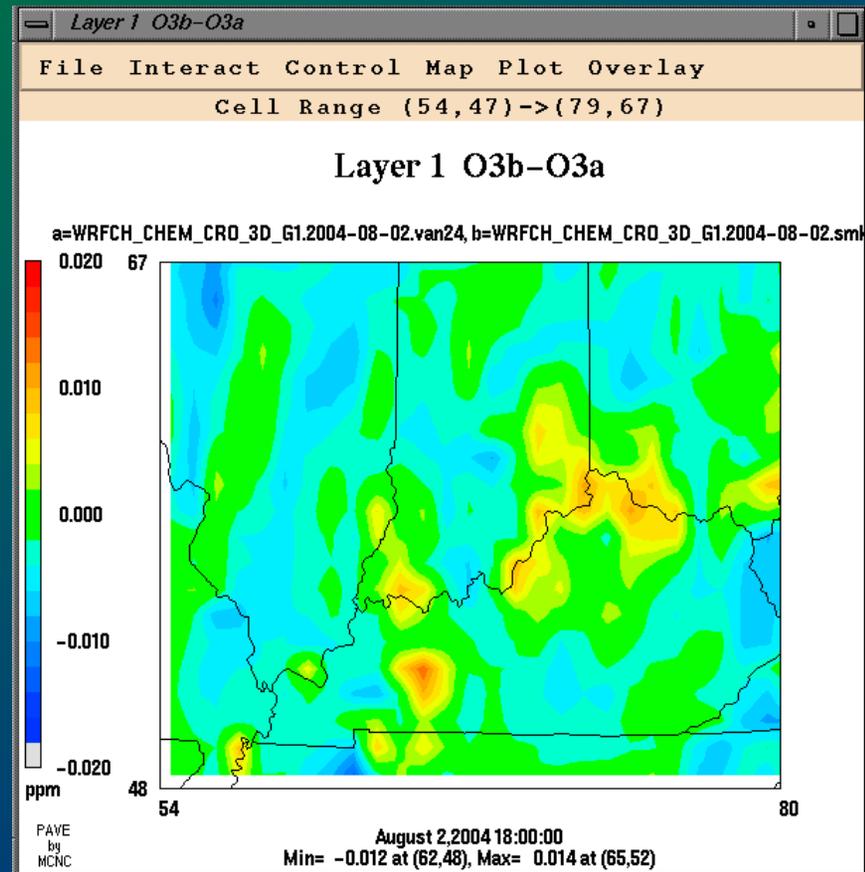
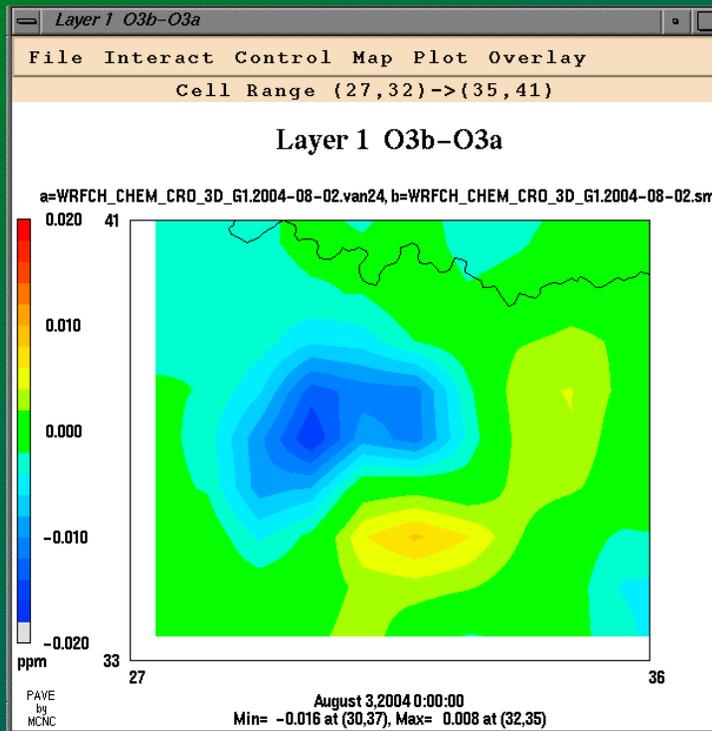


CASE Study and Results:O3 difference field at 18z



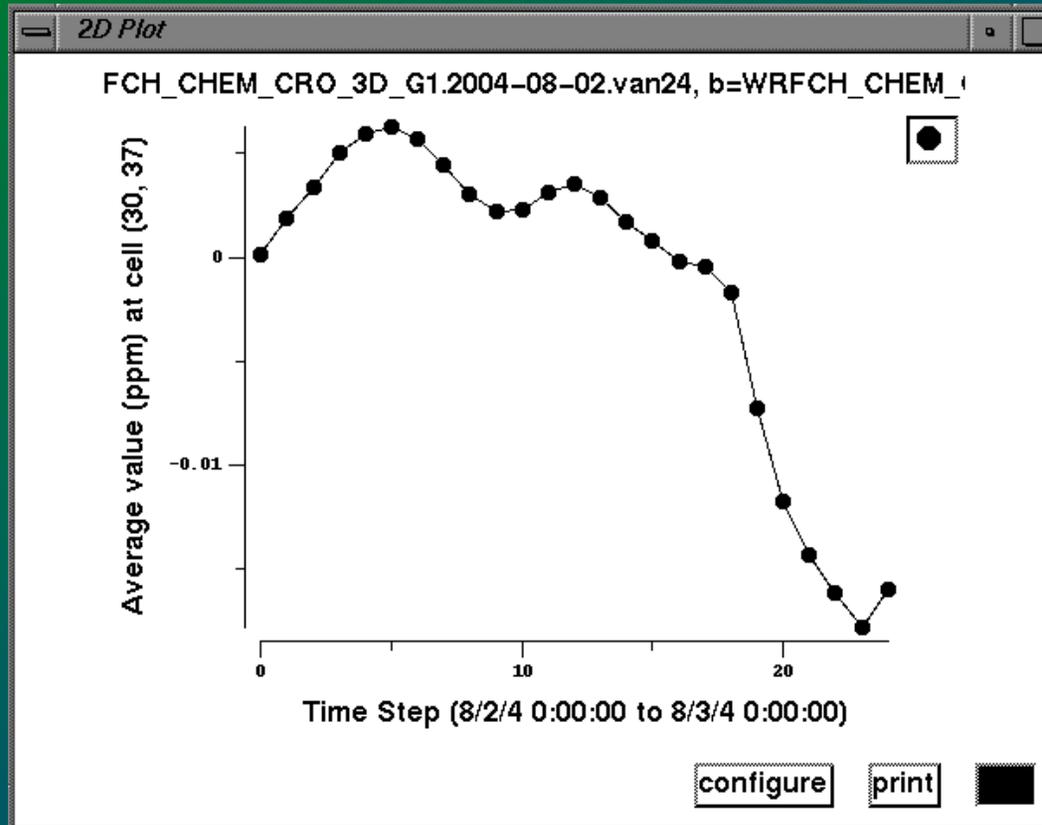


CASE Study and Results: Regional O3 Difference fields at 18z [DFW and Ohio Valley]





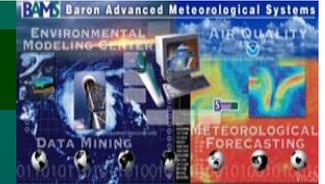
**CASE Study and Results: Regional O3
Difference Time Series near DFW: note
difference of nearly 20PPB**





Case Study Scientific Conclusions

- Results of a 24hour 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***



STATUS

- **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



Acknowledgements

- **Ken Schere of NOAA's Atmospheric Sciences Modeling Division (RTP, NC) for sponsoring this work; and his staff for many useful interactions**
- **Georg Grell and Steven Peckham of the Forecast Systems Lab for many useful discussions regarding WRF-Chem; and help where needed.**
- **John Michelakes of NCAR's MMM division for discussions regarding the WRF software architecture**
- **Nelson Seaman for many useful and engaging discussions concerning the WRF and WRF architecture**



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