BAMS
BARON ADVANCED METEOROLOGICAL SYSTEMS

Forecasting a Better Future

Results of Coupling the WRF-Chemistry Model with the SMOKE Emissions Processing/Modeling System

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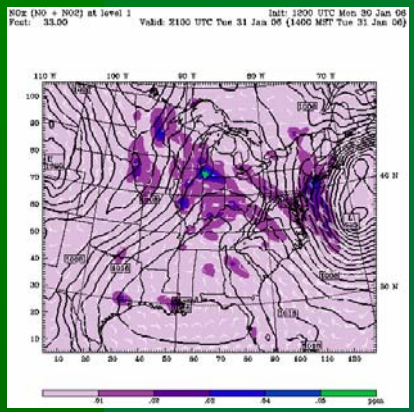
Talk Outline

- Background and Motivation
- WRF-Chem SMOKE design concept
- From SMOKE to SMOKE-RT for WRF
- Case Study and Results
- Conclusions and Acknowledgments

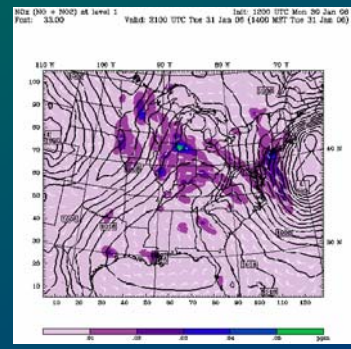
Background and Motivation



The WRF - Chemistry Model

- Calls to the chemistry driver are in-lined within the WRF meteorological driver (using the EM (I.e. ARW) core)
- Two choices in "legacy" chemical mechanisms:
  - RADM2, RACM [with or without aerosols (MADE - SORGAM)]
- 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 contain aqueous chemistry

Background and Motivation



The WRF 2.1 - Chemistry Model

- **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

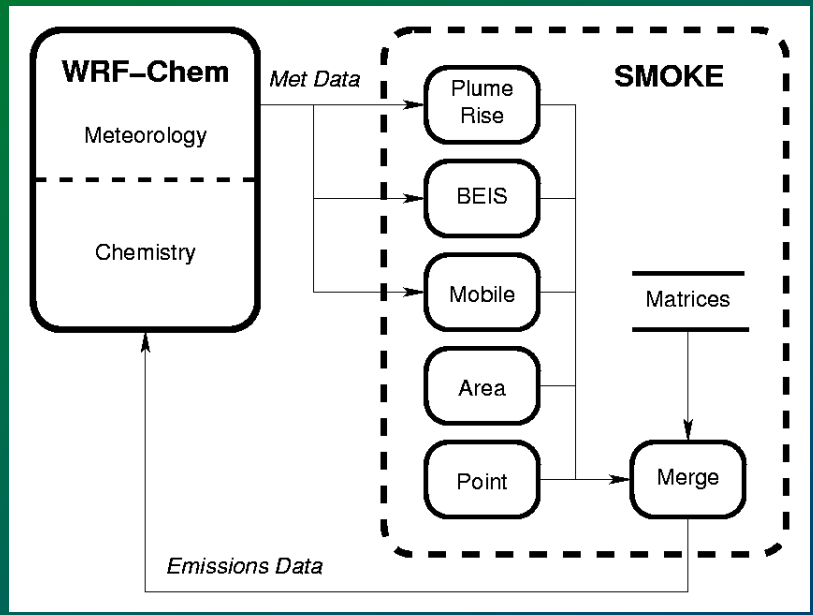
The Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System

- Computationally efficient state-of-the-art emissions modeling system
- Used by CMAQ, MAQSIP, MAQSIP-RT, CAMx, UAM, REMSAD
- Standardizing on inventory source order turns most emissions modeling computations into sparse matrix multiplications:
- Hundreds of times faster than data-processing style emissions modeling

WRF-CHEM SMOKE DESIGN CONCEPT

- **SMOKE Uses the EPA/MCNC/BAMS Models-3 I/O API (*M3IO*)**
  - **Gridded, observational, inventory, sparse matrix data types: definition, storage, arithmetic operations**
  - **Persistent file storage layered on top of *netCDF* and native-binary files with peripheral support for *GRIB* and other formats.**
  - **Communication/coordination layered on top of *PVM* (looks to the program just like file storage)**
  - **not just a file-format broker, rather, a full API (Applications Programming Interface)**
    - **High level data access routines, time-keeping, map transforms, utilities**
- ***M3IO* is now built into WRF and WRF-Chem, and can be used to both read and write native m3io data**

WRF-CHEM SMOKE DESIGN CONCEPT



- Met part of WRF-Chem provides meteorology data to SMOKE
- SMOKE provides model-ready met-modulated emissions back to WRF-Chem (for all emissions typologies)
- *Data exchange and interprocess scheduling are provided by the M3IO*

From SMOKE to SMOKE-RT

SMOKE-RT for WRF-Chem

- **New implementation of met-modulated sub-models:**
  - **Temporal submodels for biogenic, mobile, plume-rise**
  - **Merge processor – single-stage merge instead of multi-stage**
  - **Parallelized (via OpenMP) and much more efficient (~ 5X)**
  - **Modular design, now acts as a "time-stepped model"—OK for cooperating-process coupled modeling systems.**
- **Sub-Grid scale terrain height effects for biogenic, mobile, plume-rise, merge sub-models.**

From SMOKE to SMOKE-RT

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 model
  - 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

From SMOKE to SMOKE-RT

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**

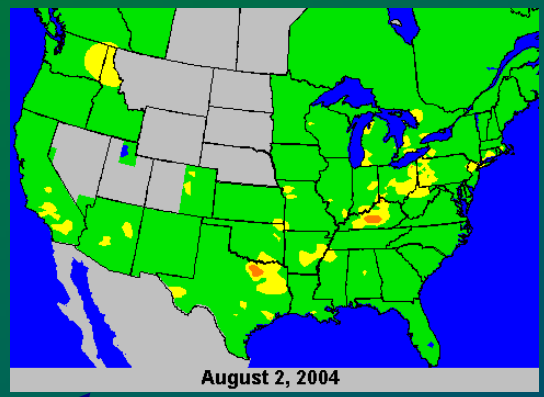
From SMOKE to SMOKE-RT

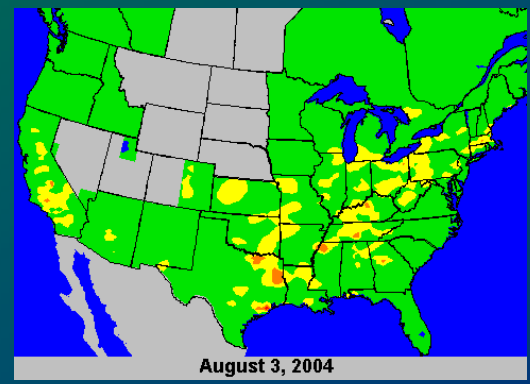
Merge Sub-Model

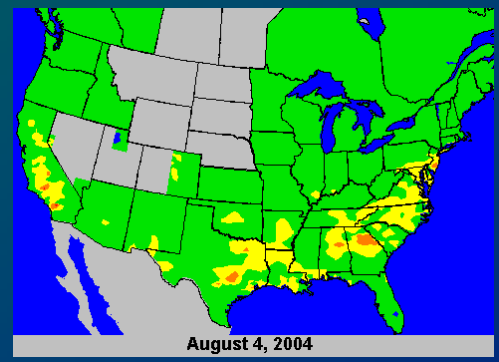
- **Single-Stage merge program**
  - Supports *multi-inventory merge*
  - Reads and combines *sparse-matrix files* for gridding, speciation, control, future/past projection
  - Optionally reads layer fractions files
  - Reads *time stepped source level* emissions files for area, point, mobile, biogenics,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







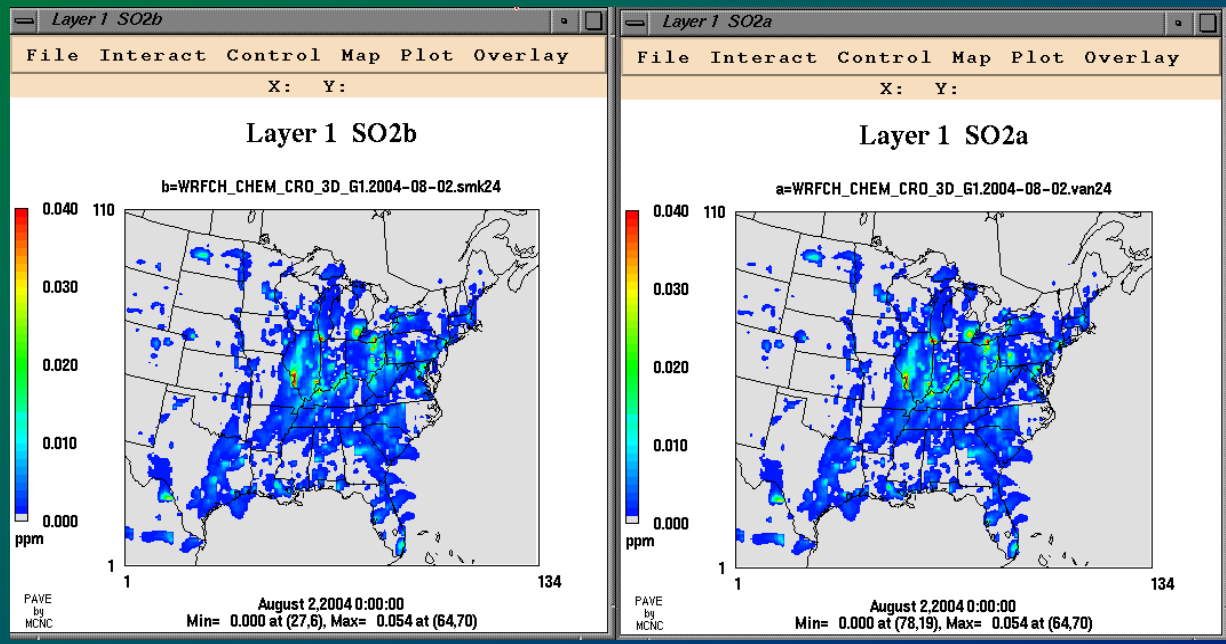
This day chosen for comparison

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"

CASE Study and Results

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

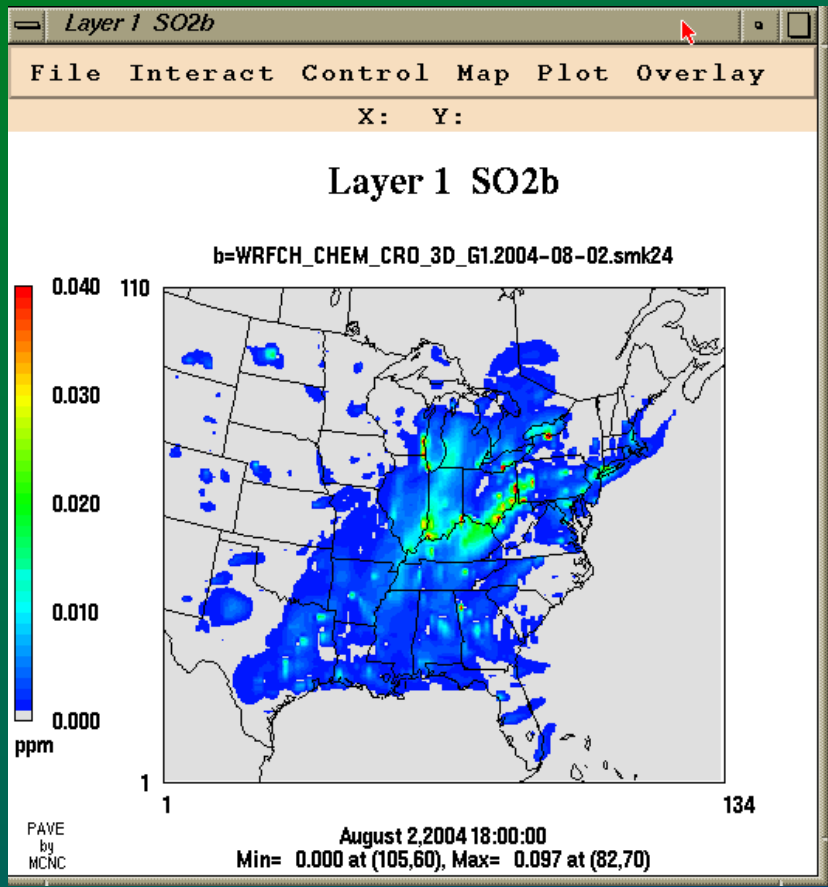


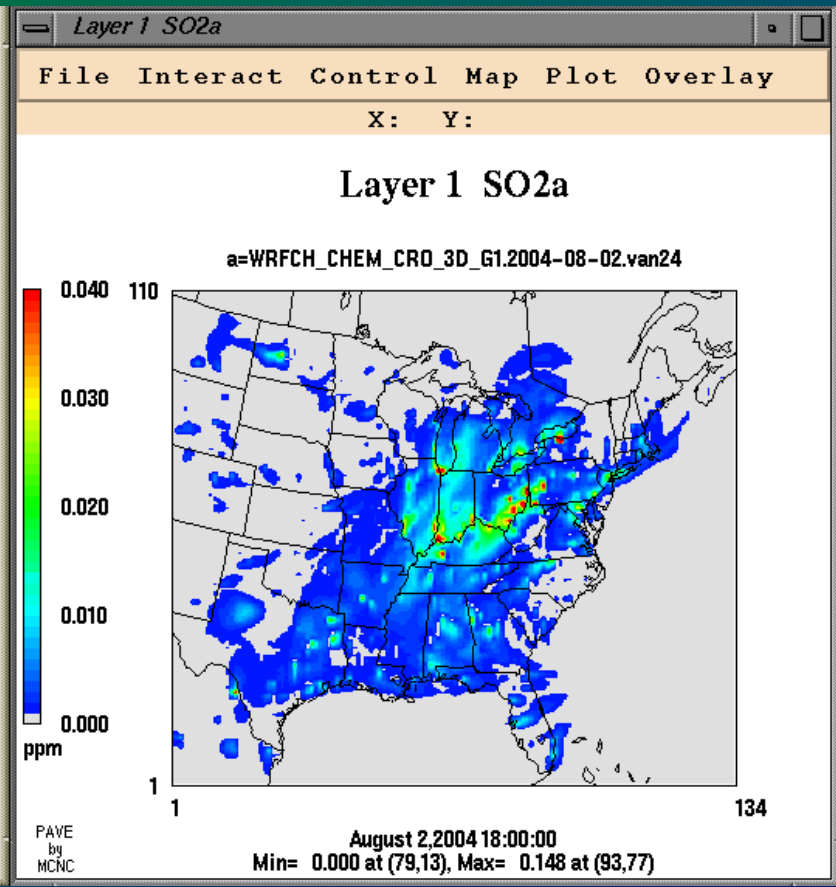
WRF-SMOKE **WRF-Vanilla**

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

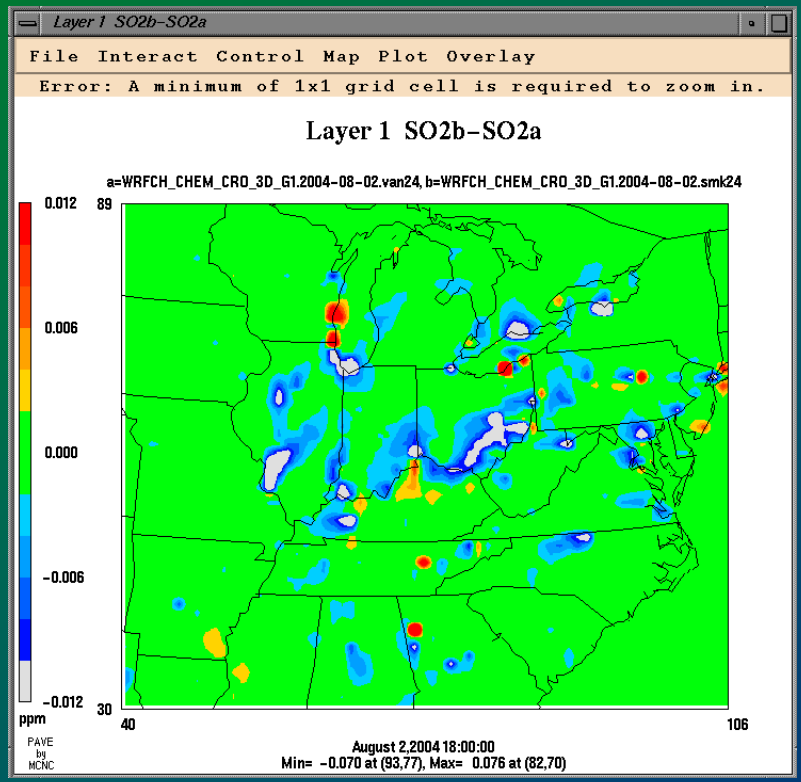


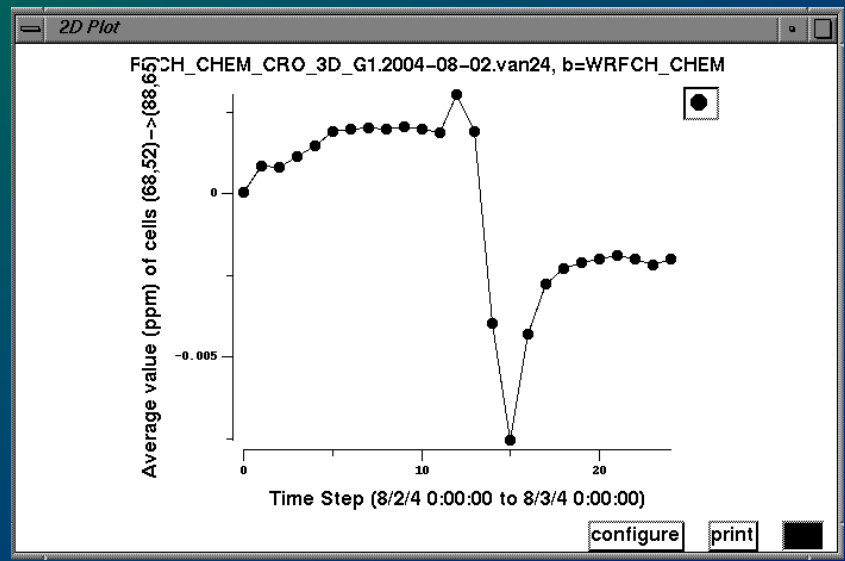


WRF-SMOKE **WRF-Vanilla**

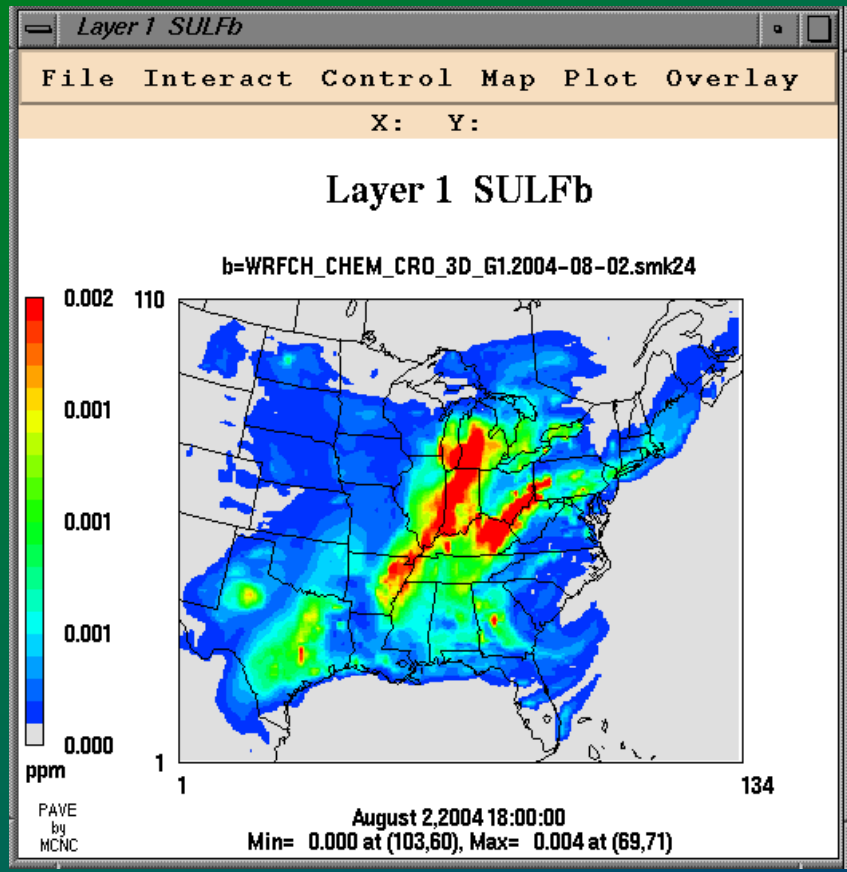
CASE Study and Results: SO2:

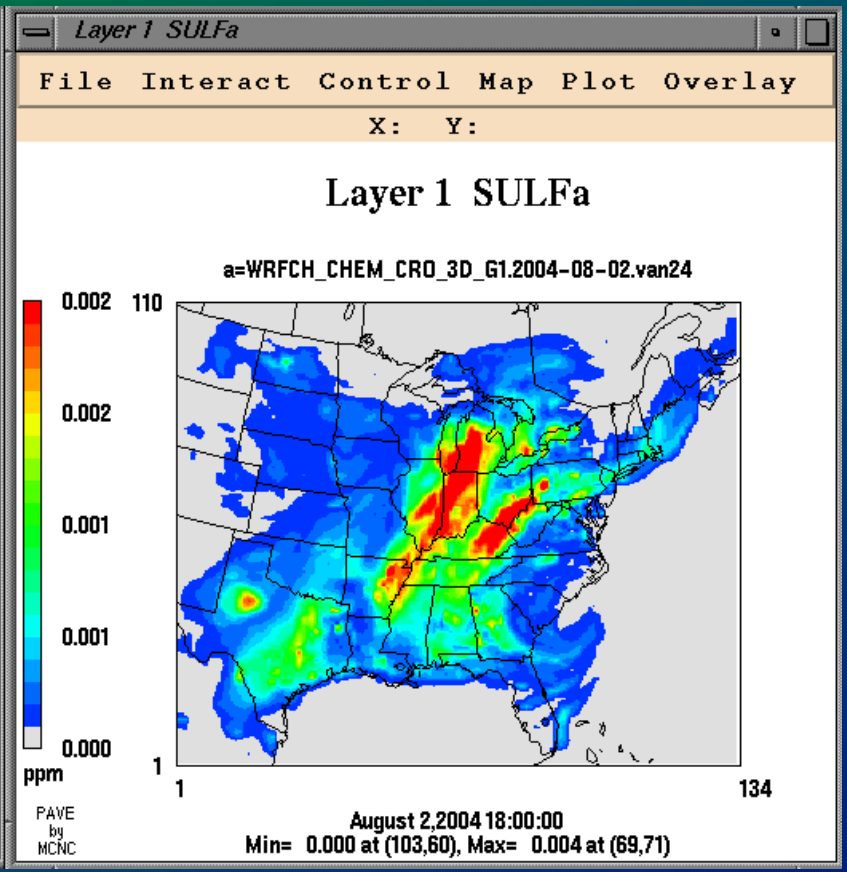
*difference field at 18z (left);
*difference time series for Ohio Valley (right)





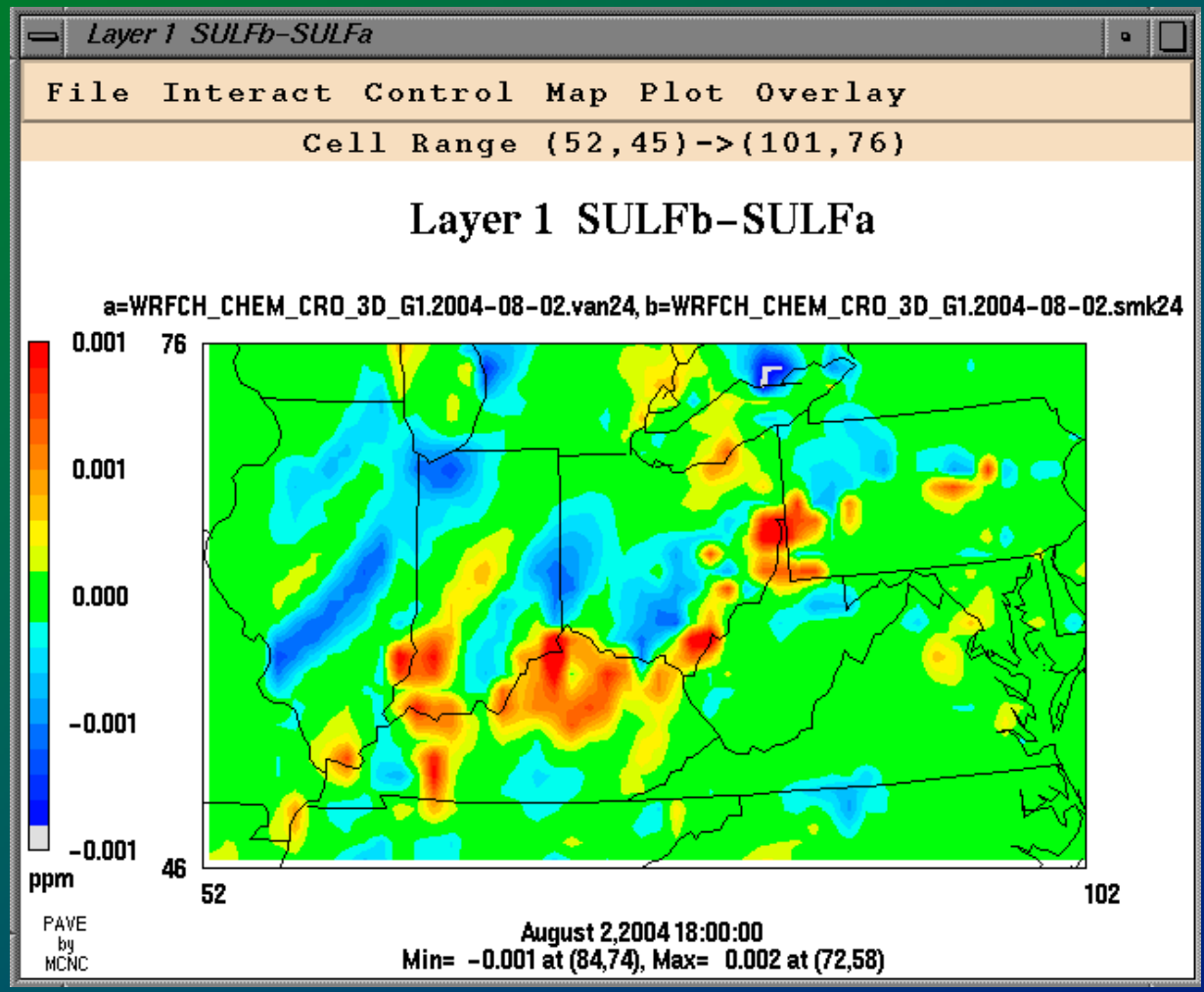
CASE Study and Results: Sulfate at 18z



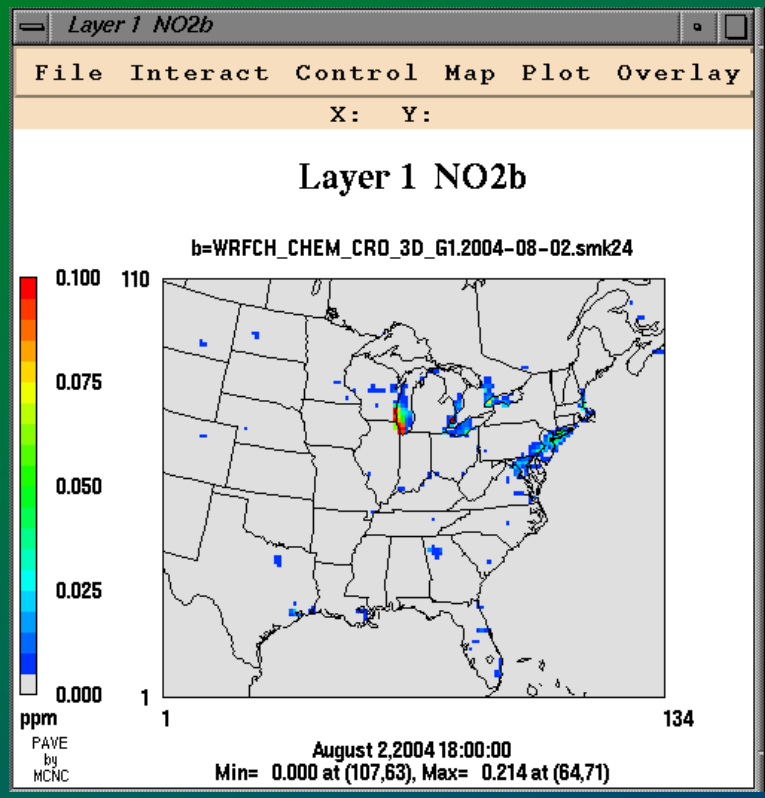


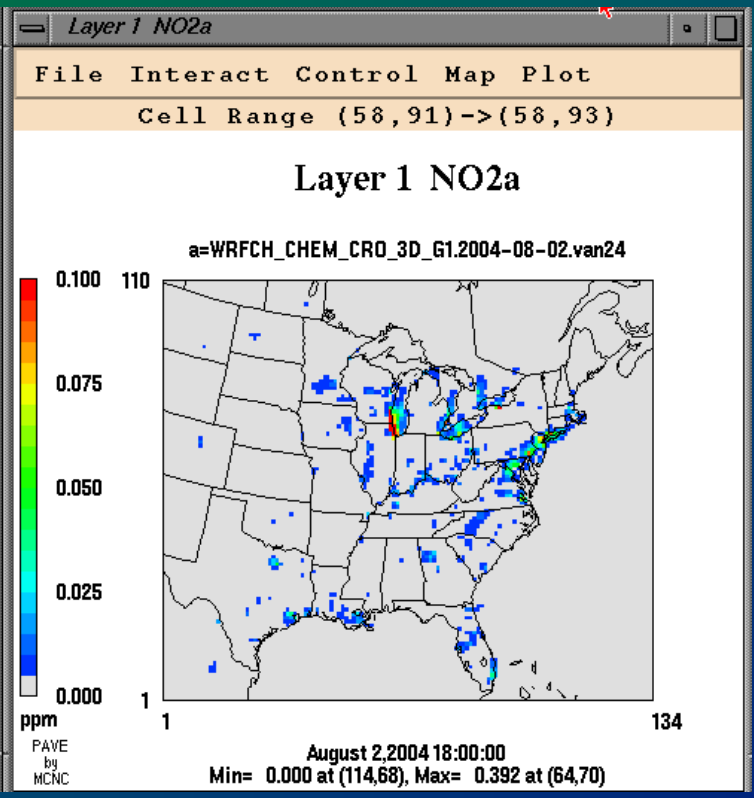
WRF-SMOKE **WRF-Vanilla**

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



CASE Study and Results: NO2 at 18z

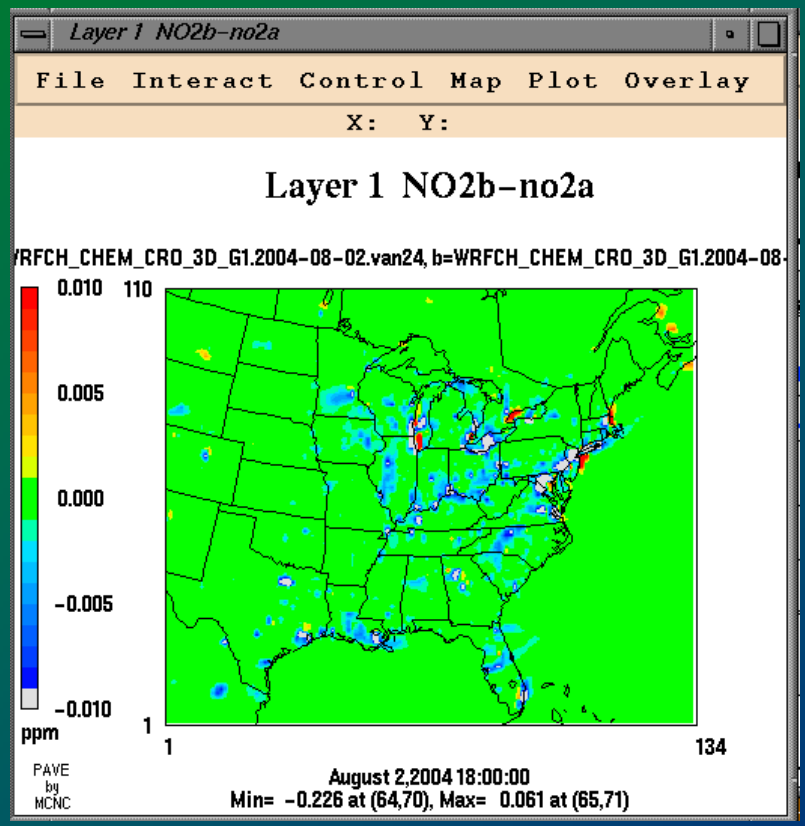


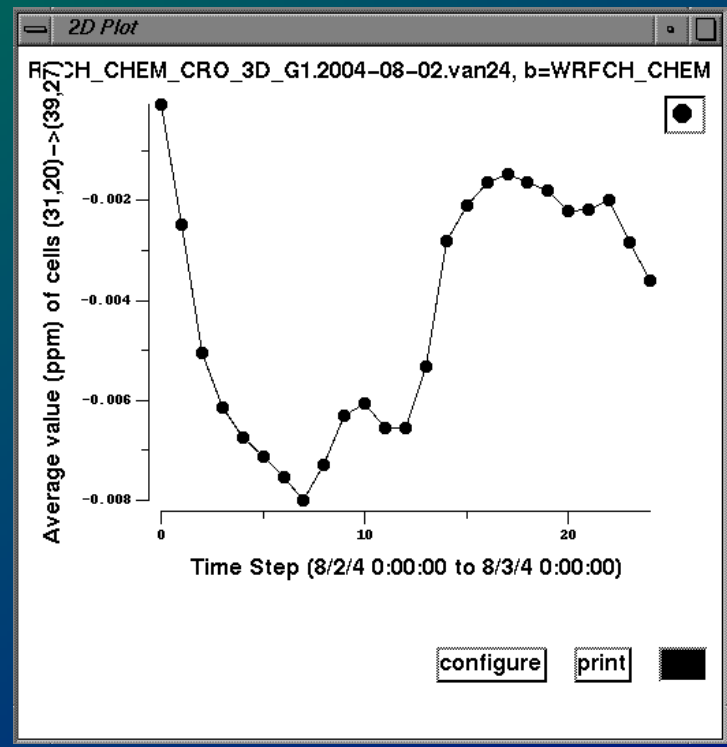


WRF-SMOKE **WRF-Vanilla**

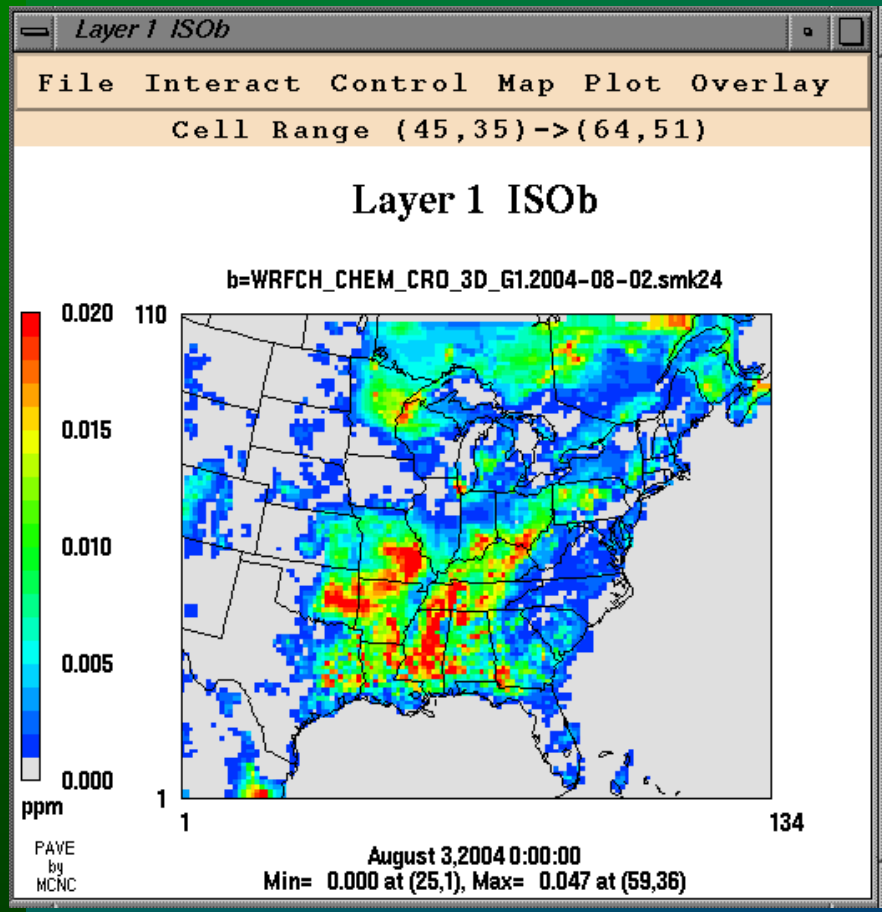
CASE Study and Results: NO2:

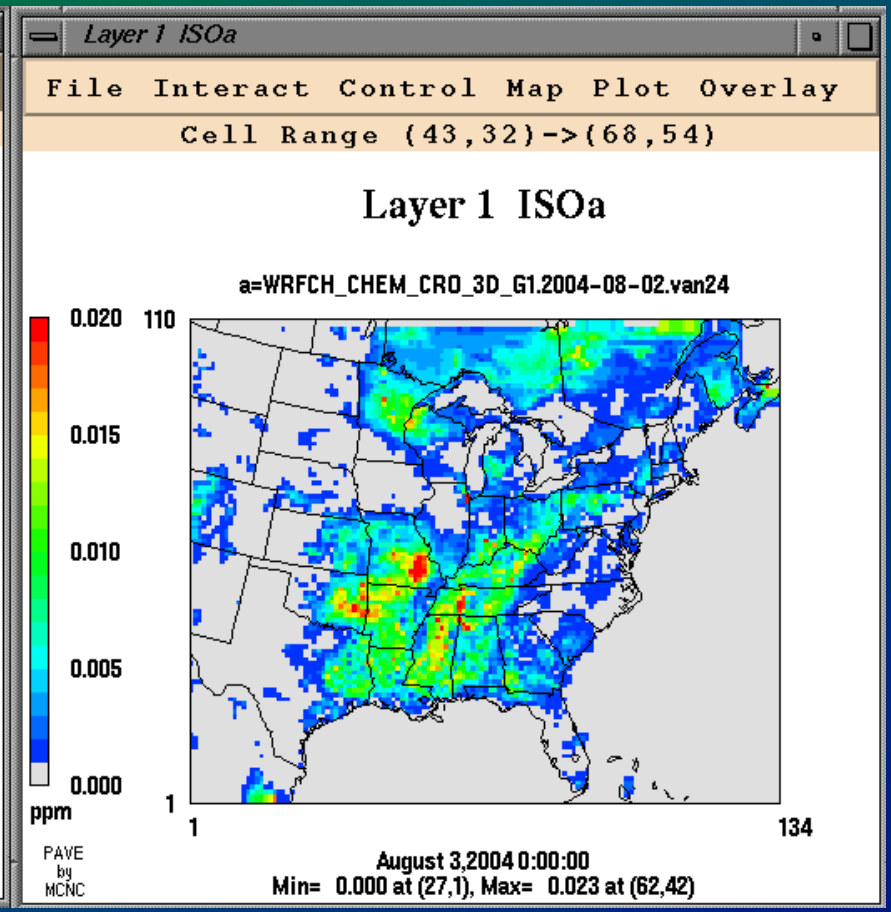
*difference field at 18z (left);
*difference time series for Houston metro (right)





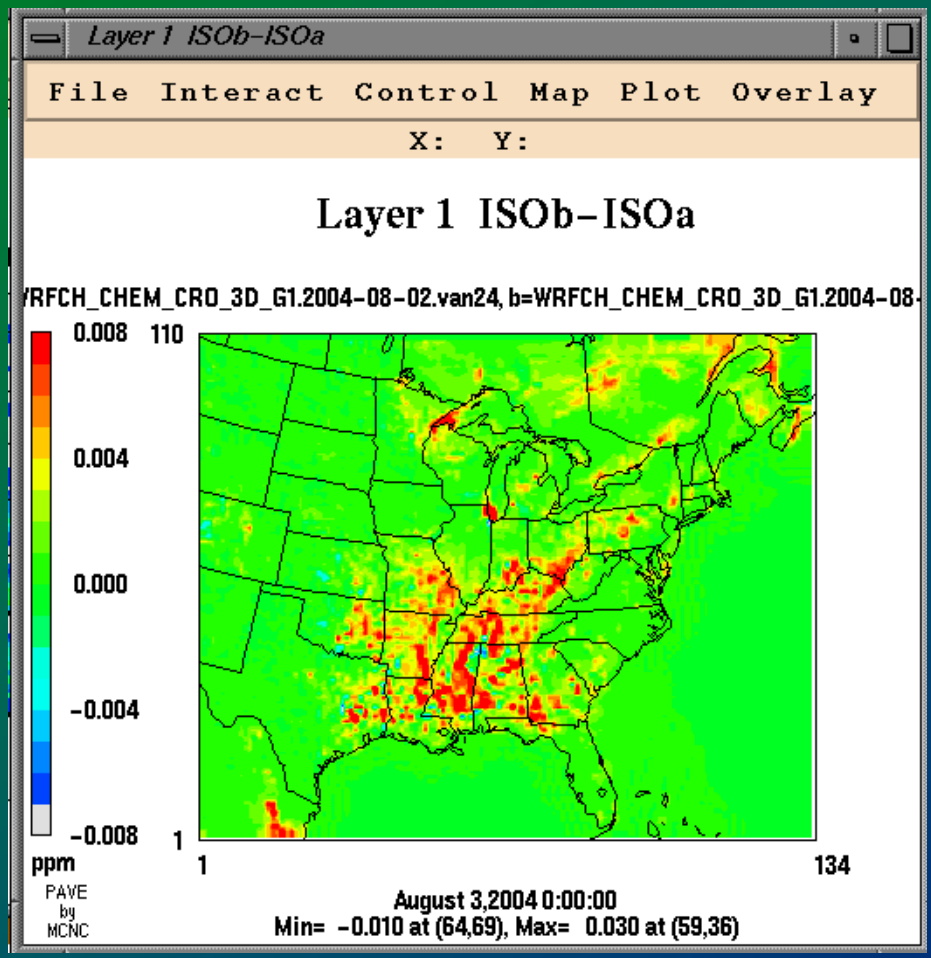
CASE Study and Results: Isoprene at "24z"

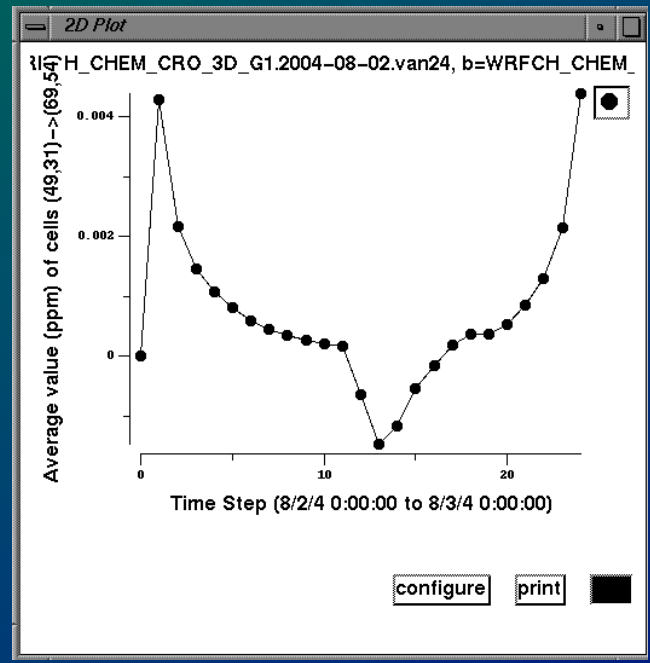




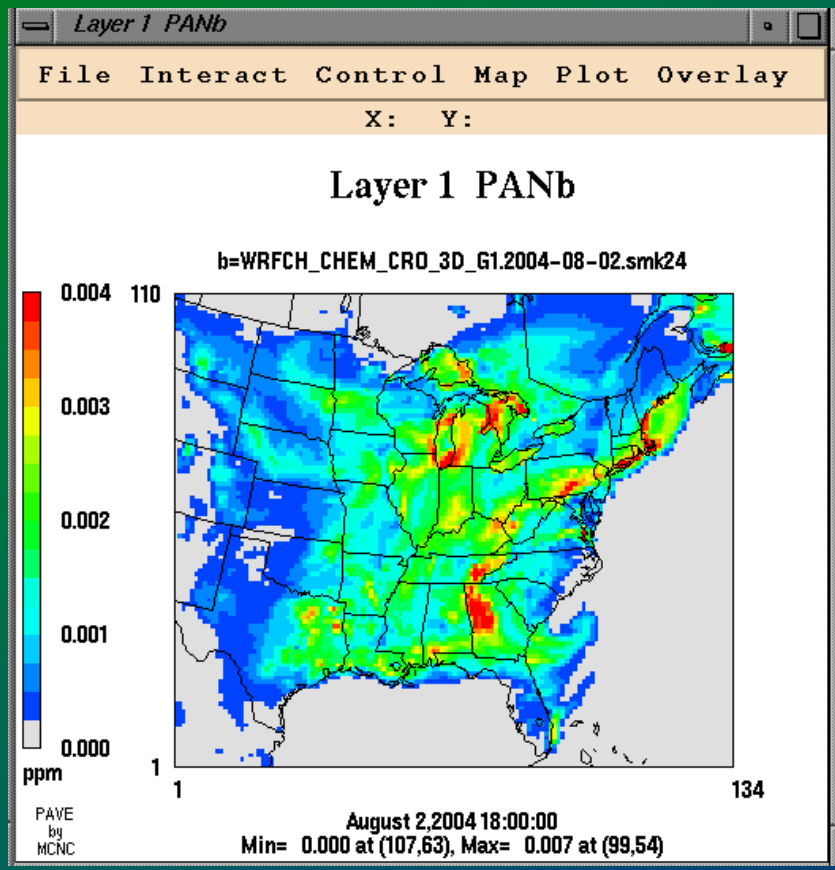
WRF-SMOKE **WRF-Vanilla**

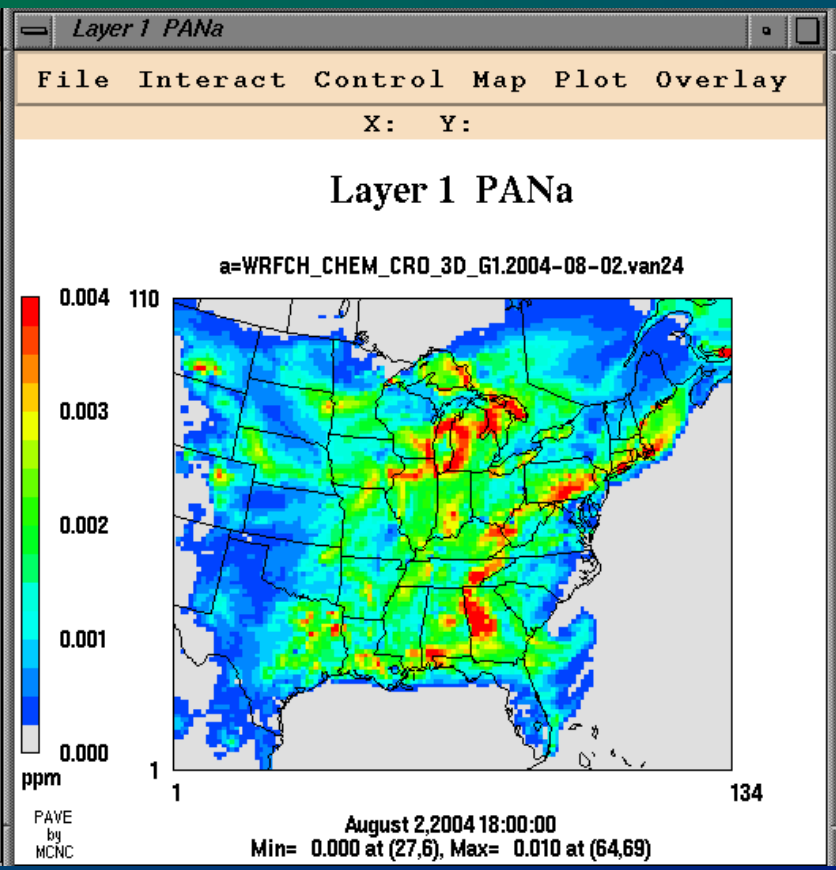
CASE Study and Results: Isoprene Difference Field after 24 hours (left): Isoprene (SMOKE) minus Isoprene (VANILLA); Difference time series (right)





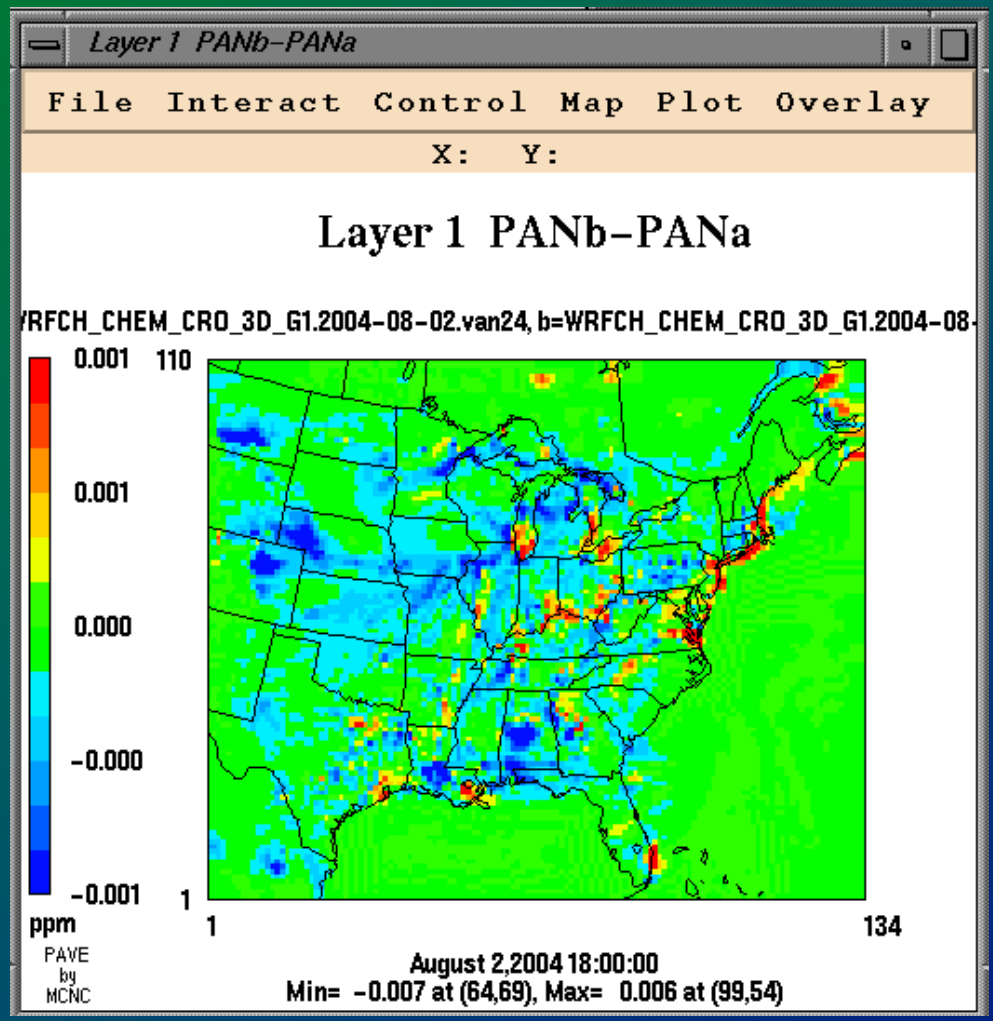
CASE Study and Results: PAN at 18z



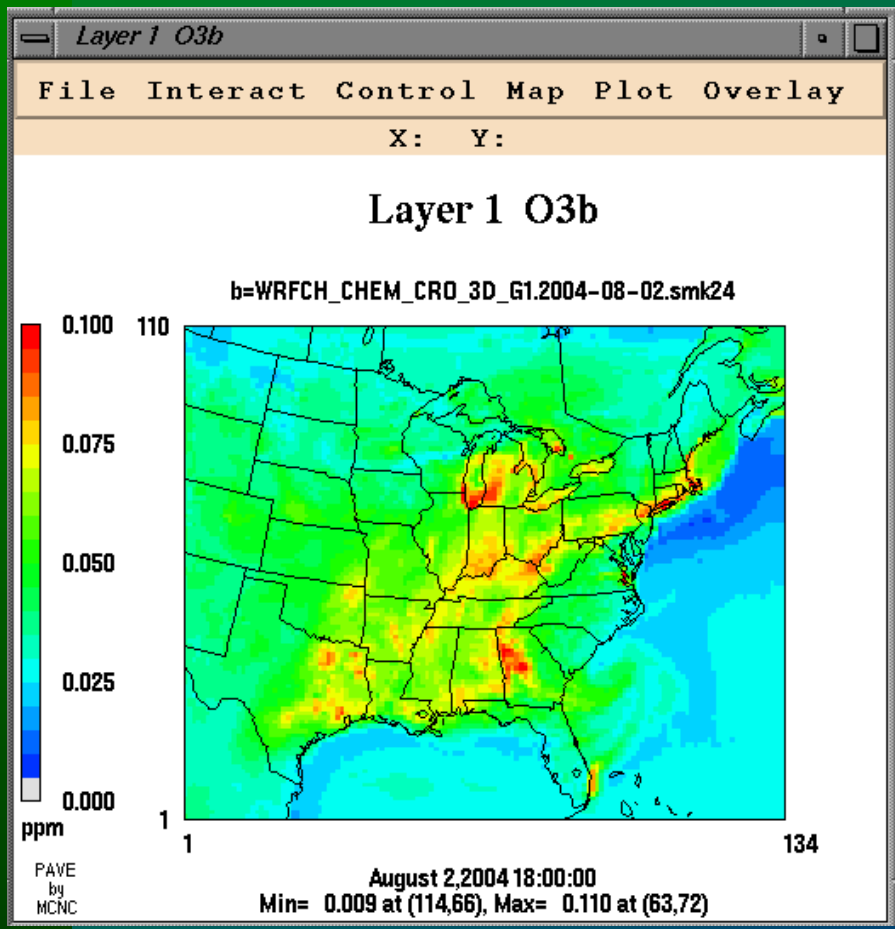


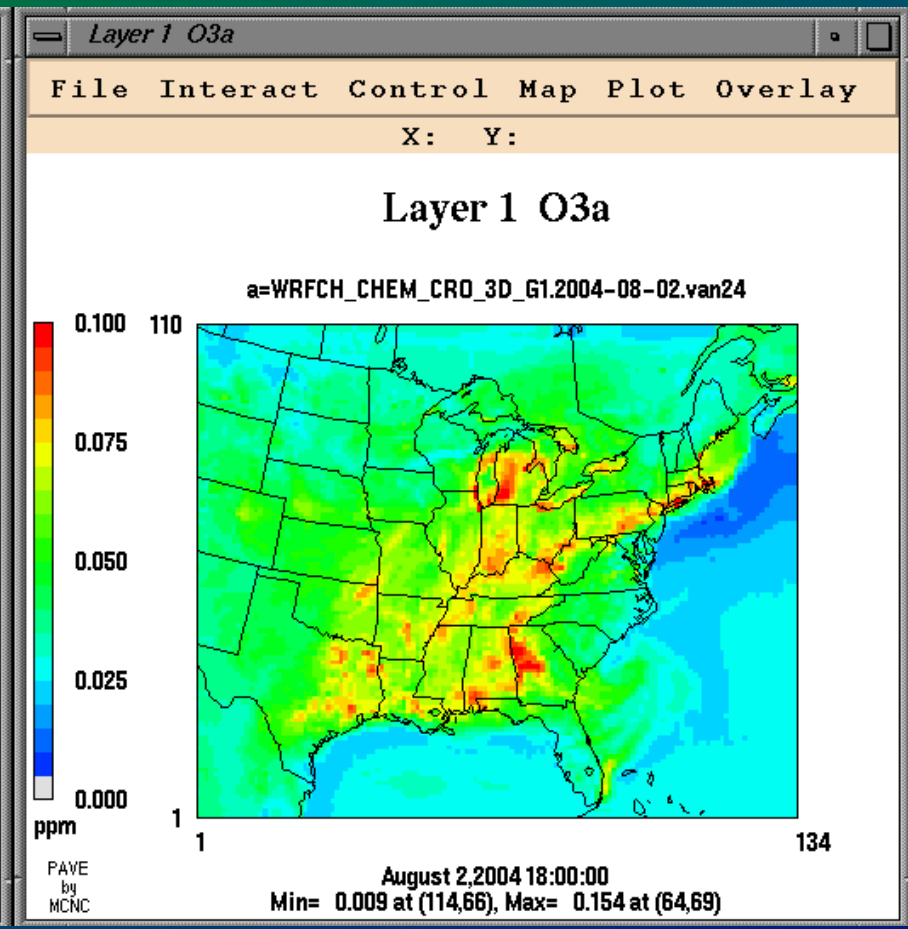
WRF-SMOKE **WRF-Vanilla**

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



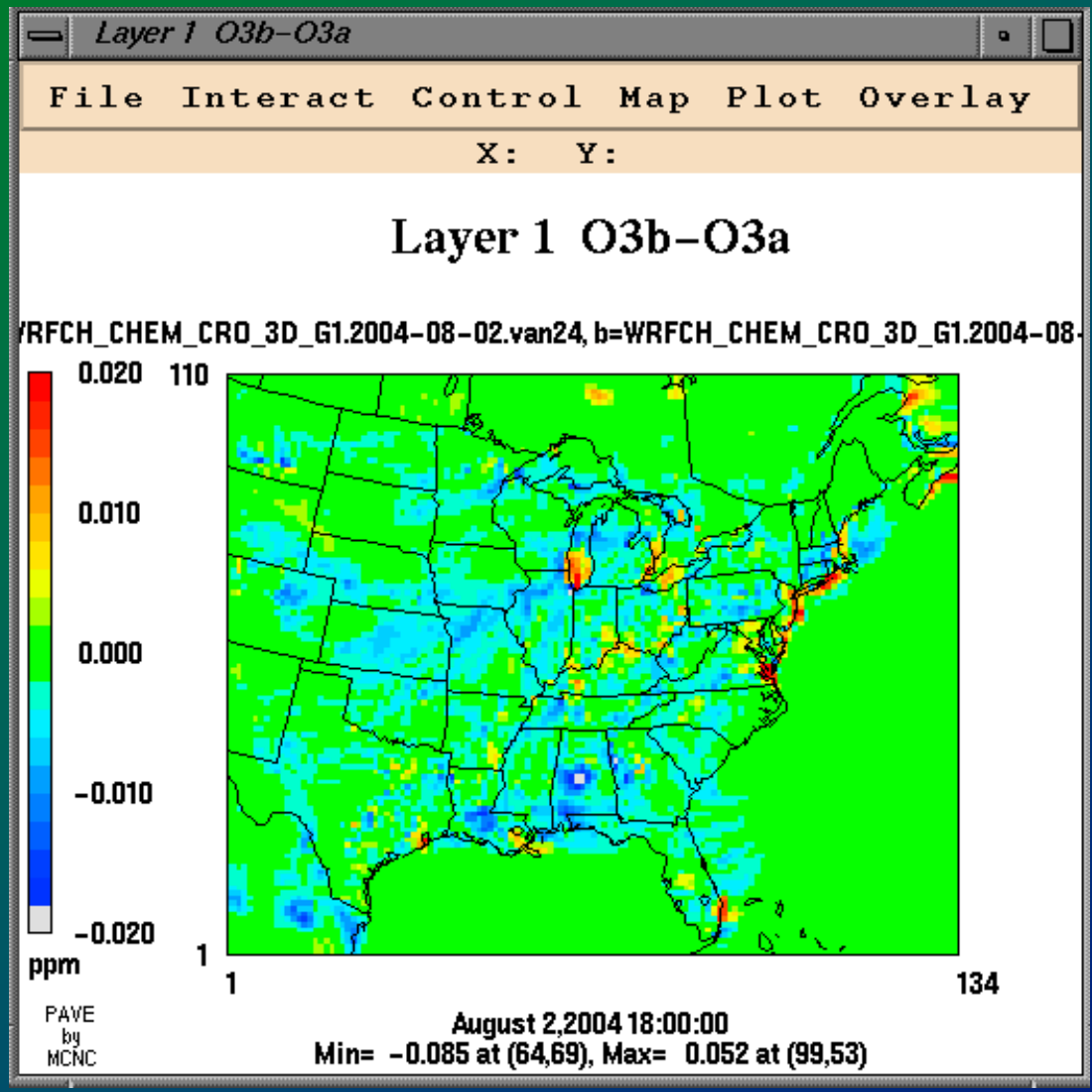
CASE Study and Results:O3 at 18z



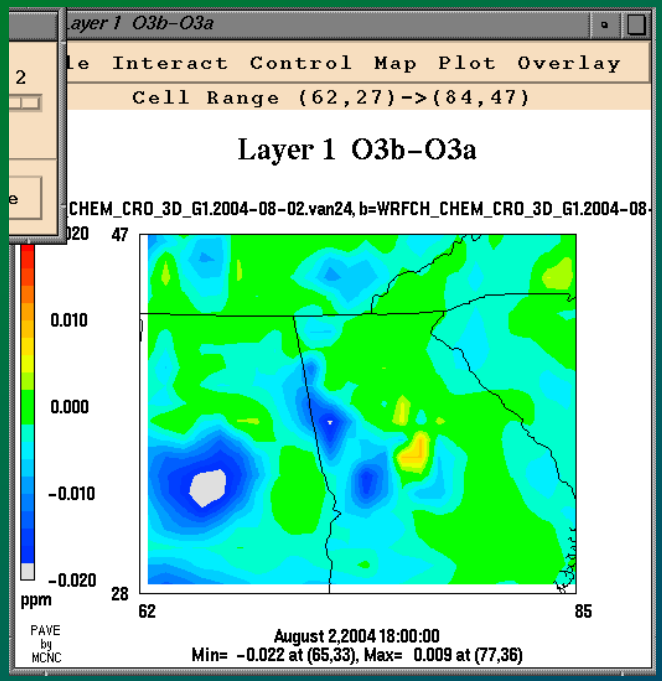


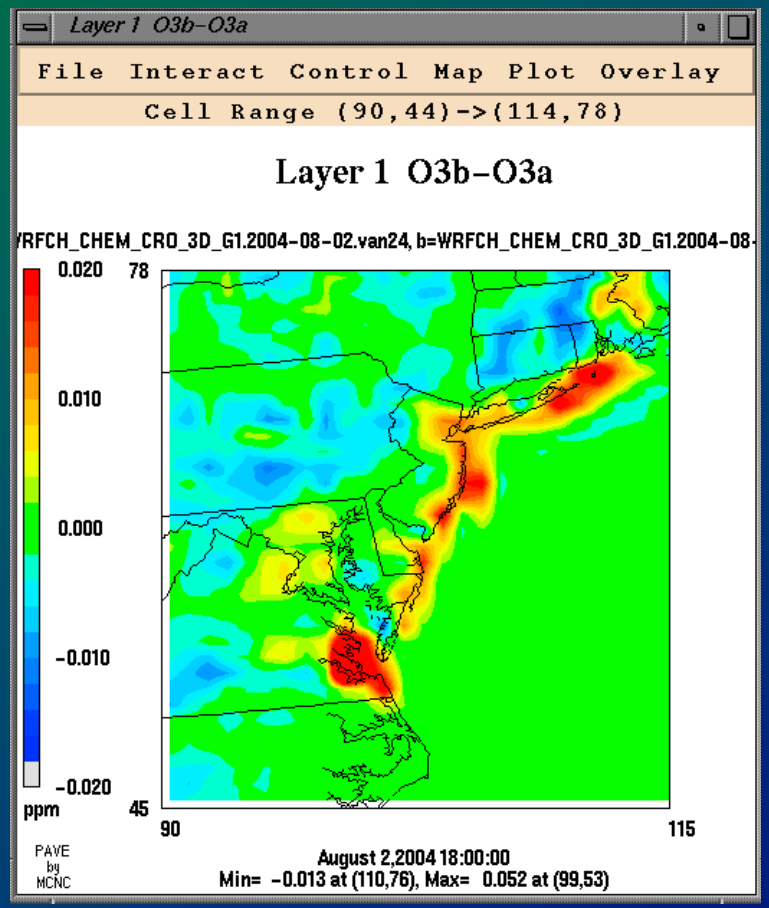
WRF-SMOKE **WRF-Vanilla**

CASE Study and Results:O3 difference field at 18z

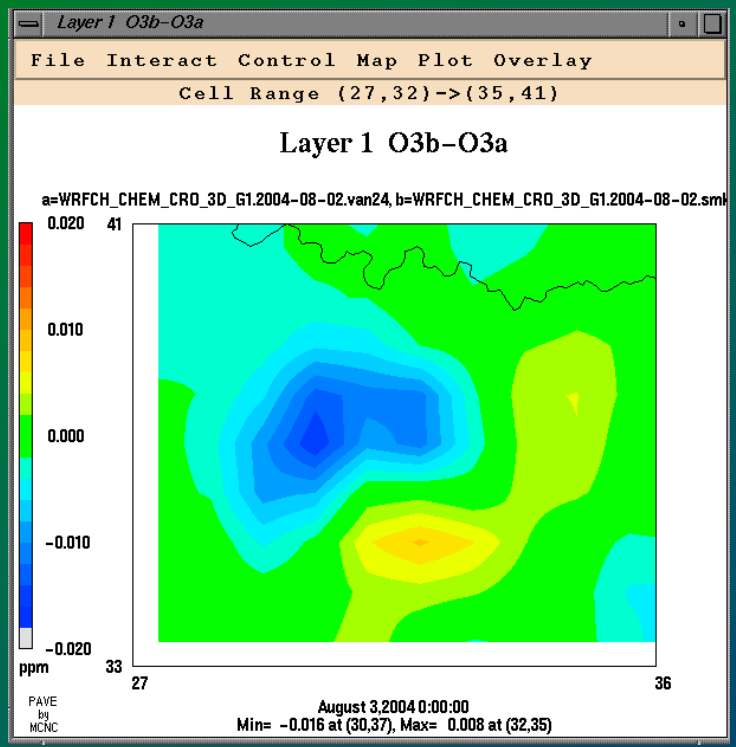


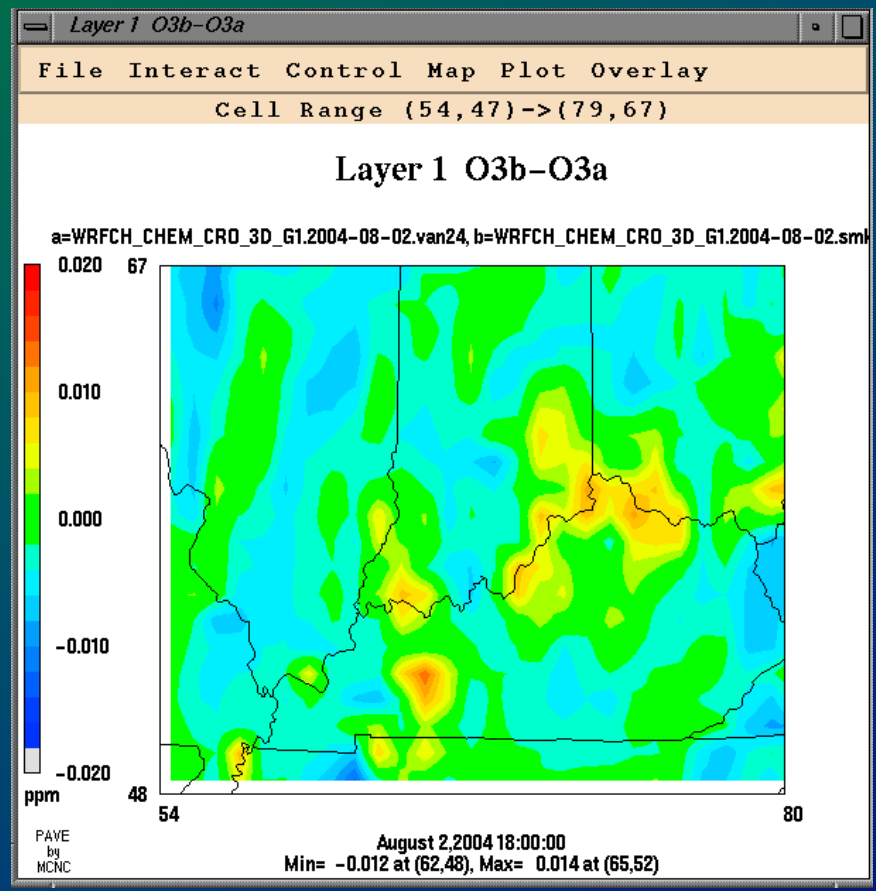
CASE Study and Results: Regional O3 Difference fields at 18z



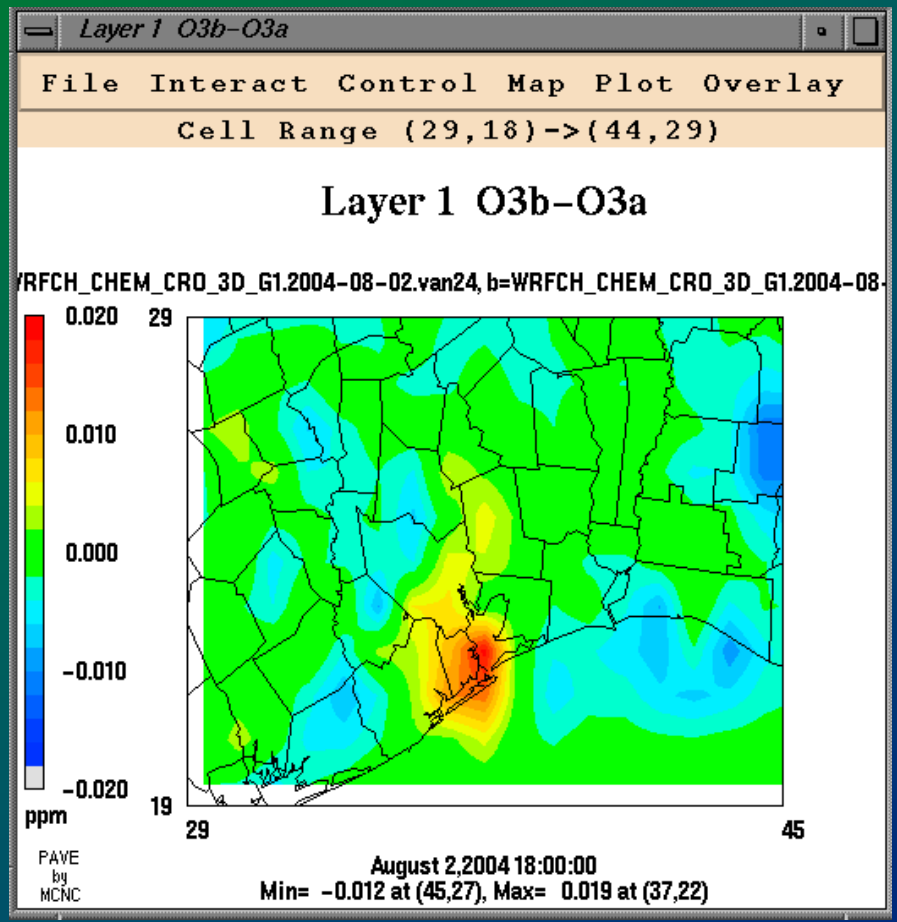


CASE Study and Results: Regional O3 Difference fields at 18z [DFW and Ohio Valley]

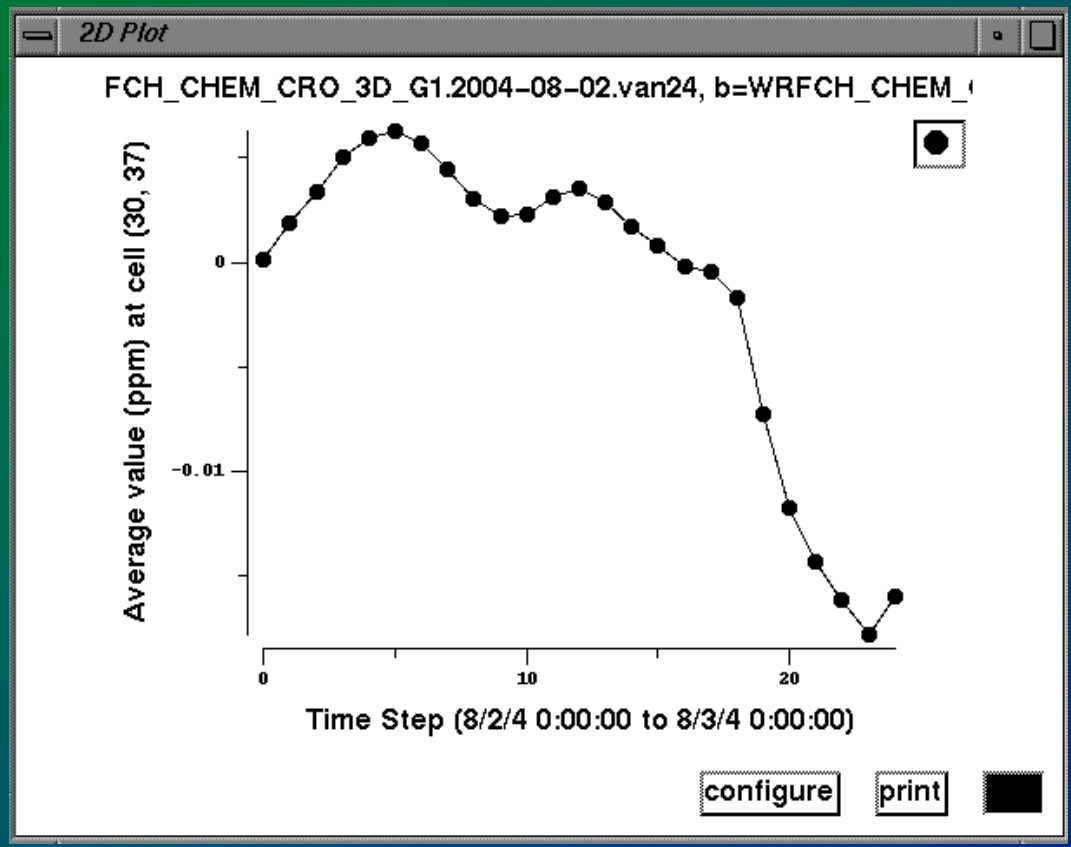




CASE Study and Results: Regional O3 Difference fields at 18z [Houston}



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



Conclusions

- **SMOKE-RT has been implemented within the WRF-Chem 2.1 modeling system**
- **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***
  - ***(See, for example, Wilczak et al., 2006 submitted to JGR) – in an ensemble study w/ 8 ozone forecast models, the authors found that "the greatest improvement in model skill can be achieved through improving spatial variations of the meteorological forecasts [sub-synoptic] as well improving local emissions variations….)***

Acknowledgements

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• George Grell and Steven Peckham of the Forecast Systems Lab for many useful discussions regarding WRF-Chem

• John Michelakes of NCARs MMM division for continuing discussions regarding the WRF software architecture

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