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

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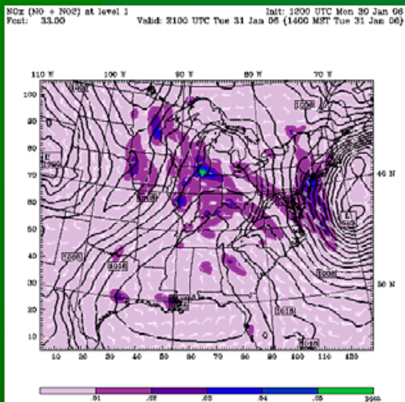
Talk Outline

- 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)

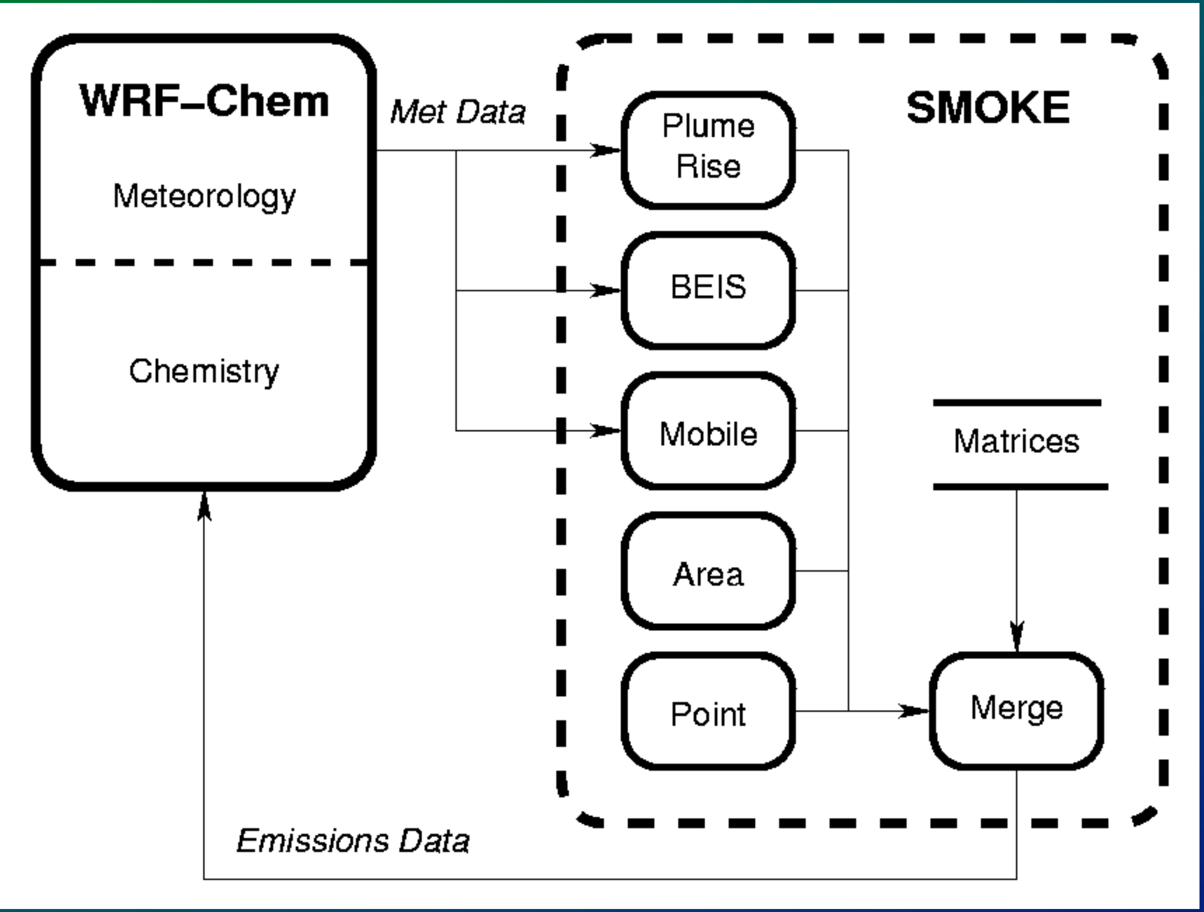
- **Emissions Approach**
  - –Online biogenic emissions:
    - BEIS 3.11 or Guenther
- **All other emissions offline**
  - –“single representative day” for point, area, and mobile sources combined in one 24 hour file
  - – July 15, 2004 used for all applications

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 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

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

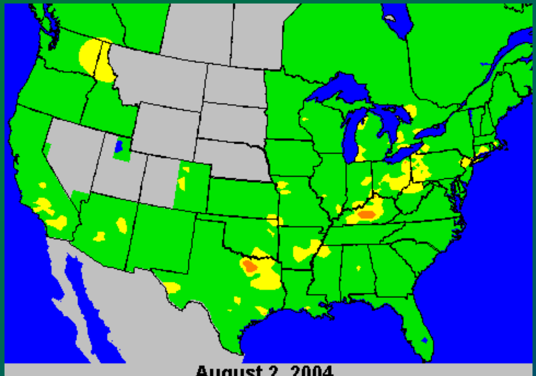
- **New driver, UI layers**
  - **Arbitrary user-selected time step**
  - **Does not override user's run-specifications**
  - **Uses *TA, QV, P, Z, U, V* from met model**
- **Same Briggs-algorithm plume-rise module**
- **Stack height re-adjustment on basis of sub-grid scale terrain is optional**

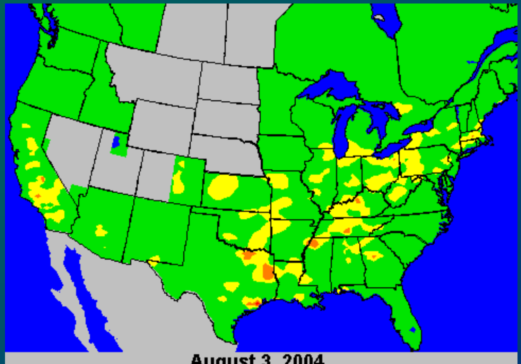
Merge Sub-Model

- 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 <u>aerosol</u> and chemical species*
  - Open-MP parallel for performance

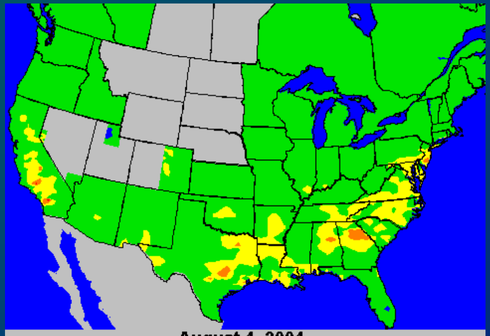
CASE Study and Results

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


August 2, 2004


August 3, 2004

This day chosen for comparison

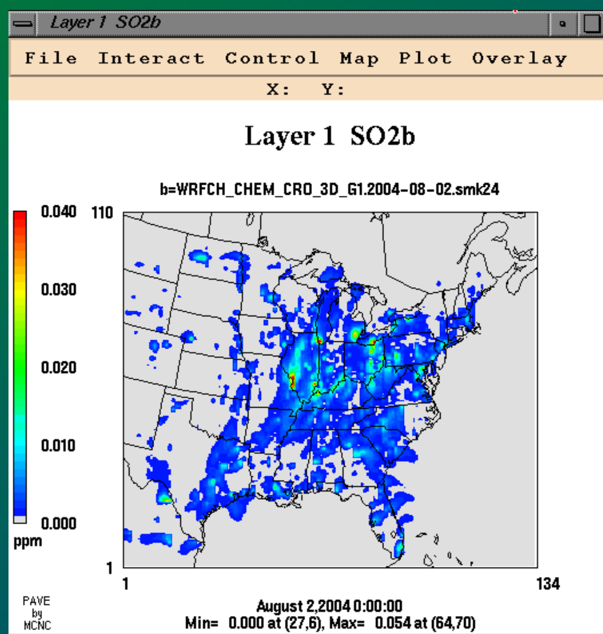

August 4, 2004

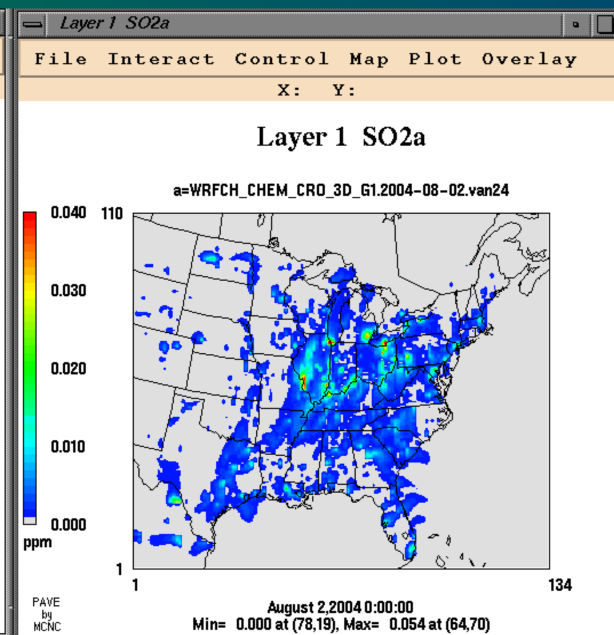
CASE Study and Results

- **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



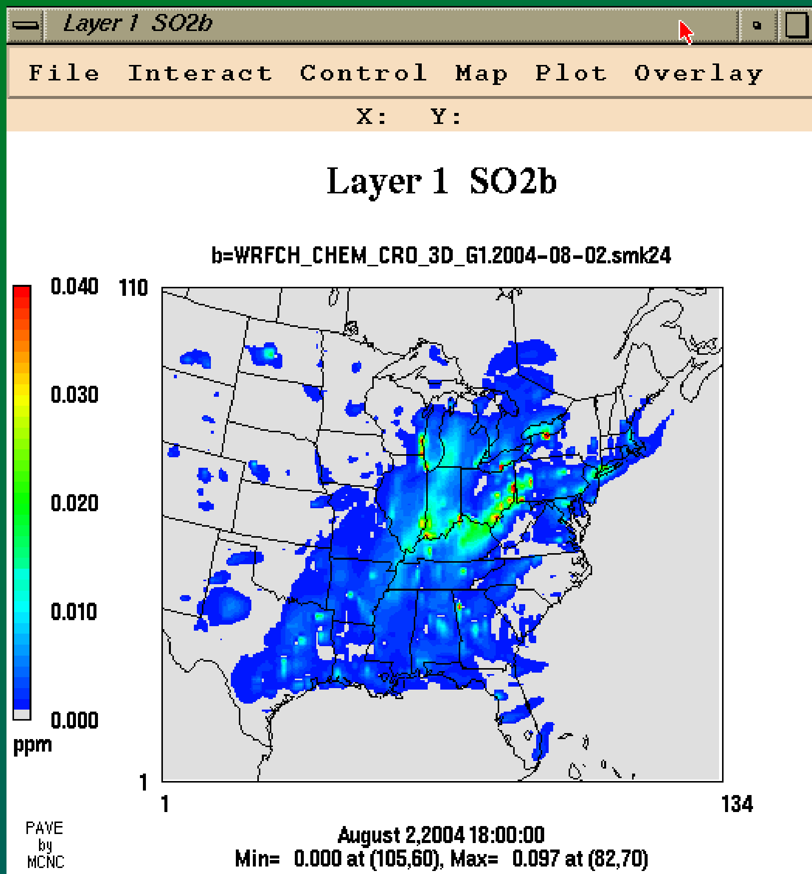


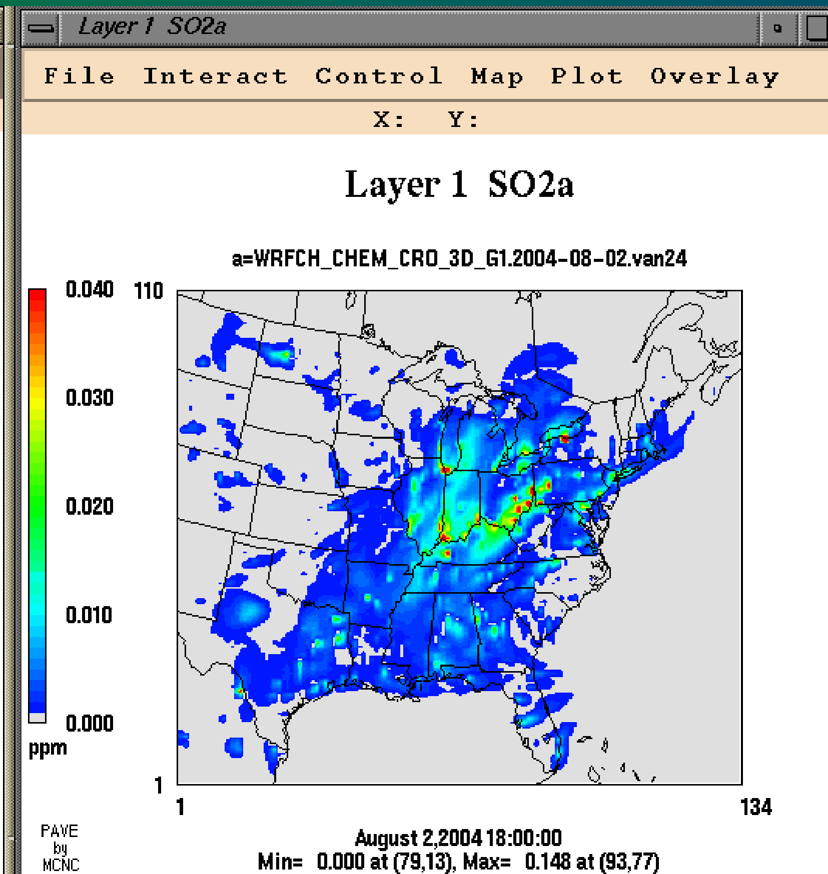
WRF-SMOKE **WRF-Vanilla**

CASE Study and Results

- **WRF-Chem Results for Aug 2, 2004:**
  - **SO_2**
  - **SULF**
  - **NO_2**
  - **ISO**
  - **PAN**
  - **O_3**
- **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

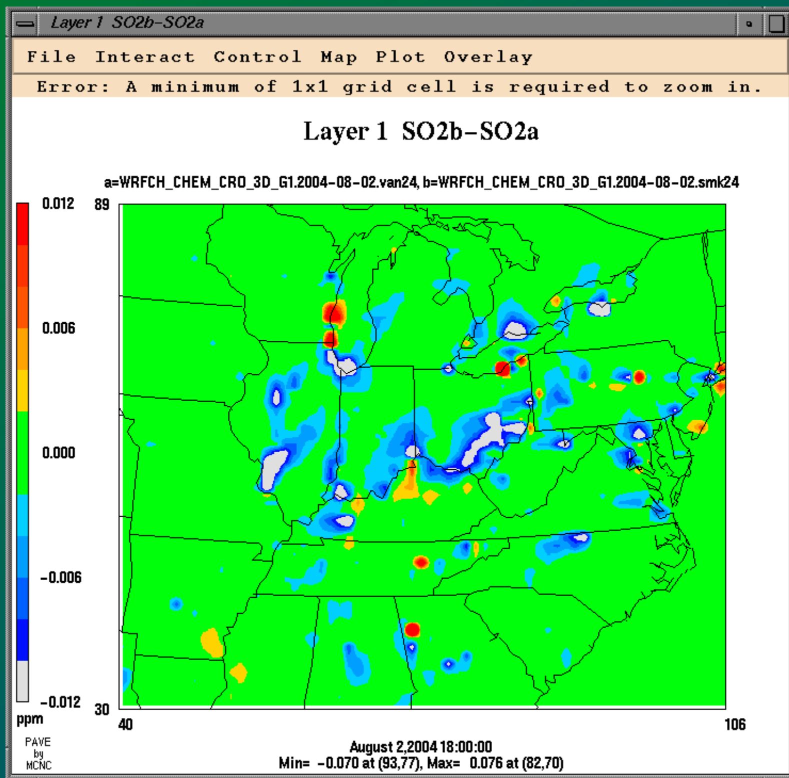


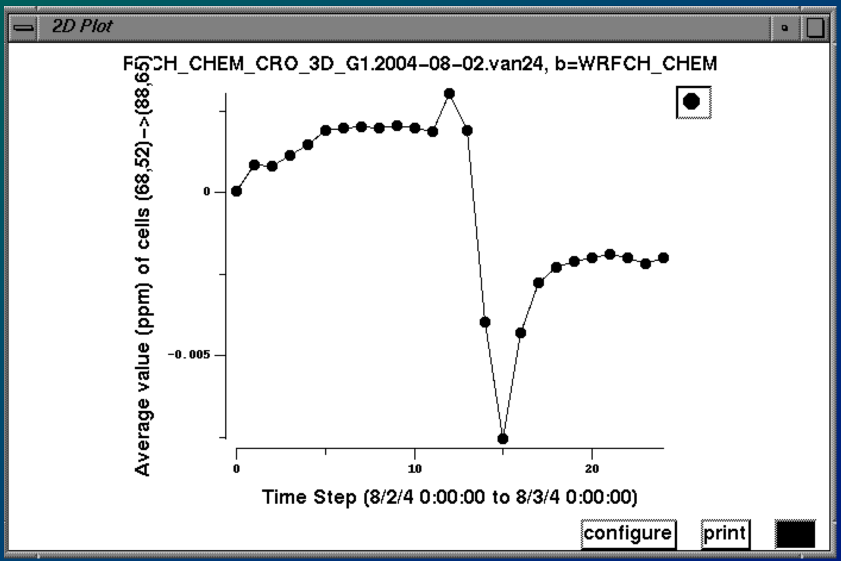


WRF-SMOKE **WRF-Vanilla**

CASE Study and Results: SO2:

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





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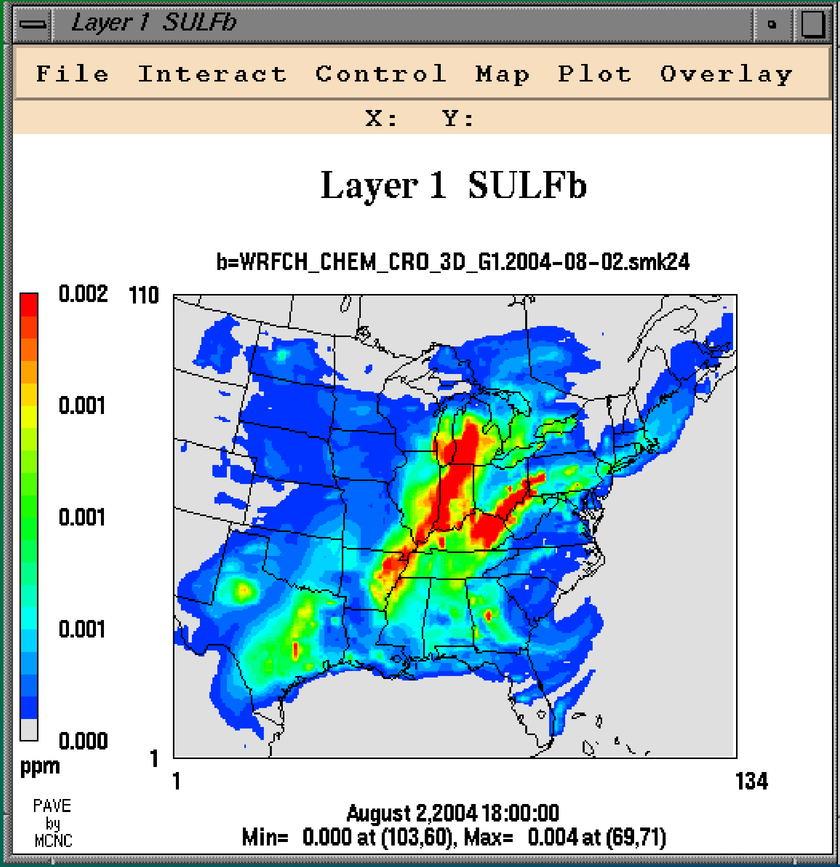
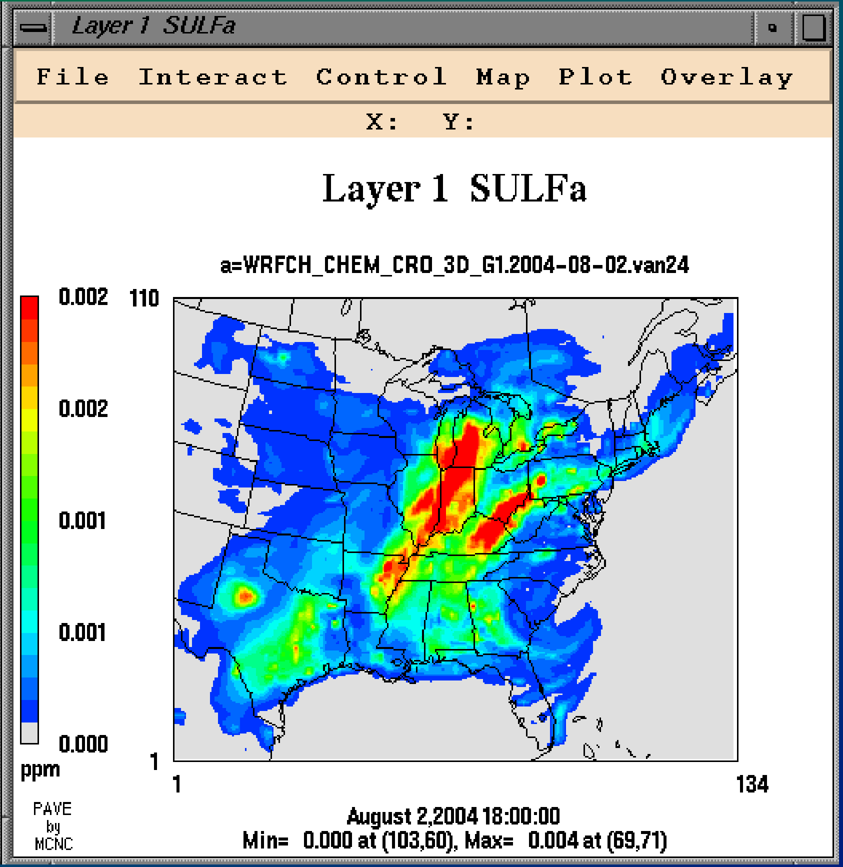
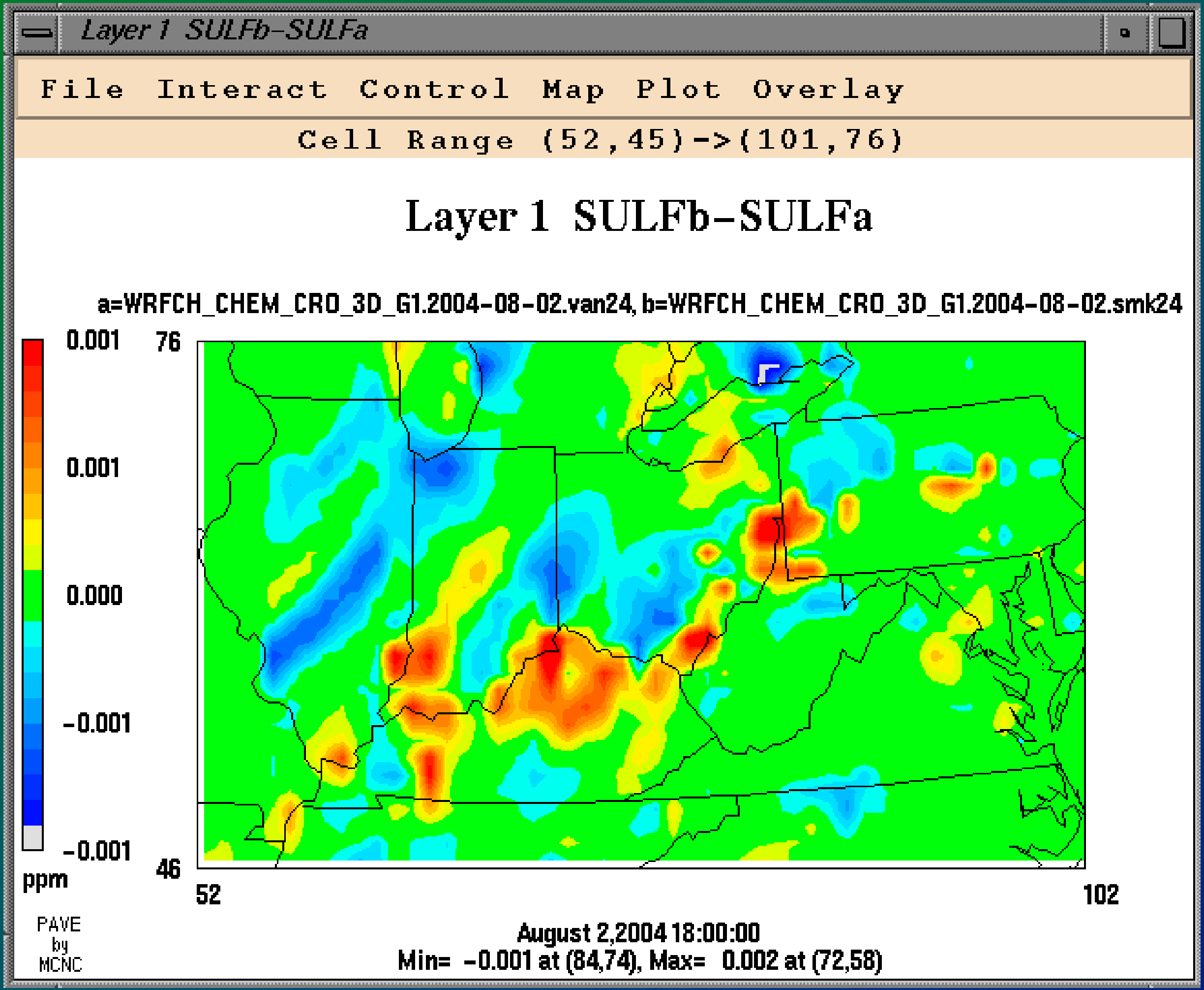
CASE Study and Results: Sulfate at 18z



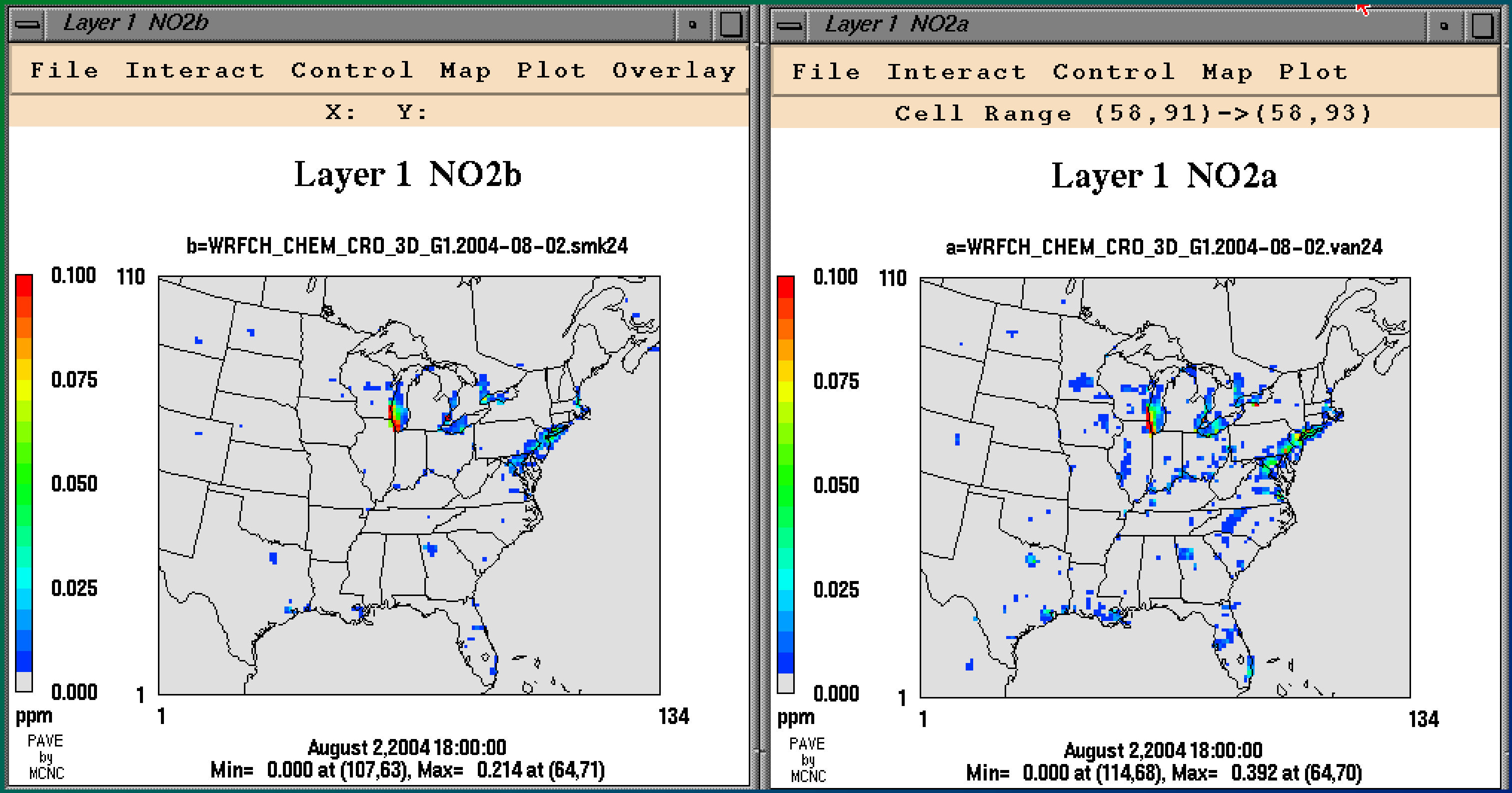


WRF-SMOKE **WRF-Vanilla**

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



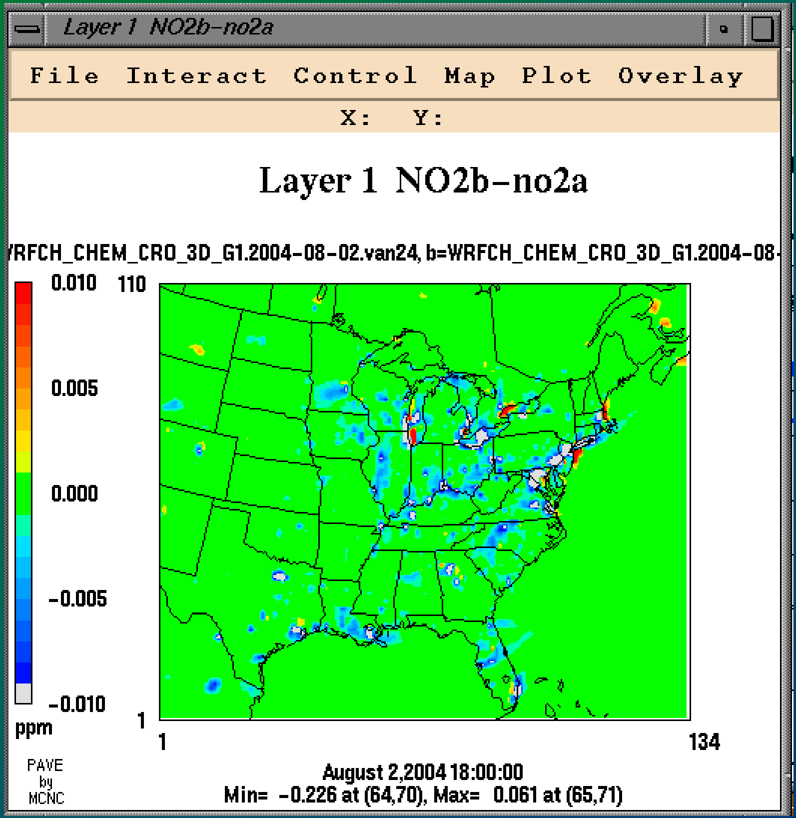
CASE Study and Results: NO2 at 18z

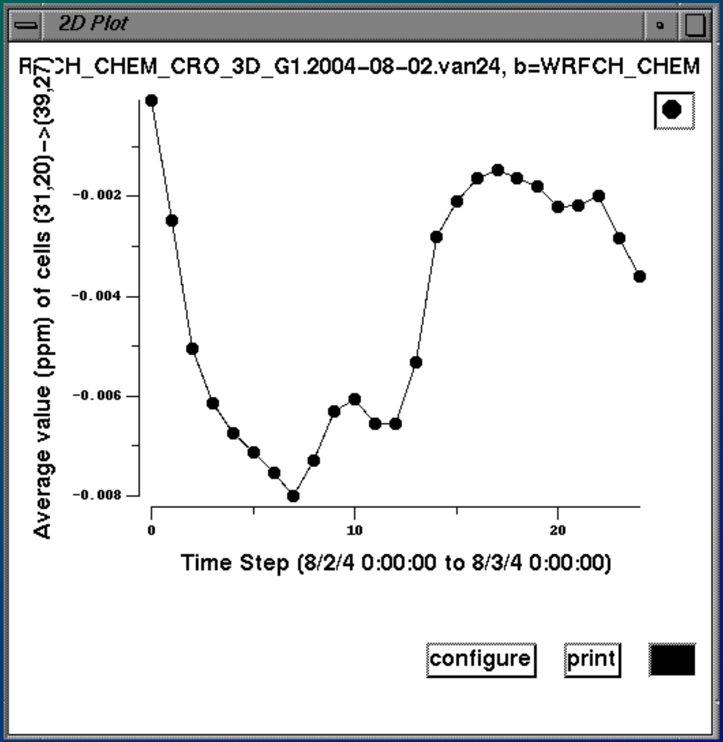


WRF-SMOKE | WRF-Vanilla

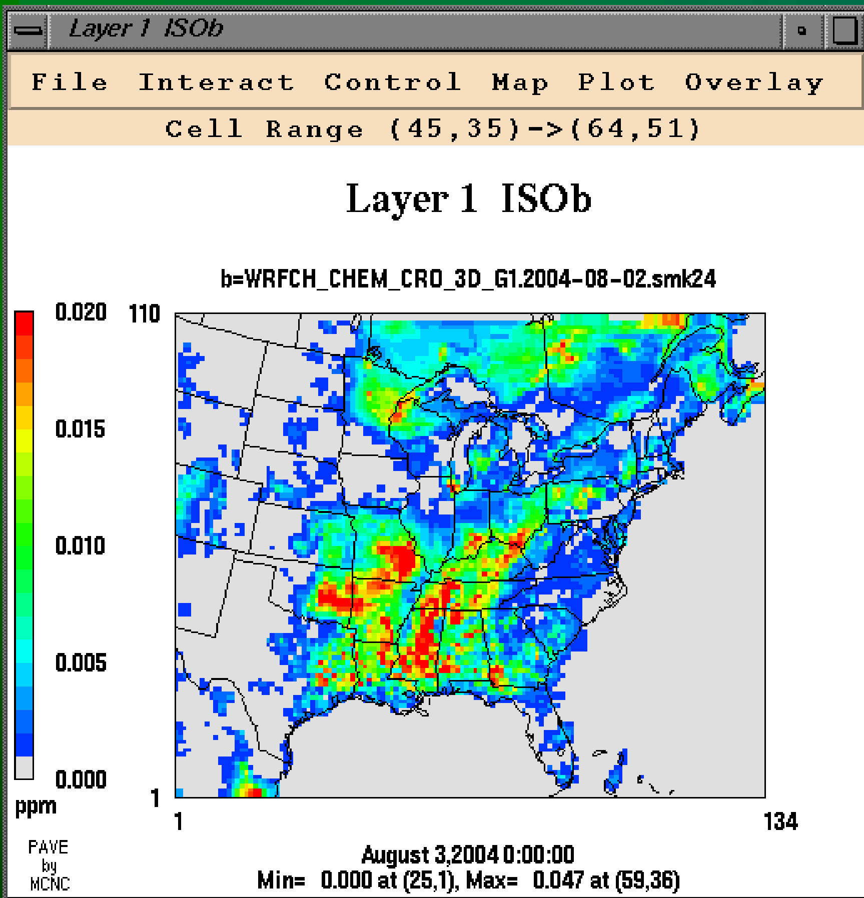
CASE Study and Results:
NO2:

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

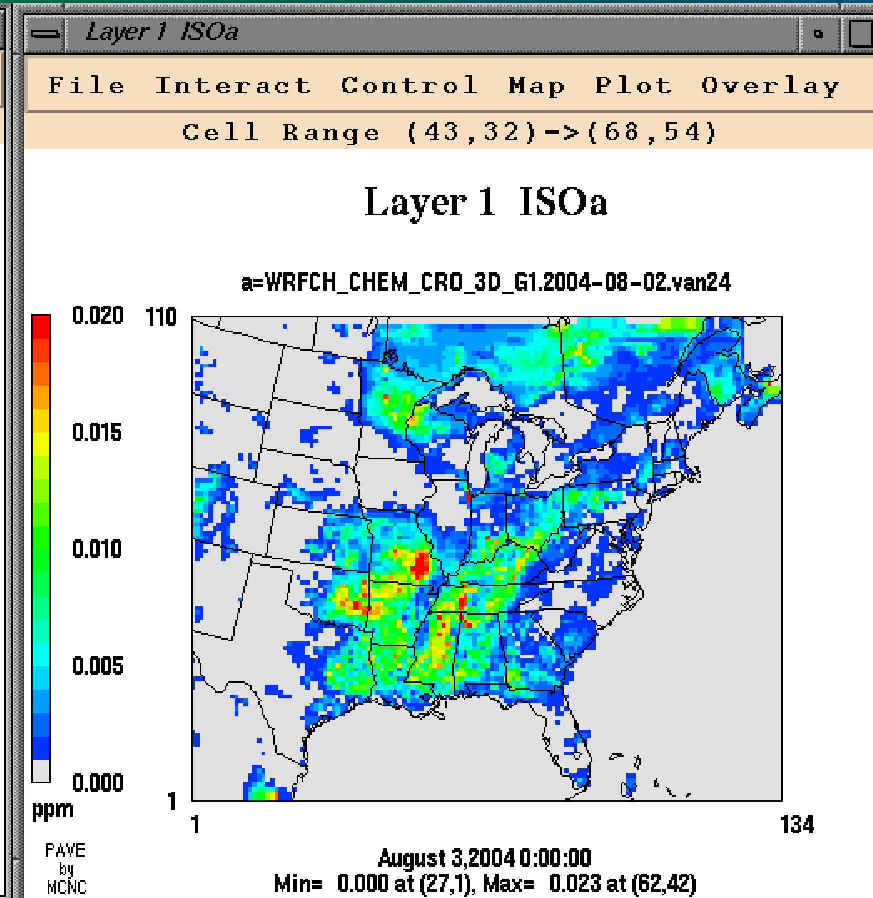




CASE Study and Results: Isoprene at “24z”

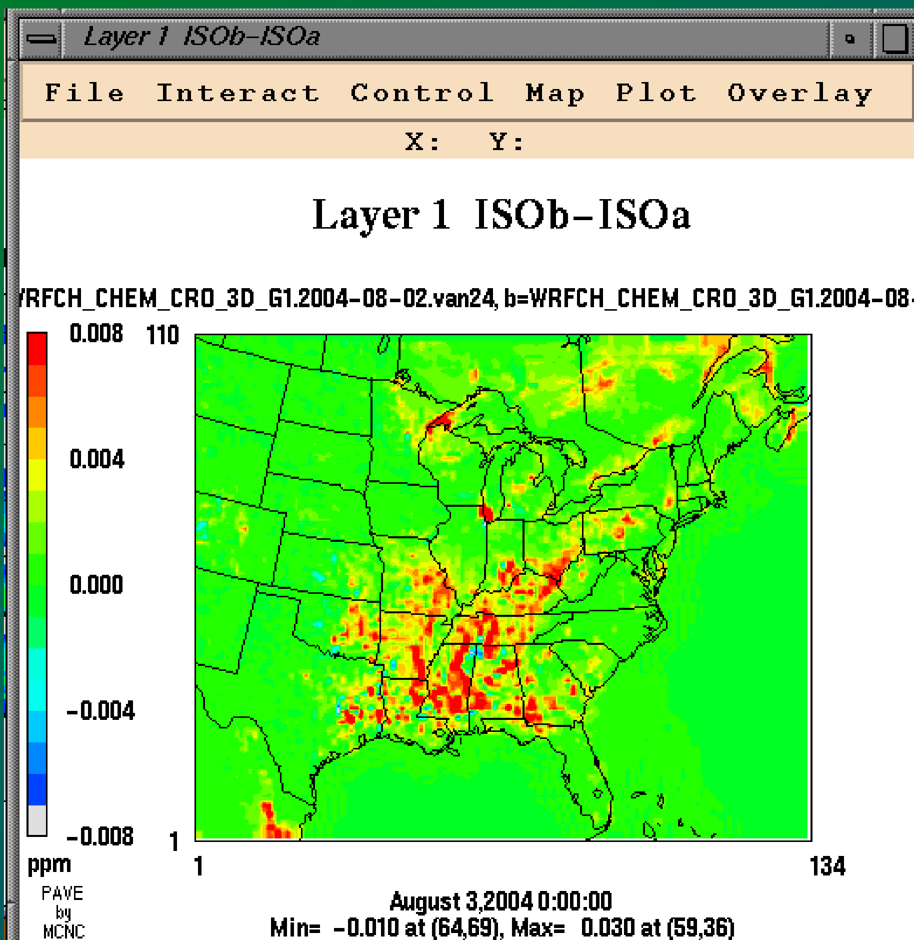


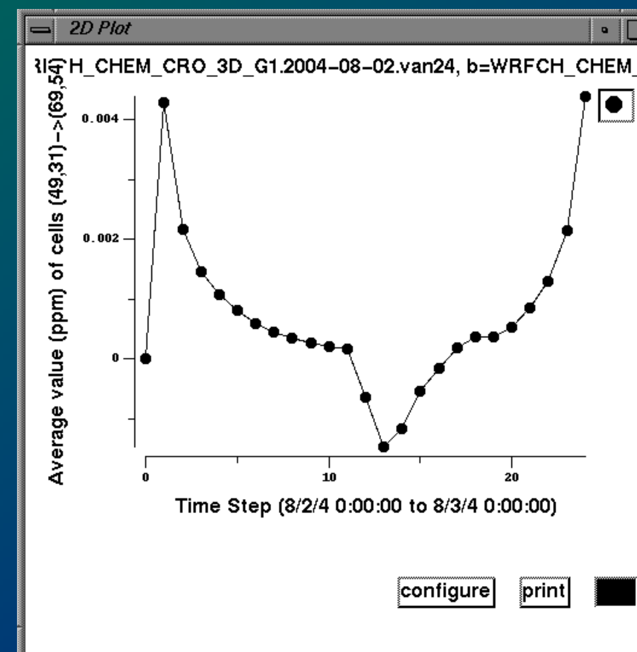
WRF-SMOKE



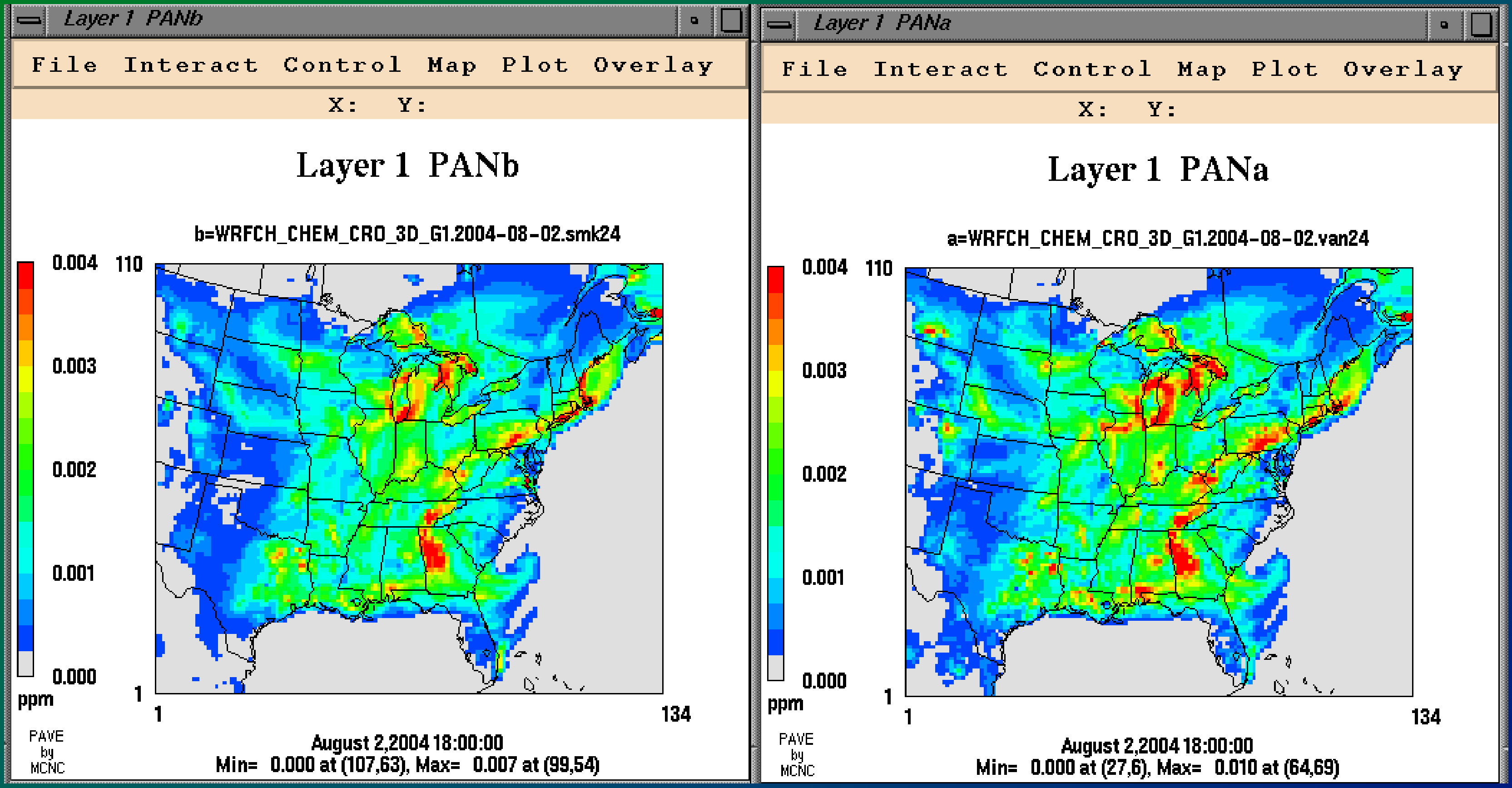
WRF-Vanilla

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



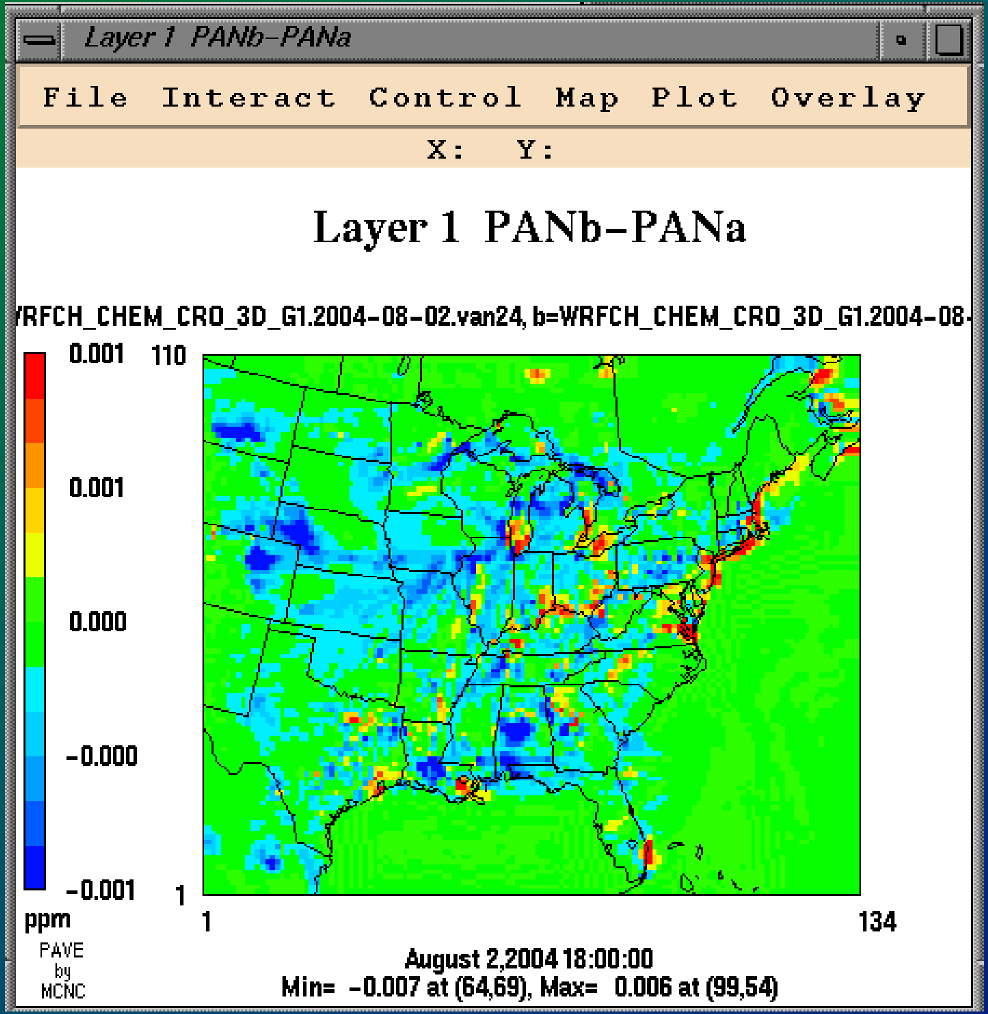


CASE Study and Results: PAN at 18z

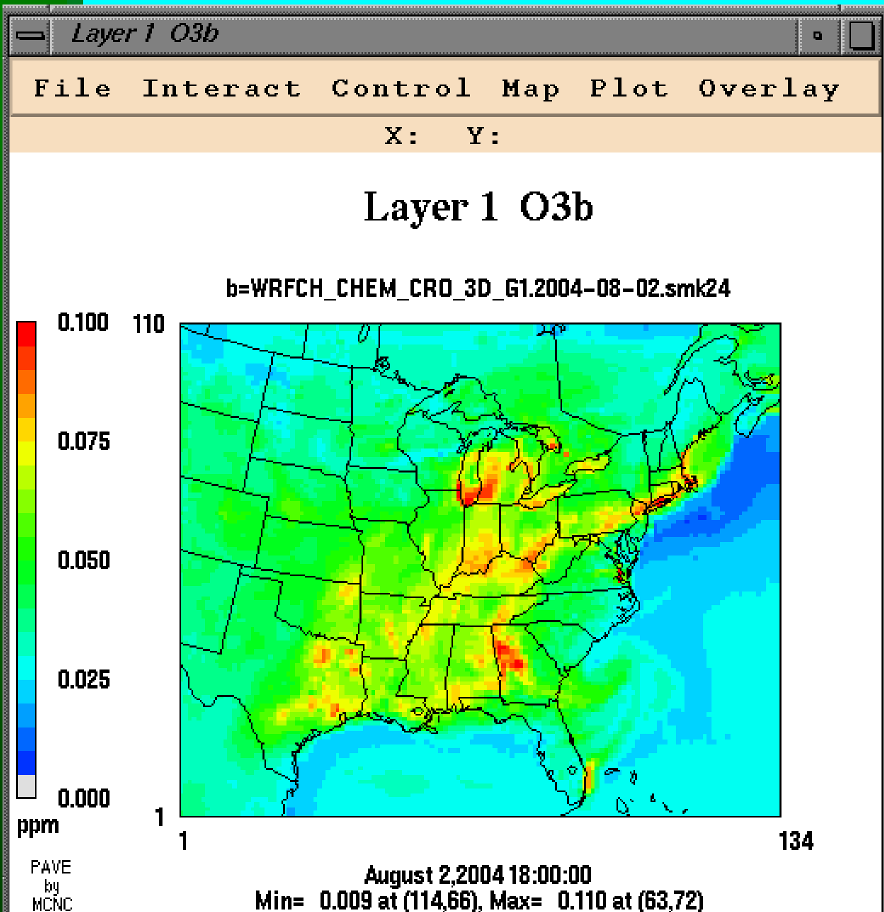


WRF-SMOKE **WRF-Vanilla**

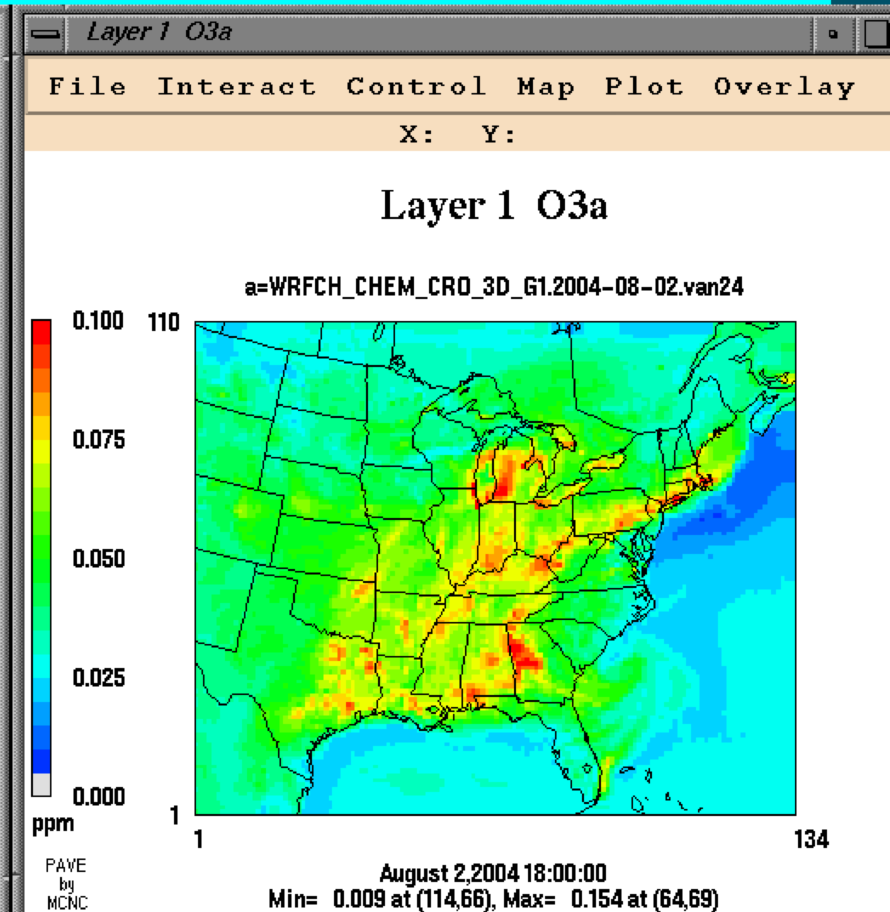
CASE Study and Results: PAN difference field (SMOKE minus VANILLA) at 18z



CASE Study and Results:O3 at 18z



WRF-SMOKE

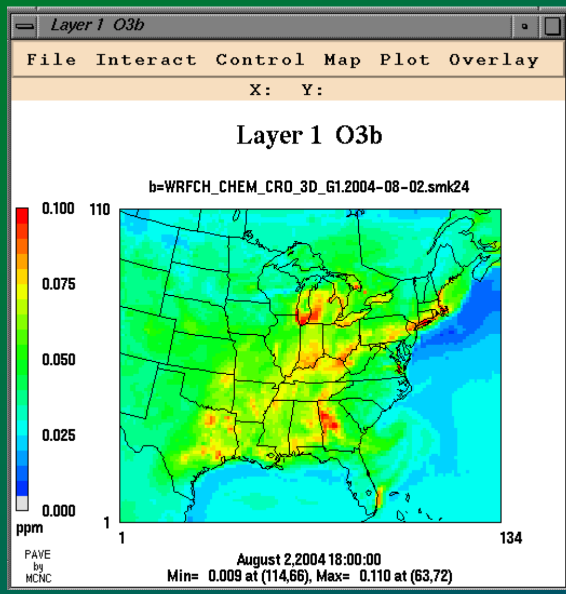


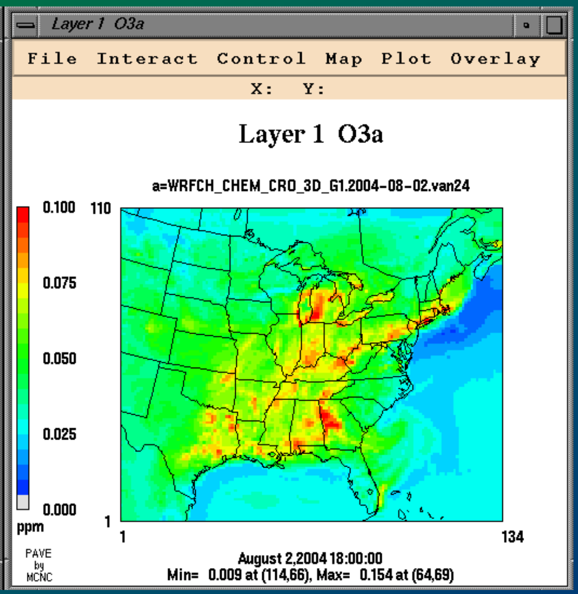
WRF-Vanilla

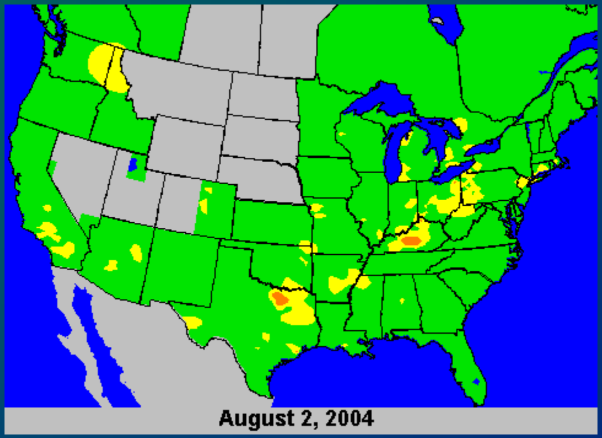
CASE Study and Results:O3 at 18z

WRF-SMOKE

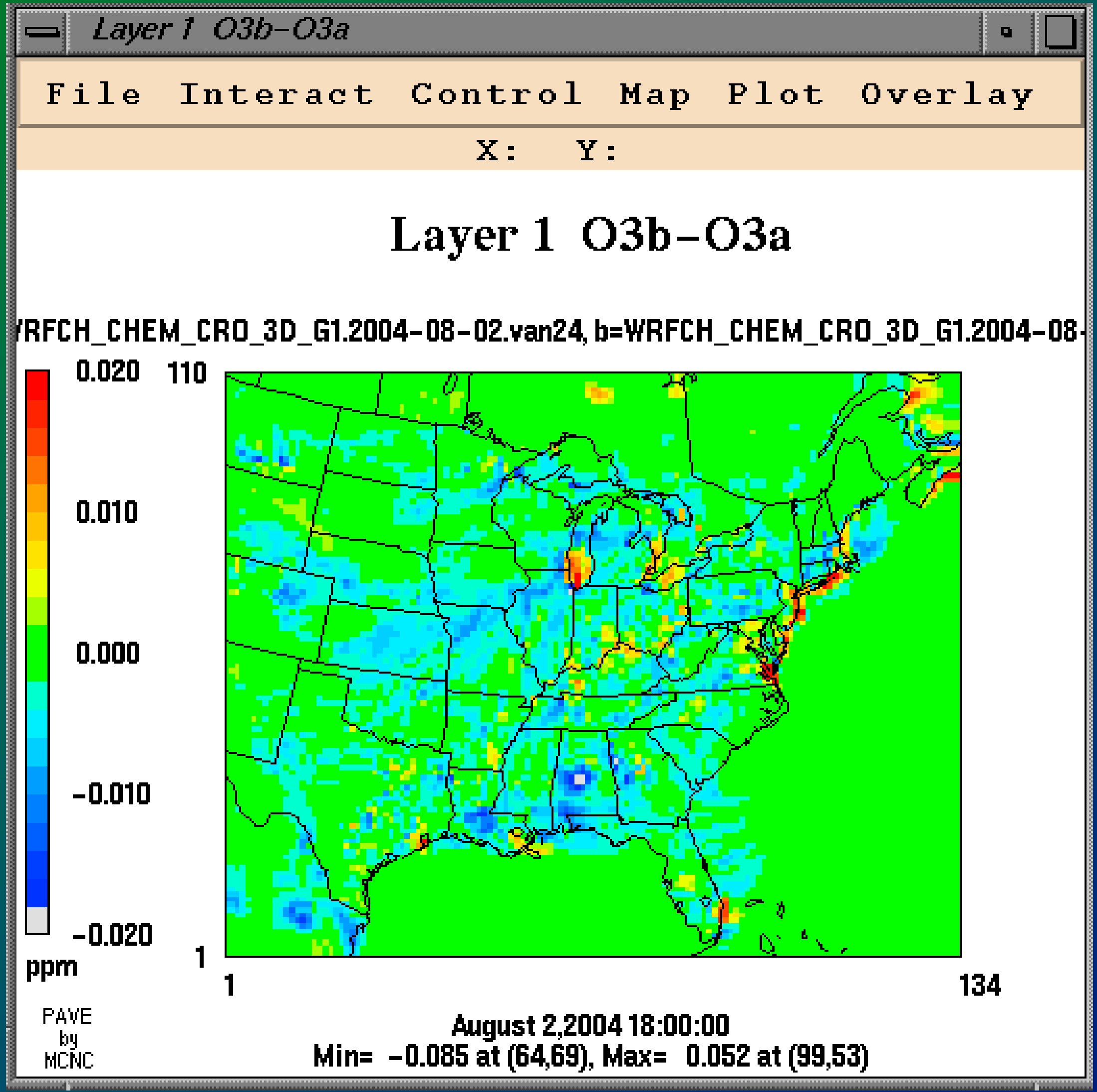
WRF-Vanilla



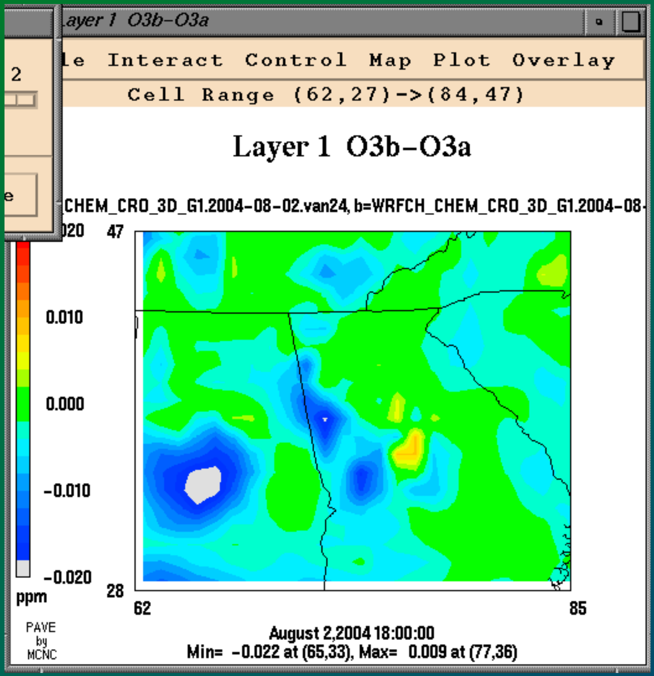


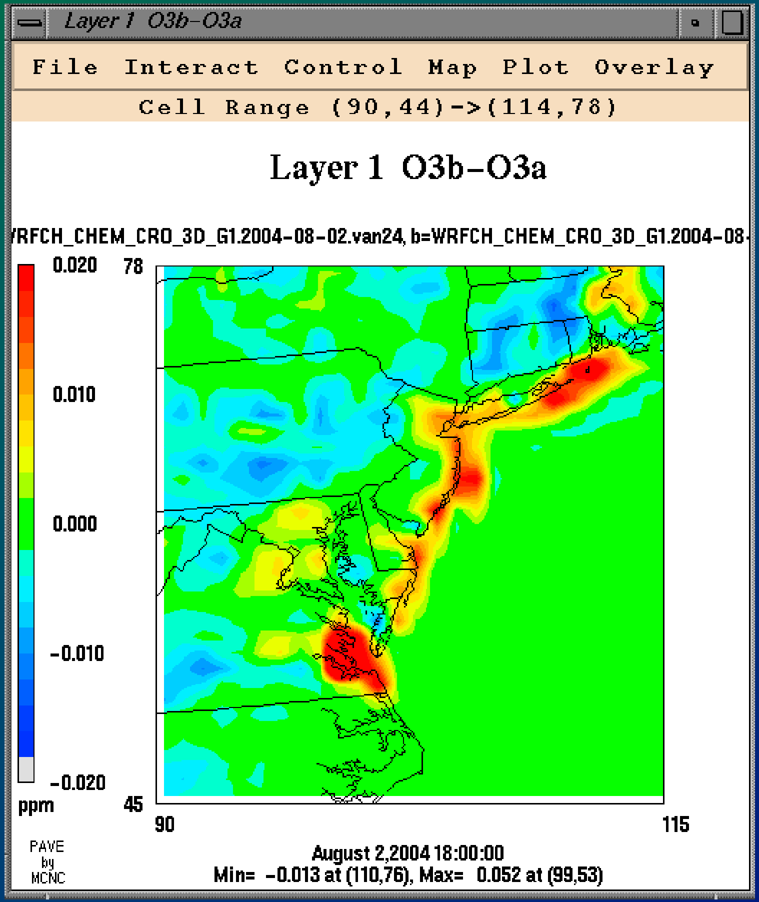


CASE Study and Results:O3 difference field at 18z

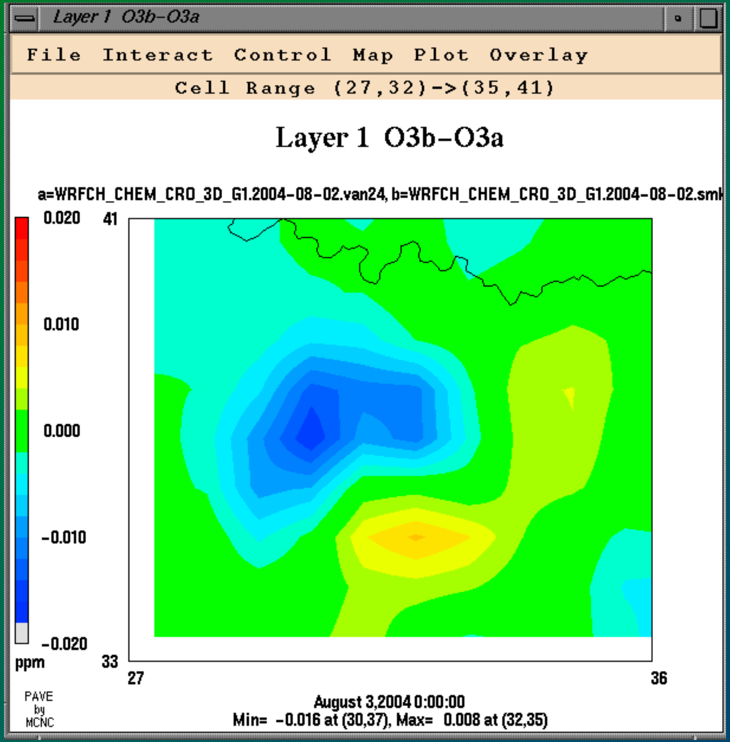


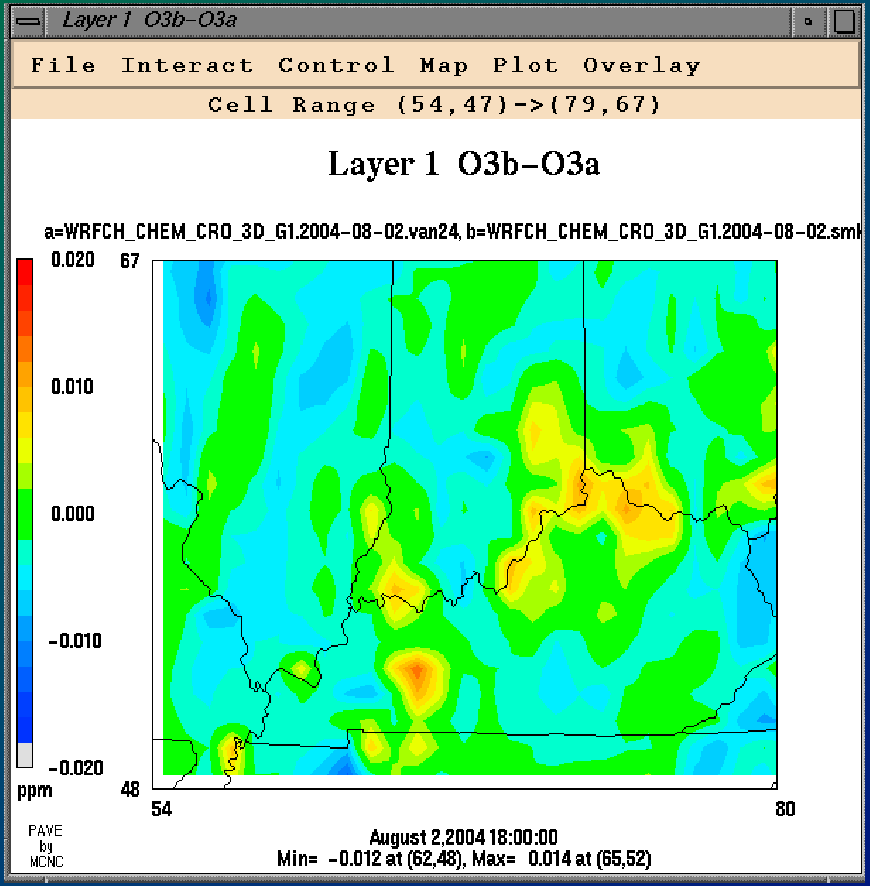
CASE Study and Results: Regional O3 Difference fields at 18z



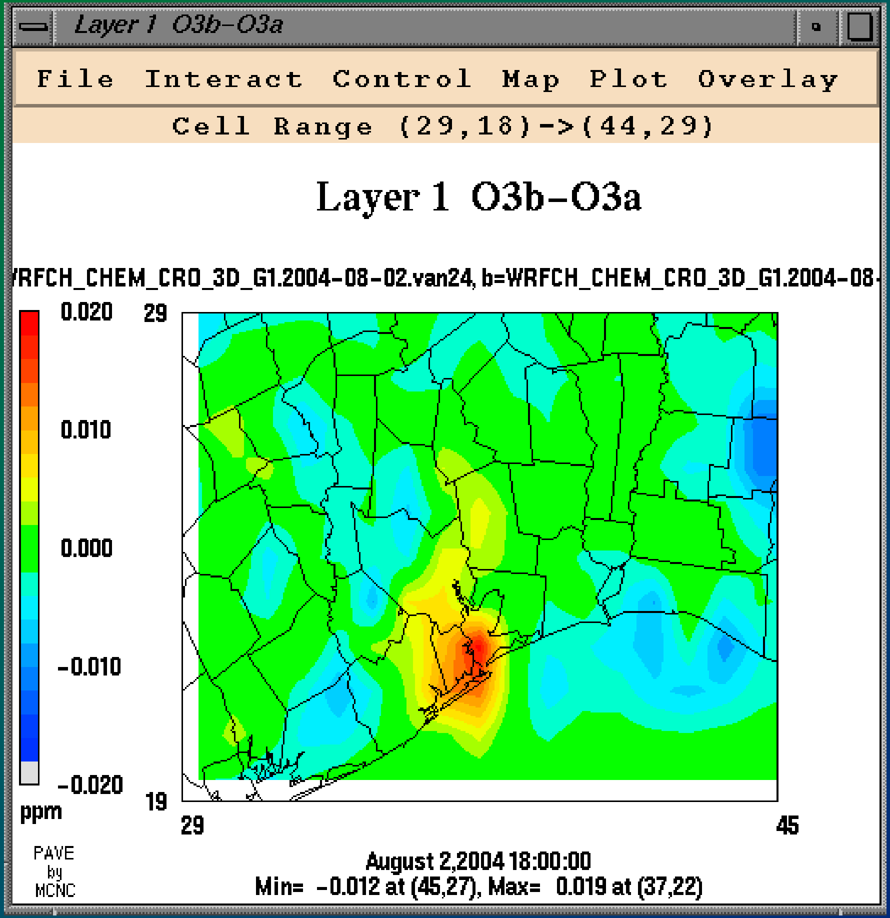


CASE Study and Results: Regional O3 Difference fields at 18z [DFW and Ohio Valley]

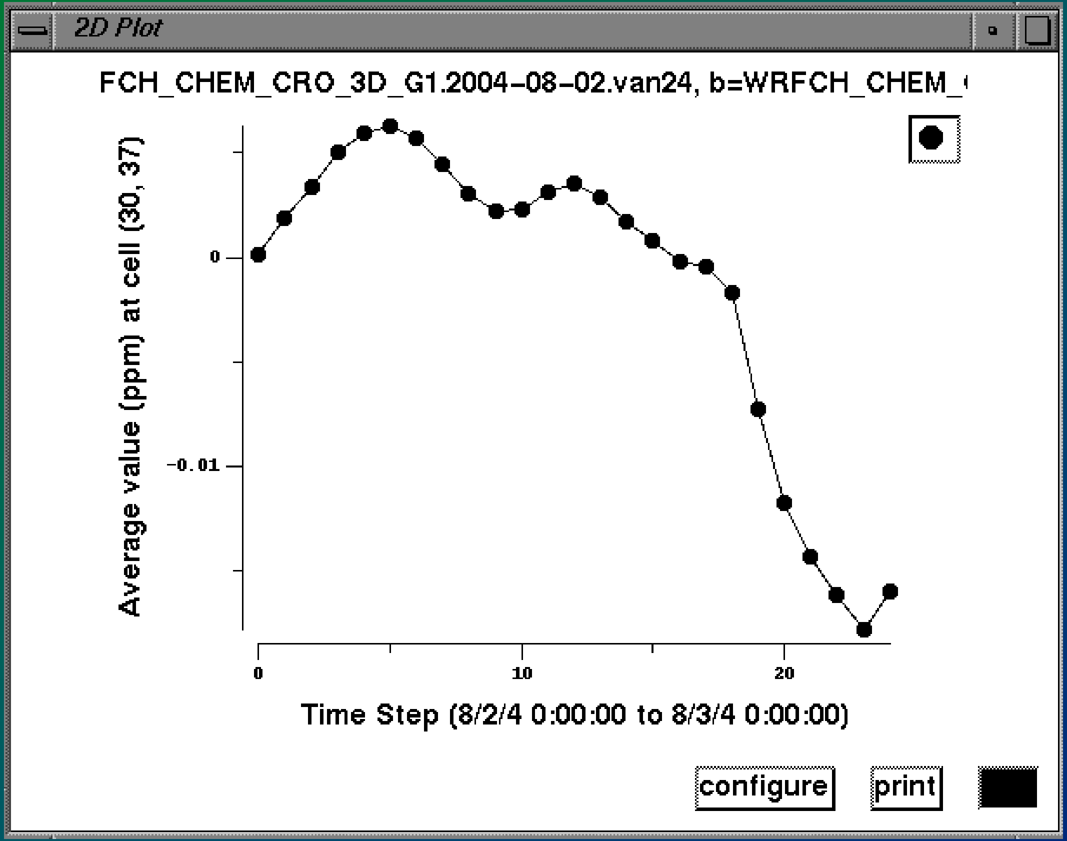




CASE Study and Results: Regional O3 Difference fields at 18z [Houston}



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



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

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- Georg Grell and Steven Peckham of the Forecast Systems Lab for many useful discussions regarding WRF-Chem; and help where needed.
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- Nelson Seaman for many useful and engaging discussions concerning the WRF and WRF architecture

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