Oil & Natural Gas Technology

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Annual Progress Report

(April 17, 2006 - April 16, 2007)

Modeling the Transport and Chemical Evolution of Onshore and Offshore Emissions and Their Impact on Local and Regional Air Quality Using a Variable-Grid-Resolution Air Quality Model

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Office of Fossil Energy

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Abstract

By the end of this project reporting period, we had completed most of the tasks that were originally planned. We identified modeling domains and case studies to perform meteorological and air quality model simulations. We evaluated the performance of two different atmospheric boundary layer schemes, and identified the best-performing scheme for simulating mesoscale circulations for different grid resolutions. Use of a newly developed surface data assimilation scheme has resulted in improved meteorological model simulations. We have also successfully ingested satellite-derived sea surface temperatures into the meteorological model simulations, leading to further improvement of simulated wind, temperature, and moisture fields. We believe that these improved meteorological fields will lead to improved simulations from our variable-grid-resolution air quality model. We are close to completing the development of a variable-grid version of SMOKE, our emissions processing model; we are currently performing further testing and evaluation of this new emissions modeling tool. Also, we have updated our emissions database to include the newly released off-shore and on-shore emission estimates over the Gulf of Mexico. Further, we have completed the development of our variable-grid-resolution air quality model (MAQSIP-VGR) and performed various diagnostic tests. We have started the test runs for MAQSIP-VGR for the Houston-Galveston domain.

Contents

1. Project Objectives

This research project has two primary objectives:

(1) To further develop and refine the Multiscale Air Quality Simulation Platform – Variable Grid Resolution (MAQSIP-VGR) model, an advanced variable-grid-resolution air quality model, to provide detailed, accurate representation of the dynamical and chemical processes governing the fate of anthropogenic emissions in coastal environments.

(2) To improve current understanding of the potential impact of on-shore and off-shore oil and gas exploration and production (E&P) emissions on O_3 and particulate matter nonattainment in the Gulf of Mexico and surrounding states.

2. Task Descriptions and Progress

Out of the eight tasks proposed under this project at its inception, Tasks 5, 7, and 8 were to be completed in the final year of the original three-year project. We have requested and been granted an extension to October 2007. The eight subsections below summarize the status of each of the tasks and describe any planned work needed to finish up the project.

2.1 Task 1: Develop Modeling Domains and Case Studies

This task is complete. We developed four domains for use in performing numerical simulations with a meteorological model, the Mesoscale Model Version 5 (MM5), to generate meteorological inputs to the MAQSIP-VGR. These meteorological modeling domains (Figure 1) are configured with different horizontal grid resolutions: 36, 12, and 4 km. To specifically study the effects of on-shore and off-shore emissions on the coastal environments, we developed two different 4-km-resolution domains for performing air quality modeling studies: one over the Houston-Galveston region and the other over southern Louisiana.

We selected an initial time period of August 23 through September 2, 2000, for our numerical simulation over the Houston-Galveston region. These dates were chosen because a severe air pollution episode occurred over the region at that time.

2.2 Task 2: Improve the Representation of Boundary Layer Processes

This task is complete. We selected the K-profile approach as the boundary layer scheme for the MM5 simulations to prepare meteorological inputs to drive the MAQSIP-VGR.

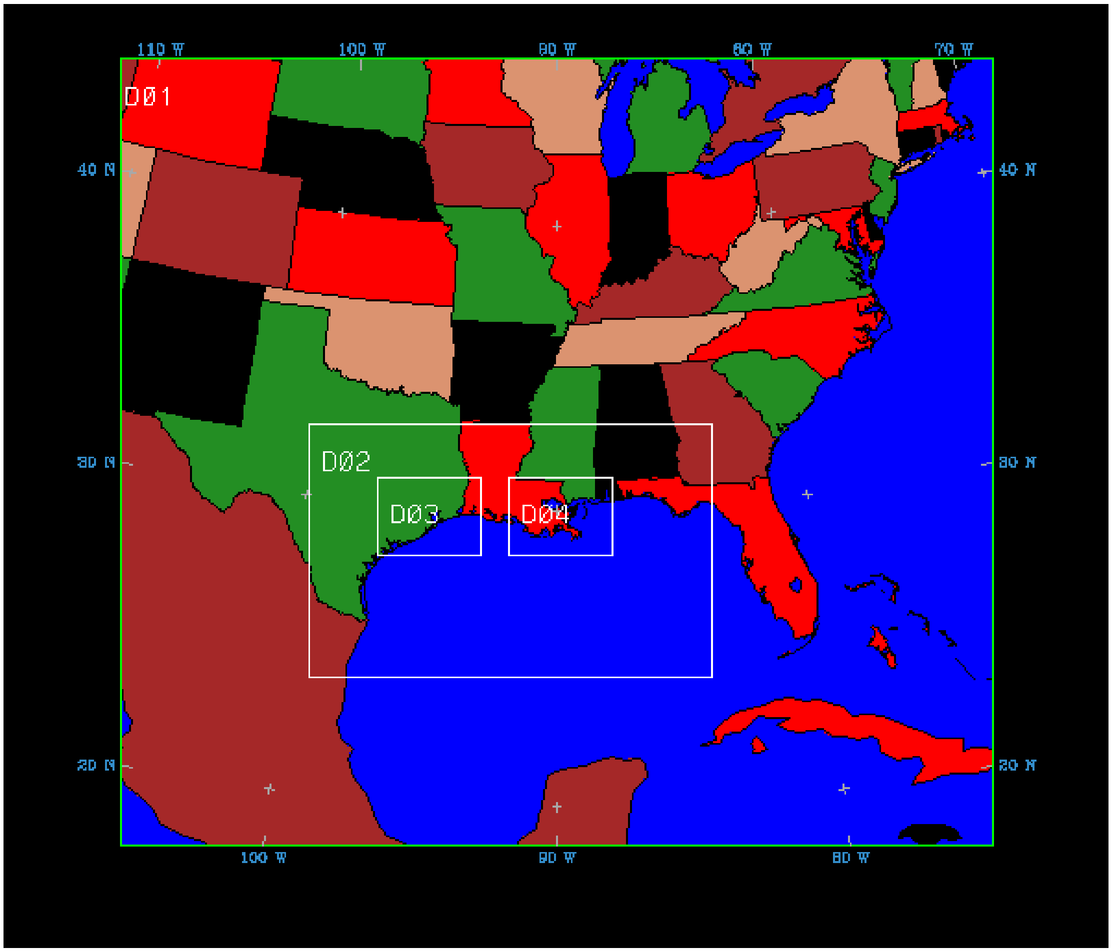


Figure 1. Simulation domains for the MM5 simulations. Domains D01 and D02 use 36- and 12-km grids, respectively, while domains D03 and D04 use 4-km grids located over the Houston-Galveston region and southern Louisiana.

2.3 Task 3: Assimilation of Surface Observations to Improve MM5 Simulations

This task is complete. We analyzed the MM5 simulations obtained using the base configuration structure and those obtained using the Flux-Adjusting Surface Data Assimilation System (FASDAS). The FASDAS-based results showed improvements in boundary layer simulations in both the 36- and 12-km-resolution domains. We completed a data assimilation exercise using GOES satellite-derived sea surface temperatures instead of the climatological sea surface temperature patterns used in MM5. The results showed considerable changes in the land-sea breeze circulations and the lower tropospheric dynamics.

2.4 Task 4: Simulate Mesoscale Circulations Using the MM5

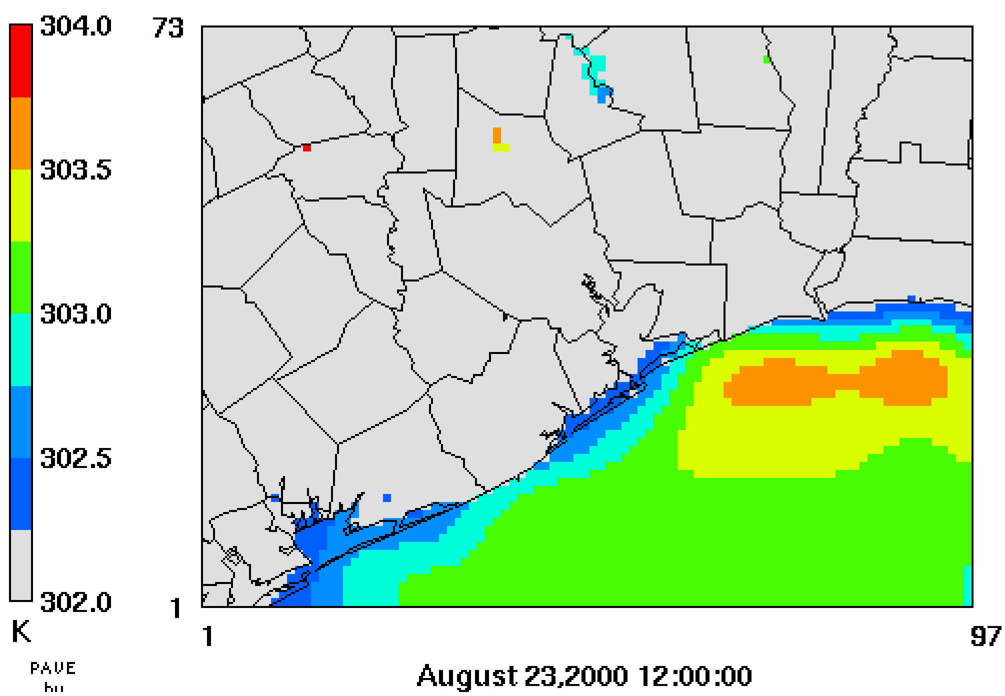
This task is complete. For the summer of 2000, we conducted an episodic MM5 simulation of domain D01 at 36-km horizontal resolution and of domain D03 at 4-km resolution (both domains are shown in Figure 1). These meteorological simulations were done on a uniform grid resolution for the period August 23 through September 2, 2000. As mentioned in Section 2.3 (Task 3), using satellite-derived sea surface temperatures instead of climatological sea surface temperatures for the Gulf region as part of domain D03 at 4 km affects the land-sea breeze circulation. This in turn affects the pollution transport in-land and off-land. As an example of the difference that results from using the two approaches for sea surface temperature, Figure 2 shows the sea surface temperature distribution based on the satellite-derive approach and on the climatological sea surface temperatures often used for meteorological modeling simulations. Noticeable is the large difference in the magnitude of sea surface temperature between the two cases (note that the scales are different) and the spatial distribution of the temperature patterns

Figure 3 shows differences in the simulated MM5 wind fields for domain D03 in the lower layer between the satellite-derived sea surface temperature case (Vsat) and the wind simulation using climatological sea surface temperatures (Vbase) for 1 September 2000 at 2000 UTC (8:00 PM local time) and 1500 UTC (9:00 AM local time). The figure reveals how using the satellite-derived sea surface temperature affects the wind strength and direction. It is also important to notice that the effect has diurnal variation (compare the morning plot with the evening plot). The differences seen in the wind vector are caused by the temperature gradients between land and sea. While the sea surface temperature can change only a little on an hourly basis due to the large heat capacity of the water surface, the land surface on the other hand generally has a relatively strong diurnal cycle. In the early hours of the morning the land surface tends to be cooler than the water surface due to the loss of heat during the night through radiative cooling. In the afternoon the land surface temperature tends to be higher than the temperature of the adjacent water surface. Such contrasts in land-sea temperature trigger land-sea breezes and control their direction (in-land or off-land) in accordance with the land-sea temperature gradient. Clearly this is an important mechanism to include in the calculation of pollution transport near coastal areas and in defining the extent of the pollution reach (in-land or off-land).

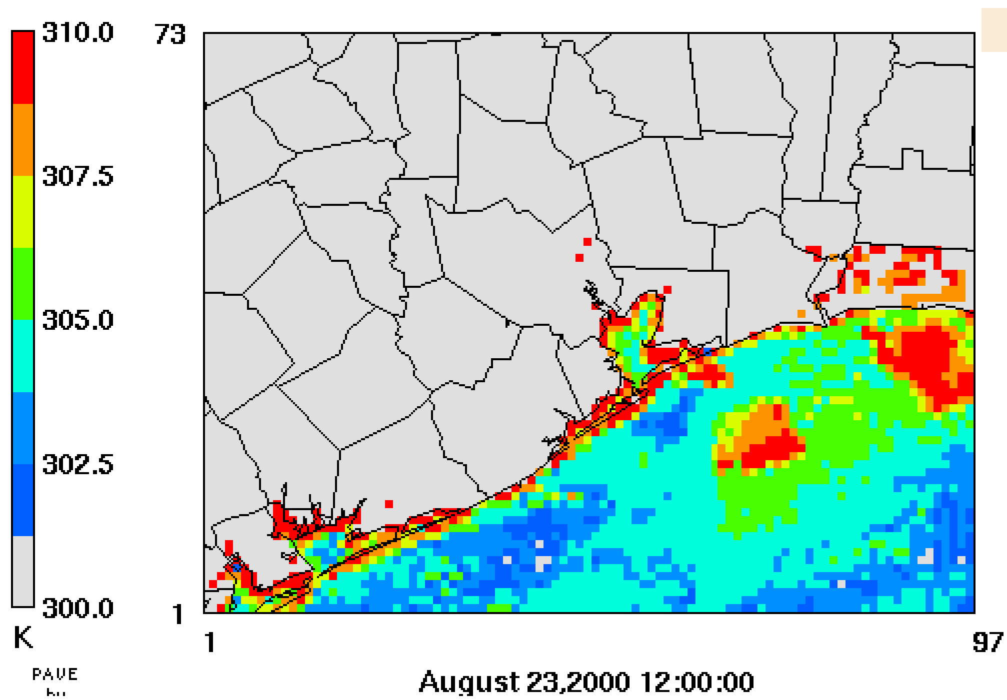
2.5 Task 5: Develop Emission Estimates

We are using the National Emissions Inventory (NEI) 1999 Version 3. Updates in this NEI version include revisions to area, nonroad, and point sources. For updating mobile sources, we will use MOBILE6 with updated vehicle miles traveled (VMT) data from the Texas Commission on Environmental Quality (TCEQ). Other databases available from the TCEQ are a 1999 area/nonroad inventory and a 1997 Galveston Bay shipping inventory. Further, TCEQ has an off-shore point- and area-source inventory that we have used in the past; we will contact TCEQ for any updates. We will also use BELD3 land cover data (available at 1-km resolution) to estimate biogenic emissions. For the Mexico region, we will use the 1999 BRAVO Mexican inventory. Emissions data for the Outer Continental Shelf in the Gulf of Mexico that are available from MM5 will also be included in updating our emissions database.

The variable-grid SMOKE (SMOKE-VGR) will be used to prepare emissions estimates for use in the MAQSIP-VGR. At the time of preparing this report, we are working on an issue in the variable-grid SMOKE code and expect it to be resolved shortly.

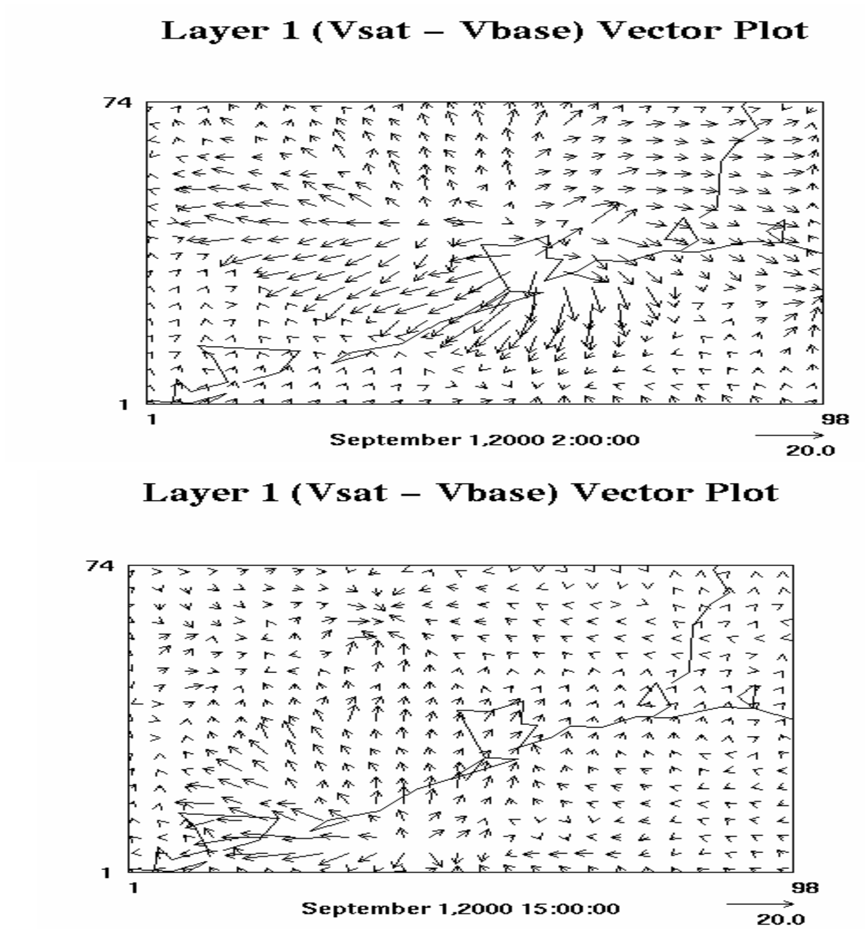


(a)



(b)

Figure 2: Comparison of spatial distributions of sea surface temperature at 1200 UTC 23 August 2000 in domain D03 obtained from (a) the climatological sea surface temperature (traditional NCEP analysis) and (b) NOAA's satellite-derived measurements. Note the difference in the scale ranges.



(a) (b)

Figure 3: Spatial distribution of the differenced MM5-simulated vector winds in Domain D03; values shown are [values from NOAA's satellite-derived measurements] minus [values from traditional climatological analysis], for 1 September 2000 at (a) 2000 UTC (8:00 PM local time) and (b) 1500 UTC (9:00 AM local time).

2.6 Task 6: Enhance Representation of Cloud Processes in the MAQSIP-VGR

We analyzed the results of a 1-D cloud model to examine the effect of the fine-resolution configuration of the variable-grid model on the cloud processes, which in turn affect the pollutant formation and deposition.

There are four primary processes by which clouds modify atmospheric chemical composition and distribution: (1) sub-grid-scale vertical turbulent redistribution of mass; (2) aqueous chemical effects, including dissolution, dissociation, and kinetic reactions; (3) rainout and wet removal due to precipitation; and (4) modification of solar actinic flux and hence the rate of photolytic reactions.

The current representation of cloud effects in the MAQSIP-VGR accounts only for attenuation of photolysis rates due to the presence of clouds and is based on the cloud fields specified by the driving meteorological fields. We will perform some sensitivity modeling analysis to examine the effect of extending the model representation of cloud processes to include the other effects discussed above by adapting the mesoscale and urban-scale cloud modules available in the uniform grid version of the MAQSIP model. This includes representation of shallow convection, deep convection, resolved-scale clouds, and sub-grid-scale layer clouds**.**

2.7 Task 7: Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain

Figure 4 shows a flow diagram of the variable-grid modeling components. MM5 simulations using a uniform grid provide the file MMOUT, which includes the meteorological simulations for specific episodes. The meteorological outputs are processed through the Meteorology-Chemistry Interface Processor (MCIP) for the same uniform grids. The variable-grid horizontal grid structure is introduced through the grid definition file ("S-Grid" in Figure 4), which provides grid information to allocate all data onto the variable grid, to process emissions through the SMOKE-VGR and to process chemistry through the MAQSIP-VGR.

Meteorological data as an output from MM5 are available from previous runs of the model on a uniform grid at horizontal resolutions of 36 km, 12 km, and 4 km (domains D01, D02 and D03, shown in Figure 1).

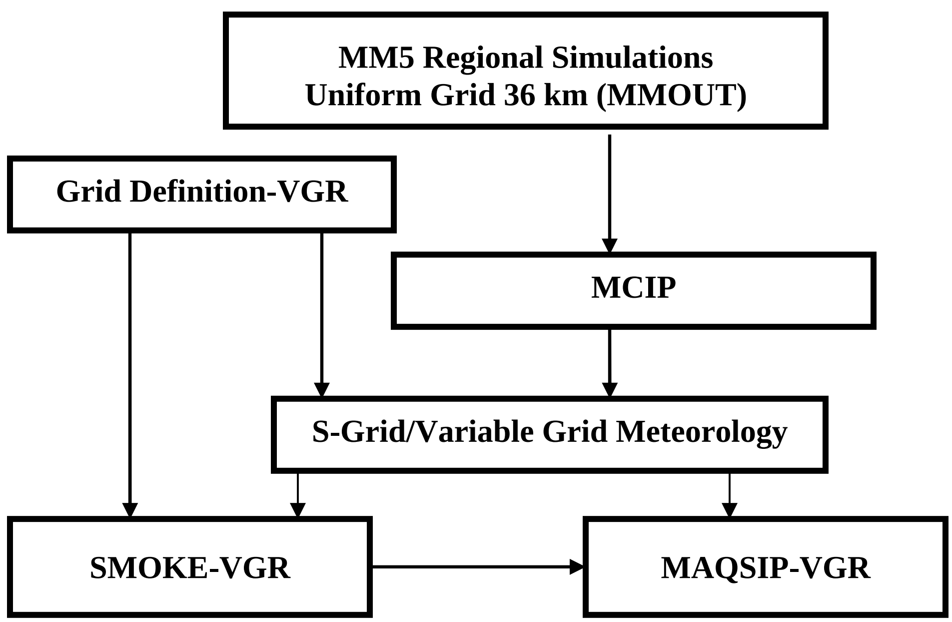


Figure 4: Flow diagram of the variable-grid modeling components.

We are currently processing the data needed to generate the meteorological variable-grid inputs for the Houston-Galveston domain. The Houston case will use the meteorological inputs of the 10-day summer episode noted earlier (August 23 through September 2, 2000) to demonstrate the variable-grid modeling concept. As described above and shown in Figure 4, the meteorological output data from MM5 and MCIP will be processed to prepare variable-grid meteorology data that feed into the SMOKE-VGR to prepare variable-grid emissions. The meteorological and emissions data on the variable grid are the two main inputs to MAQSIP-VGR.

Terrain heights are another input to the MAQSIP-VGR. Figure 5 compares terrain model input data when using a uniform grid at 36 km (domain D01), a uniform grid at 12 km (domain D02), a uniform grid at 4 km (Domain D03), and a variable grid (domain D01).

We used the visualization package NCL to create the variable-grid graphics.

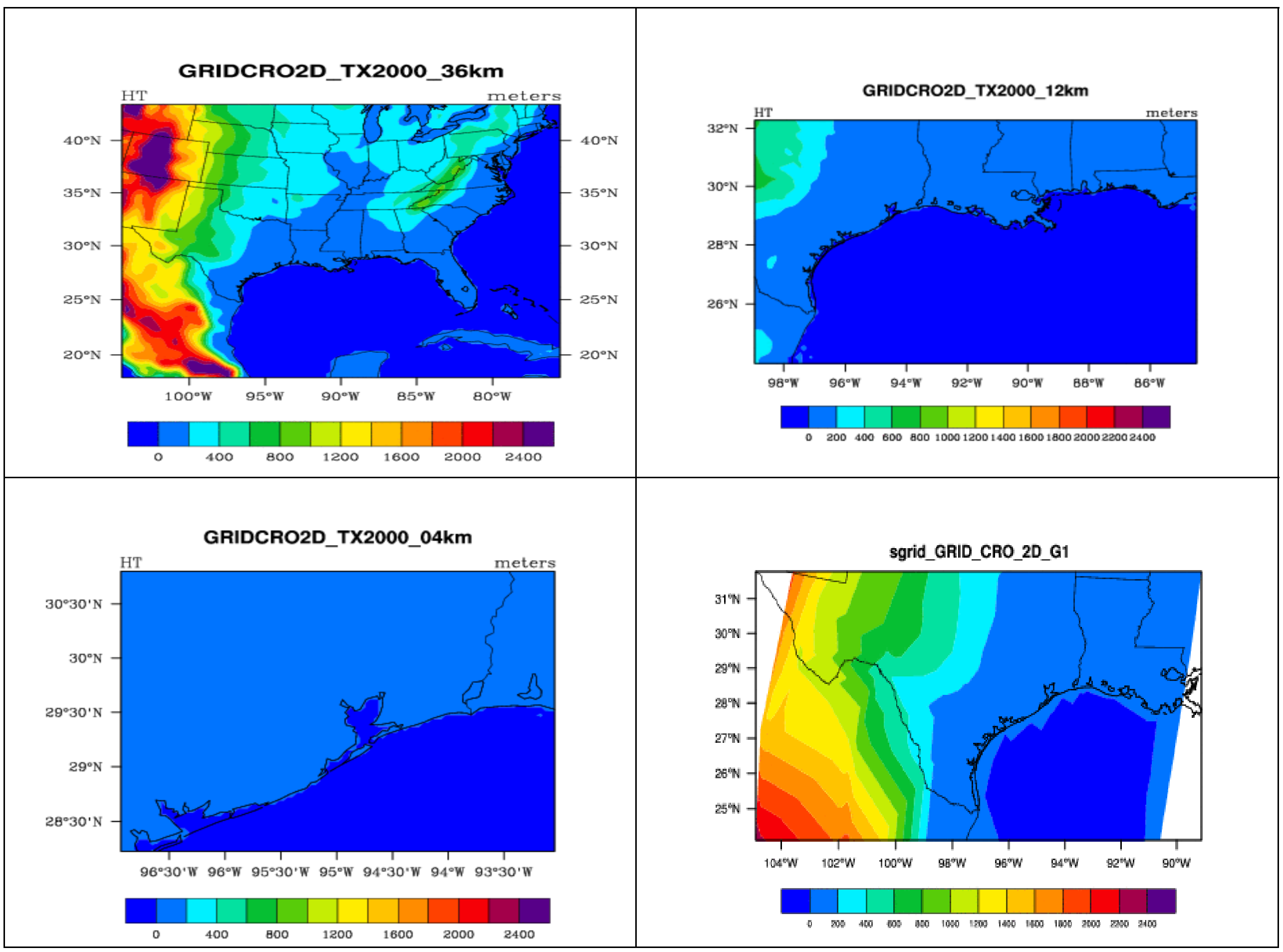


Figure 5: Terrain height from uniform grid 36 km (top left), 12 km (top right), 4 km (bottom left) and from variable-grid (bottom right).

2.8 Task 8: Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain

Following the completion of MAQSIP-VGR simulations over the Houston-Galveston region, we will perform MAQSIP-VGR simulations for selected periods during 1998 and/or 2000 over the northeast Gulf domain (the D04 southern Louisiana region in Figure 1). Model simulations will focus on assessing the impact of off-shore emissions from oil and gas E&P facilities on local and regional air quality in the southern states. Model simulations of ozone will be compared to available measurements from the EPA Air Quality System (AQS) database (U.S. EPA; http://www.epa.gov/air/data/index.html).

3. Project Publications

1) A presentation and review of the project's tasks and results were presented during

> DOE/PERF Air Program Review, August 22-23, 2007, Annapolis, MD. Hosted by Argonne National Laboratory. (The presentation is an appendix in this report.)

2) An abstract has been submitted for presentation at the American Meteorological Society annual meeting in January 2008:

> "Application of a Variable-Grid Air Quality Model to Simulate On-shore/Off-shore Emissions Near Coastal Areas" – Hanna, Alapaty, Mathur, Arunachalam, Xiu, and Shankar

3) Following the completion and analysis of all the variable-grid simulations, a journal article will be prepared (Dr. Alapaty will be the lead author) to document the methodology and results in a scientific journal.

4) A project web site has been prepared to display the results of the project (at this time it is password protected). Web site URL:

> http://www.ie.unc.edu/cempd/projects/variable_grid/index.cfm

Appendix

This appendix contains the presentation given at the DOE/PERF Air Program Review, August 22-23, 2007, Annapolis, MD.

Modeling the Transport and Chemical Evolution of Onshore and Offshore Emissions and Their Impact on Local and Regional Air Quality Using a Variable-Grid-Resolution Air Quality Model

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August 22, 2007

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Department of Energy
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Kiran Alapaty and Rohit Mathur (Co-PIs)
UNC-Chapel Hill

Objectives

- **Develop and refine an advanced variable-grid-resolution (VGR) air quality modeling tool to provide detailed, accurate representation of the dynamical and chemical processes governing the fate of anthropogenic emissions in coastal environments**

- **Improve the current understanding of the potential impact of onshore and offshore exploration and production (E&P) emissions on O_3 and particulate matter nonattainment in the Gulf of Mexico and surrounding states**

Approach

- Three components of the air quality modeling system (MM5, SMOKE, MAQSIP)
- Development of detailed emission estimates for offshore sources
- Improvements in the simulation of dynamical and thermodynamical processes influencing pollutant dispersion and transport in coastal and marine environments
- Modeling of the transport and chemical evolution of emissions from onshore and offshore E&P facilities using the VGR model
- Detailed evaluation of our modeling system's simulations

Raw Meteorology Data

Fifth-Generation
Mesoscale Model (MM5)
Creation of Meteorology Data Fields

Emissions Inventories
(Data on Area, Mobile, Point,
& Biogenic Sources)

Met-Chem Interface Processor (MCIP)
Meteorology Data Processing for Input
to CMAQ & SMOKE

SMOKE
Anthropogenic & Biogenic
Emissions Processing

MAQSIP-VGR Air Quality Model

Hourly, 3-D, Gridded Output
Chemical Concentrations (e.g.,
Ozone, Particulate Matter)

Multiple Domain Simulations

36 km, 12 km, 4 km

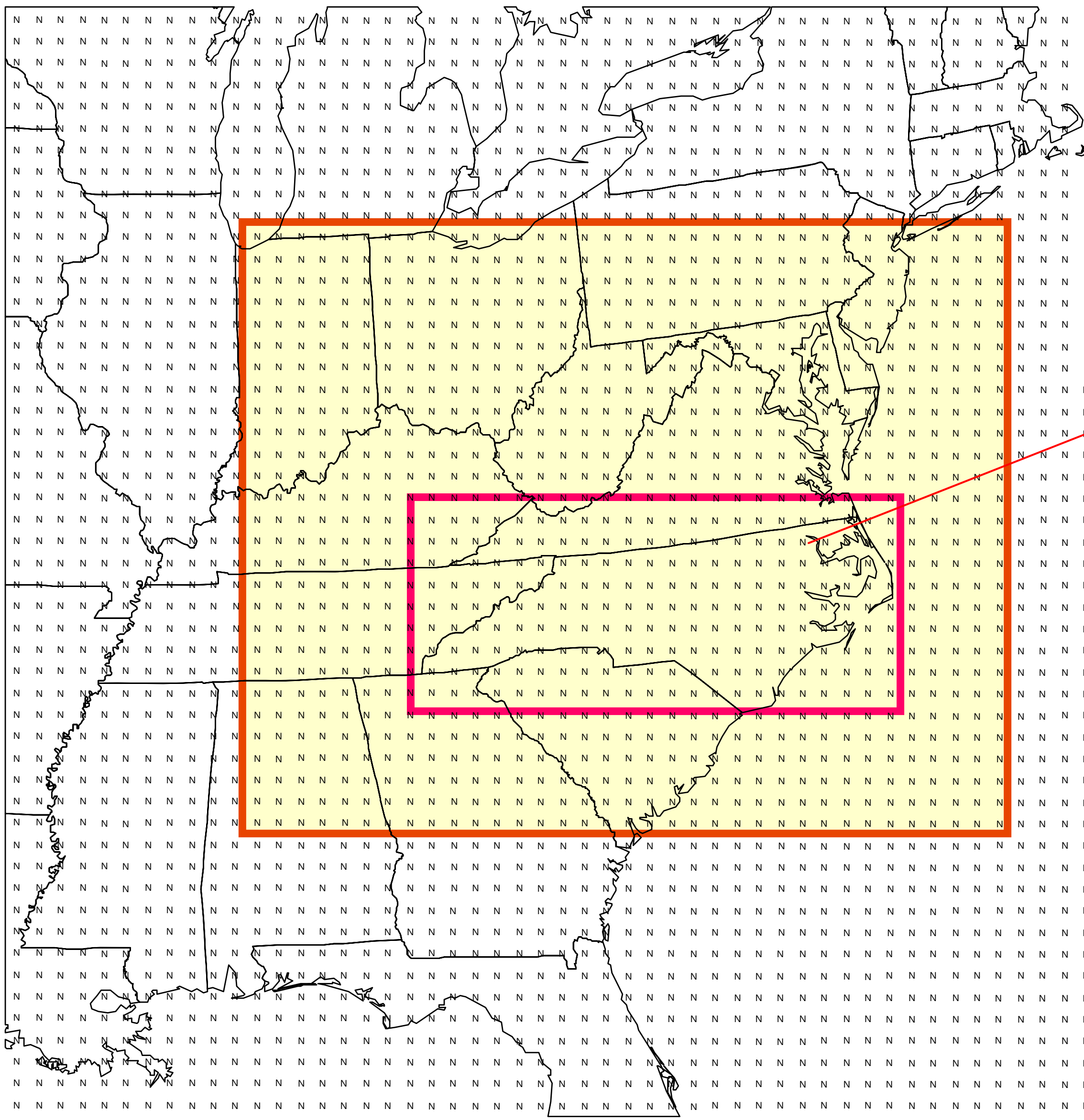
36 km

LBC

12 km

LBC

4 km



Domain of Interest

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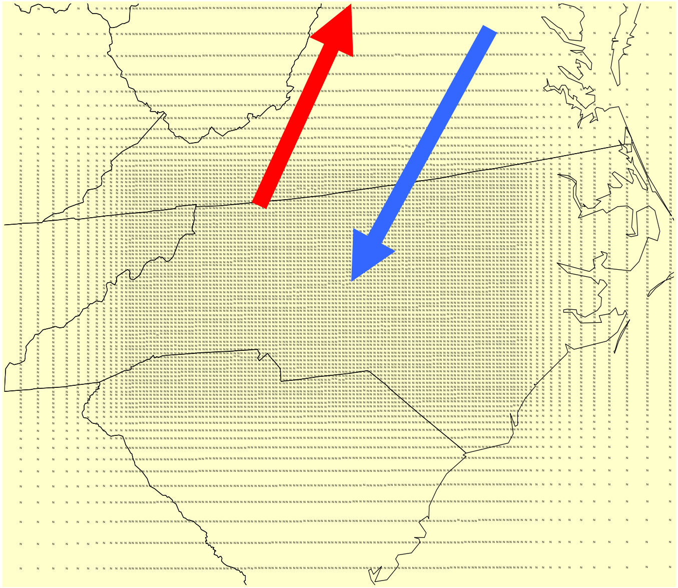
Multiple Simulations Are Inherent in Nesting Methodology

- In 1-way nesting, cannot "communicate" with outer domains
- There are issues with lateral boundary conditions (LBC) in nested models
- Lack of robust 2-way nesting methods
- Mass balance issues with 2-way nesting
- Large computer resources required

Variable-Grid-Resolution (VGR) Model

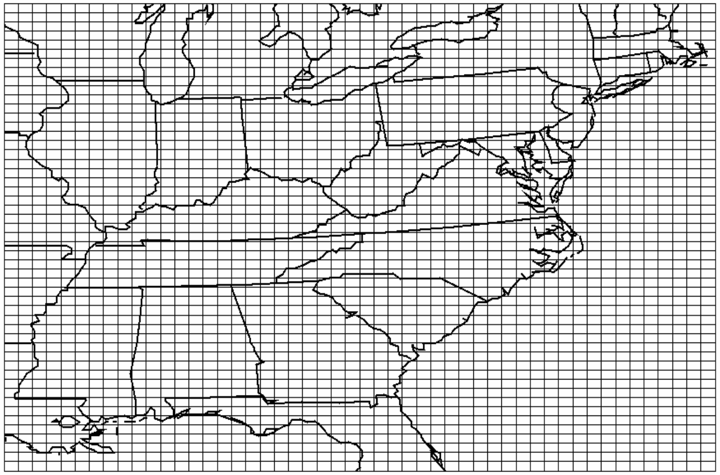
(partial domain shown)

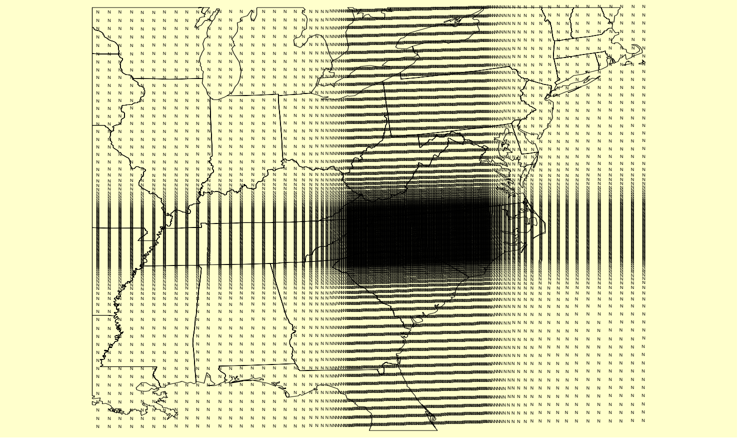


- "Natural" transport of plumes downstream from high- to low-resolution grids and vice versa
- "Avoids" nesting
- "True" scale interaction
- Single domain covers many resolutions
- One model run

Variable-Grid Concept

- **VGR avoids multiple domain requirements**
- **No LBC for interior grid cells are needed**





What Is Involved in Developing a VGR Modeling System?

- Grid generation
- Generation of meteorological fields
- Development of SMOKE-VGR (emissions)
  - MMS data (Gulf-wide Offshore Activities Data System [GOADS])
- Development of (MAQSIP/CMAQ)-VGR (handling processes such as advection, diffusion, and clouds)
- Visualization and analysis package

Grid Generation

$$S_i = \frac{\Delta X_i}{\Delta X_{i-1}}$$

$S_i = 1$ → **Uniform Grid**

$S_i > 1$ **or** $S_i < 1$ → **Variable Grid**

Processes

$$\frac{\partial C}{\partial t} = -\nabla_H \bullet (\vec{V}C)$$ ← Horizontal Advection

$$-\dot{\sigma}\frac{\partial C}{\partial \sigma}$$ ← Vertical Advection

$$+\frac{\partial}{\partial \sigma}\left(K_\sigma \frac{\partial C}{\partial \sigma}\right) + V_{d\sigma}C$$ ← Vertical Diffusion & Dry Deposition

$$+\nabla^2 K_h C$$ ← Horizontal Diffusion

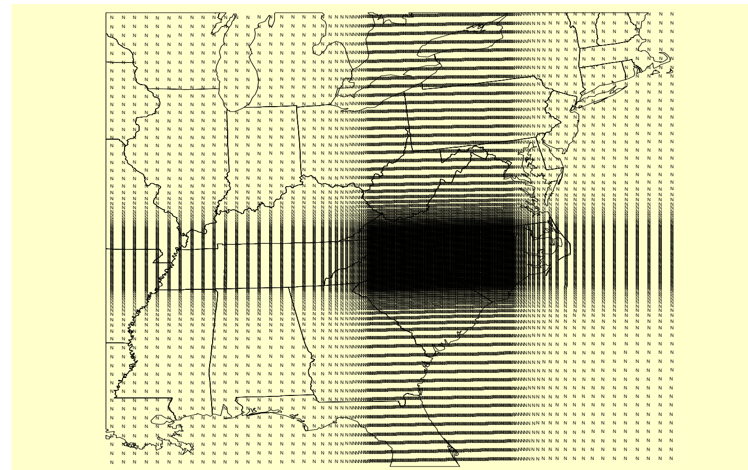
$$+(P - LC)$$ ← Chemistry

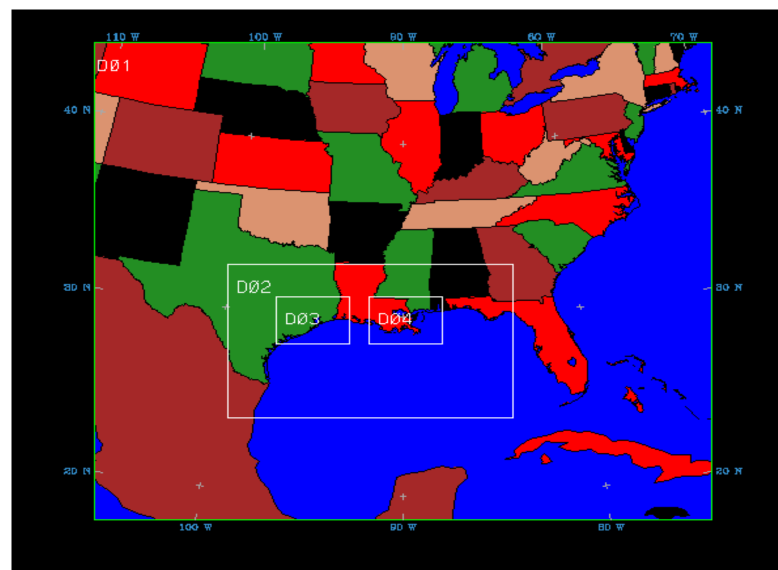
$$+(A_w - D_w)$$ ← Clouds (resolved & subgrid)

$$+E$$ ← Emission Source

Case Studies

- **NC Case Study**
  - 36- to 4-km variable grid
  - 5 days starting 19 June 1996
  - PPM for advection; CBIV Gas Phase; K-profile PBL
- **Gulf Case Study**
  - August 2000
  - Houston-Galveston (D03)
  - NE Gulf region (D04)

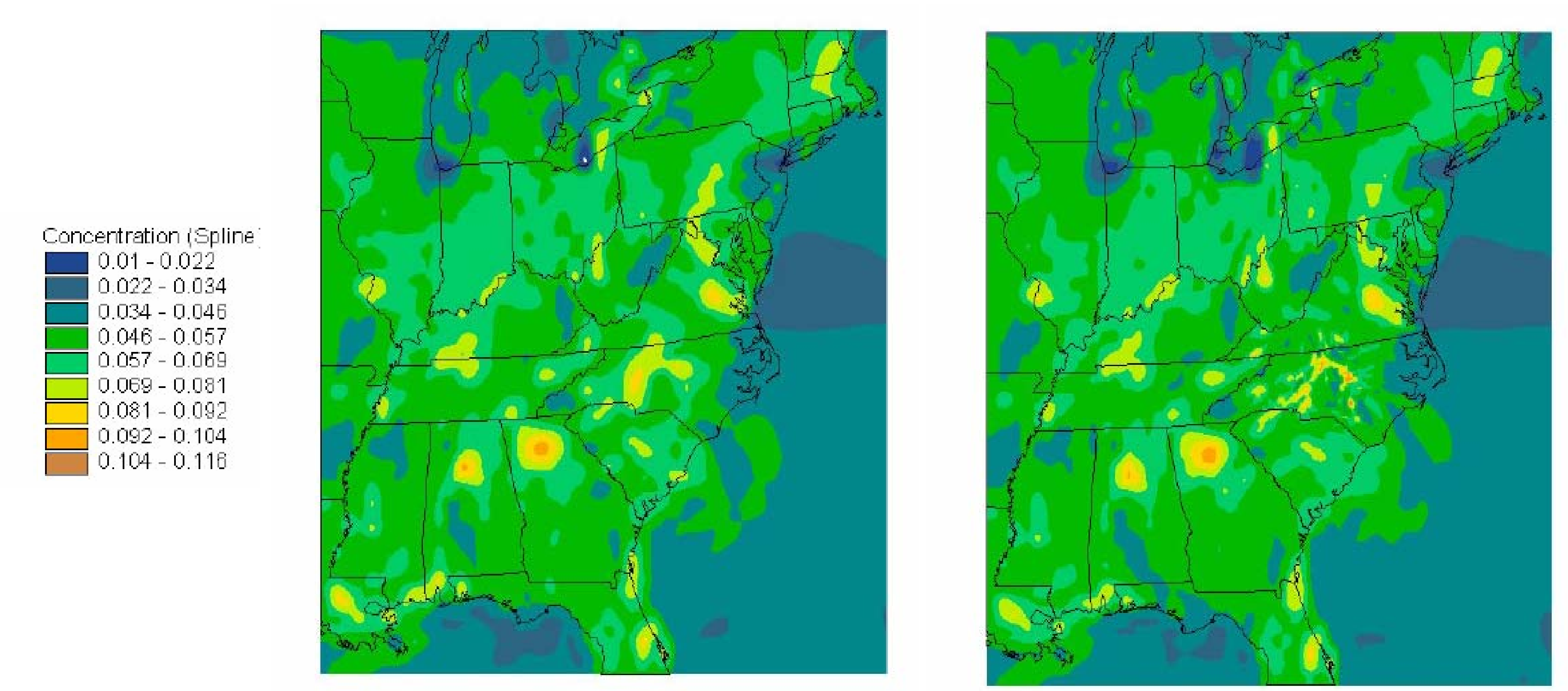




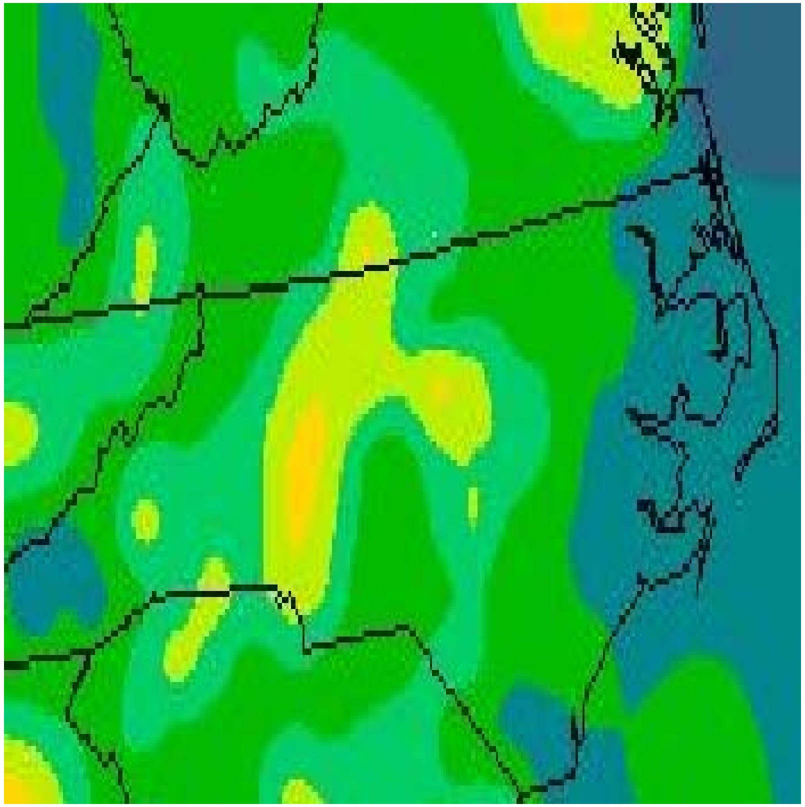
NC Surface Ozone Simulations

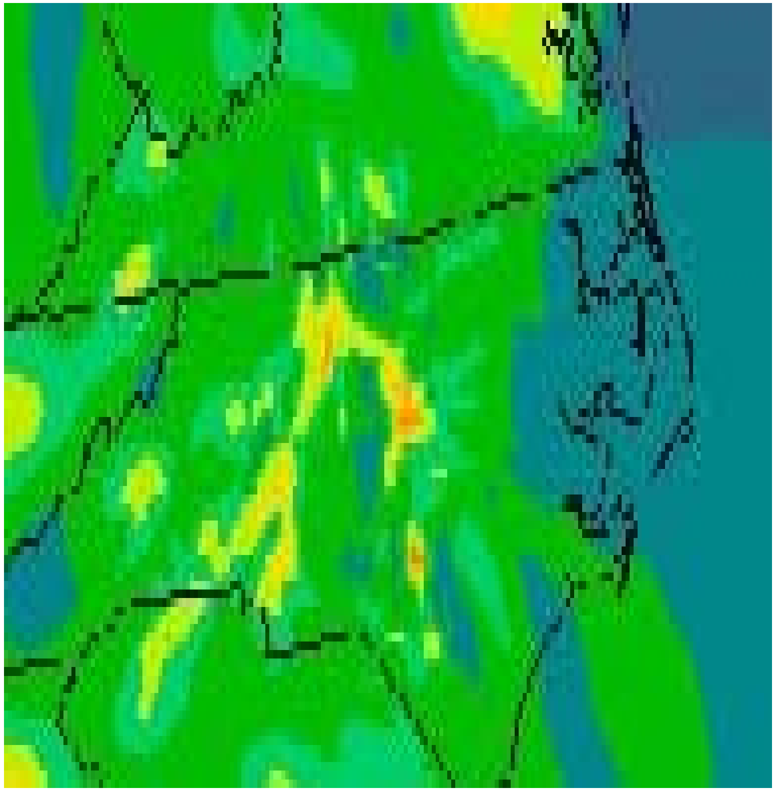
36 km

Vgrid 36 – 4-km

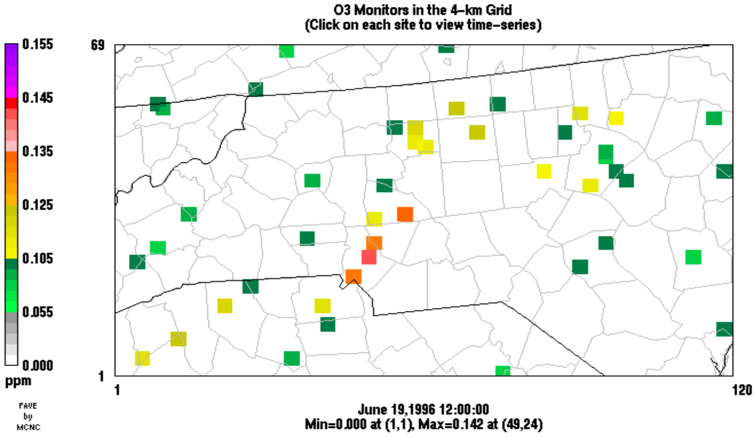


NC Simulation (36-km vs. Vgrid)

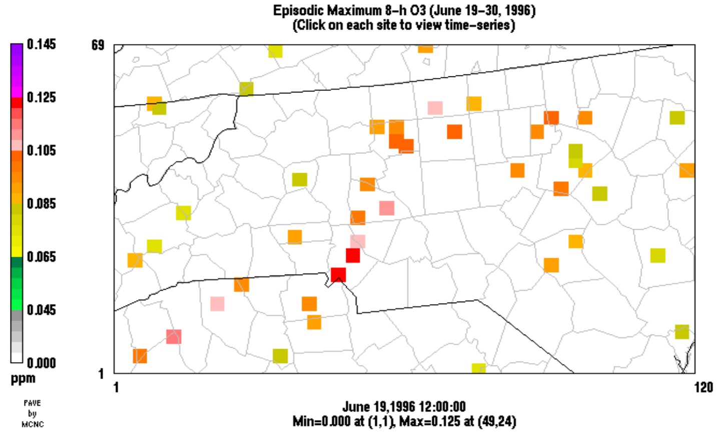




AIRS Measurement Sites

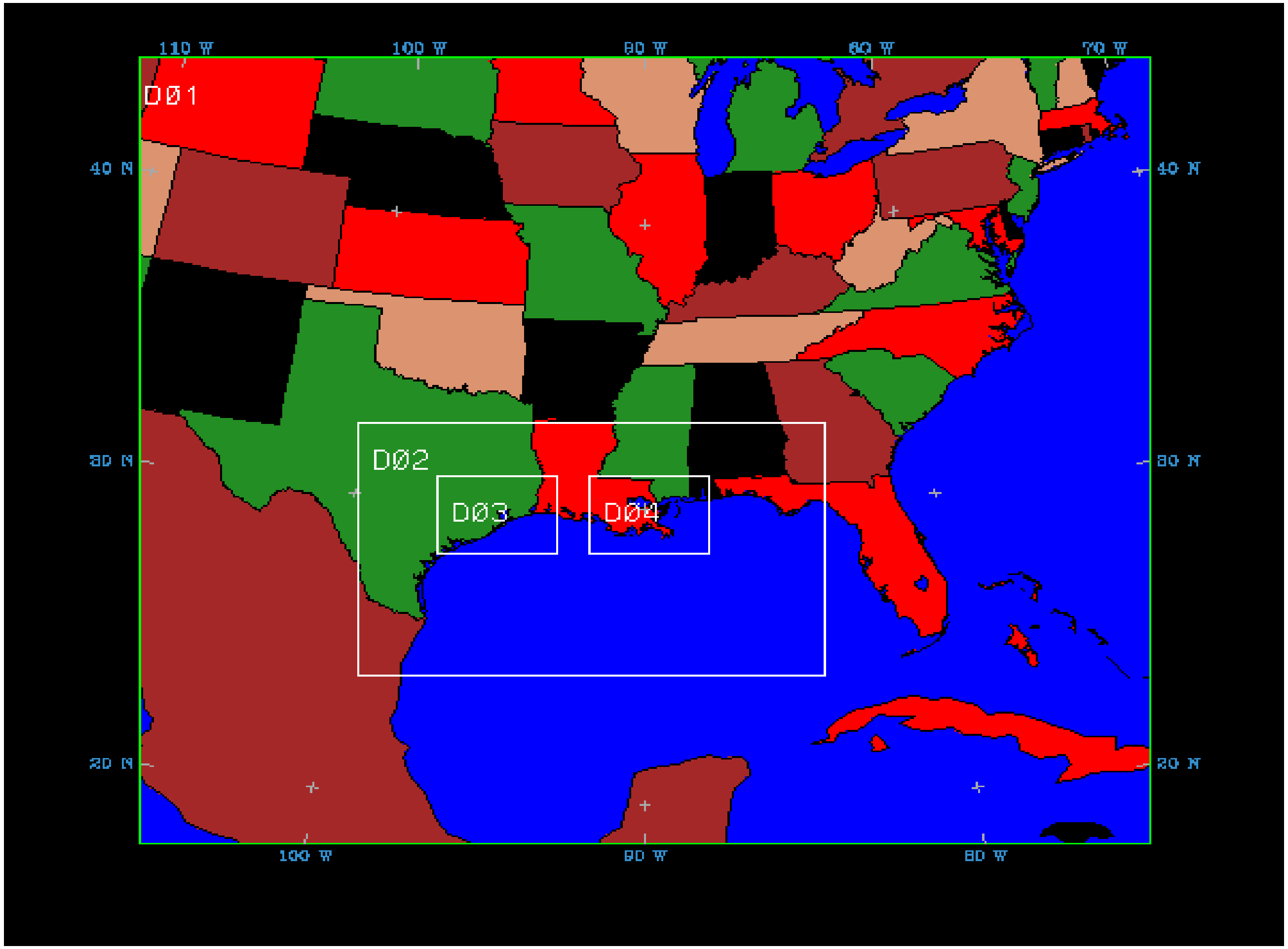


1-hour average ozone

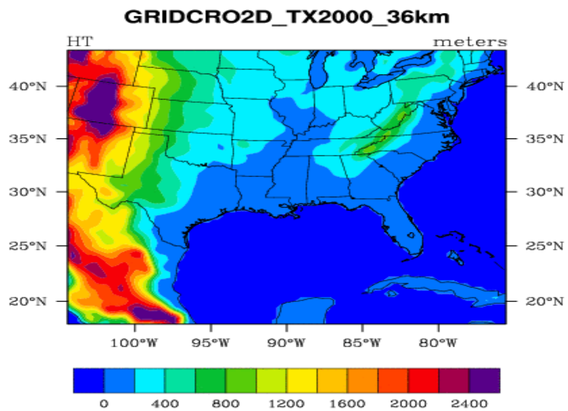


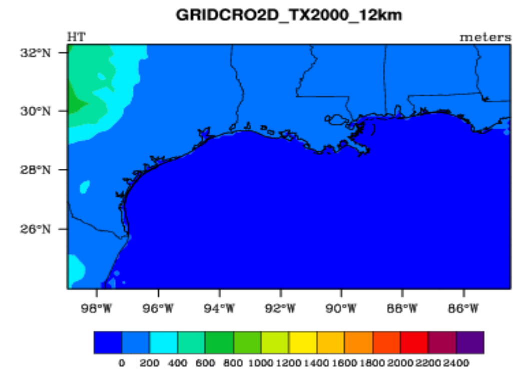
8-hour average ozone

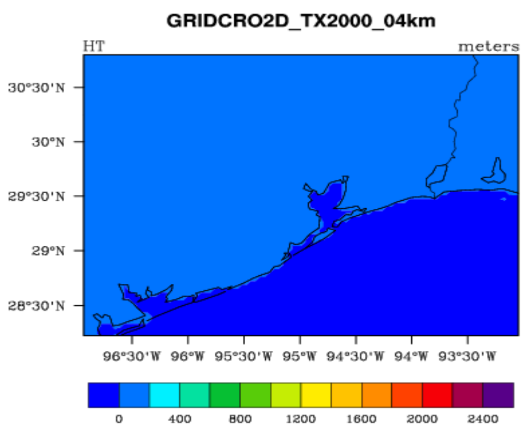
Gulf Case Study

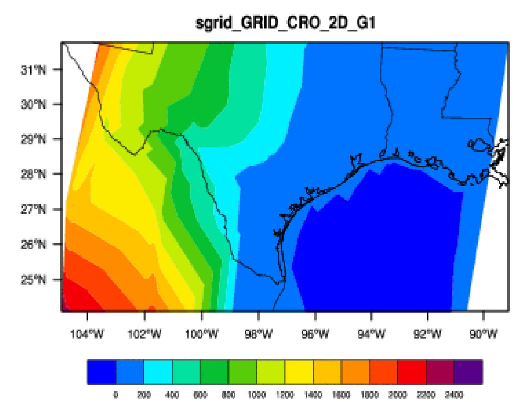


Terrain Height Uniform Grid and VGR

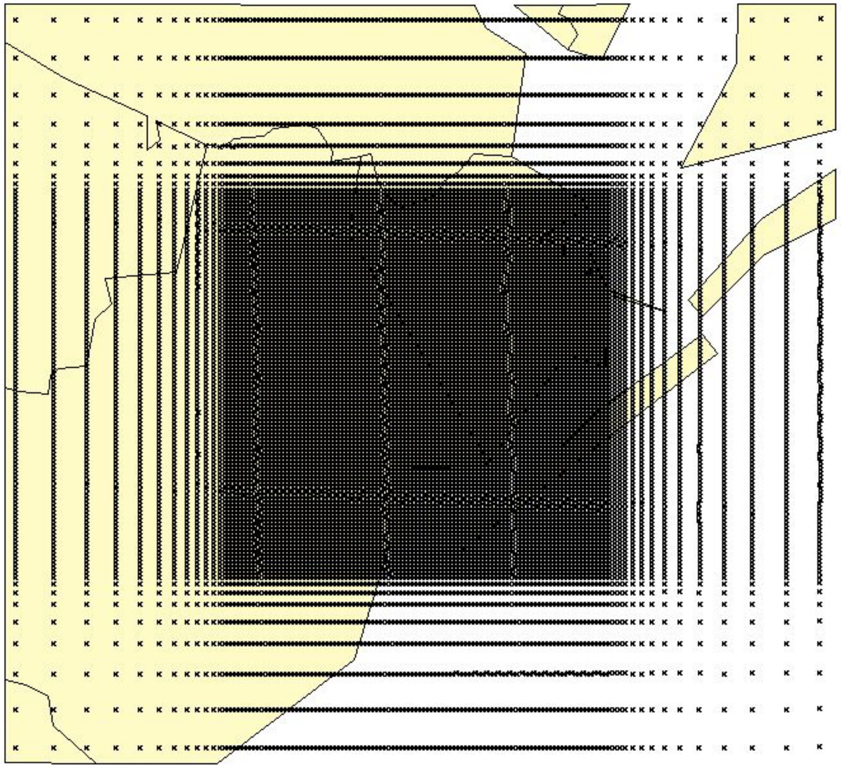




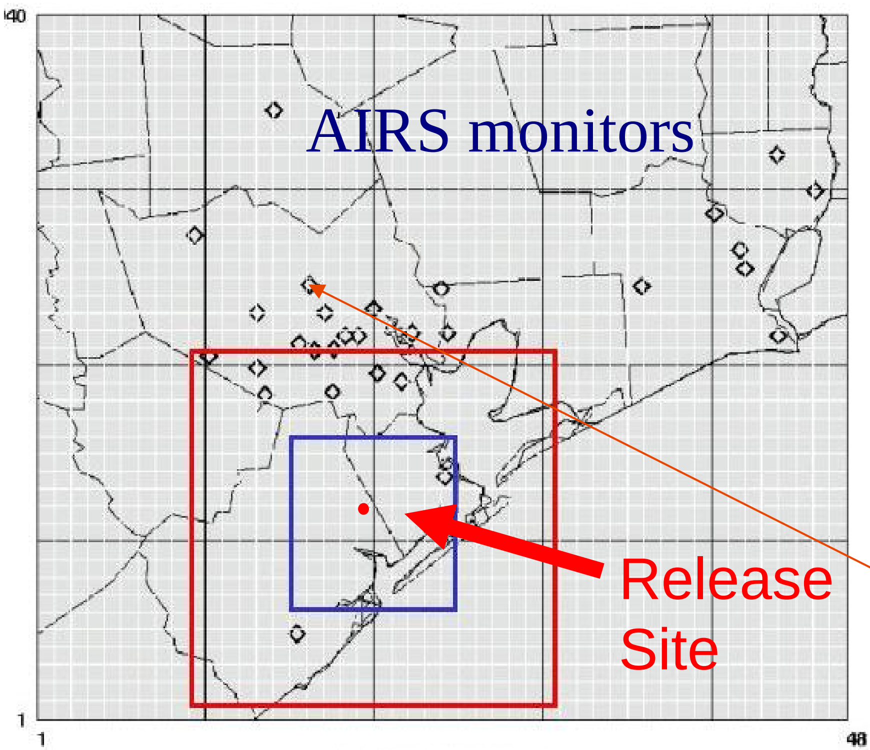




Simulation Domain with 5-km – 500-m Grids



MM5 5-km Grid Domain, VGR Domain (blue & red)

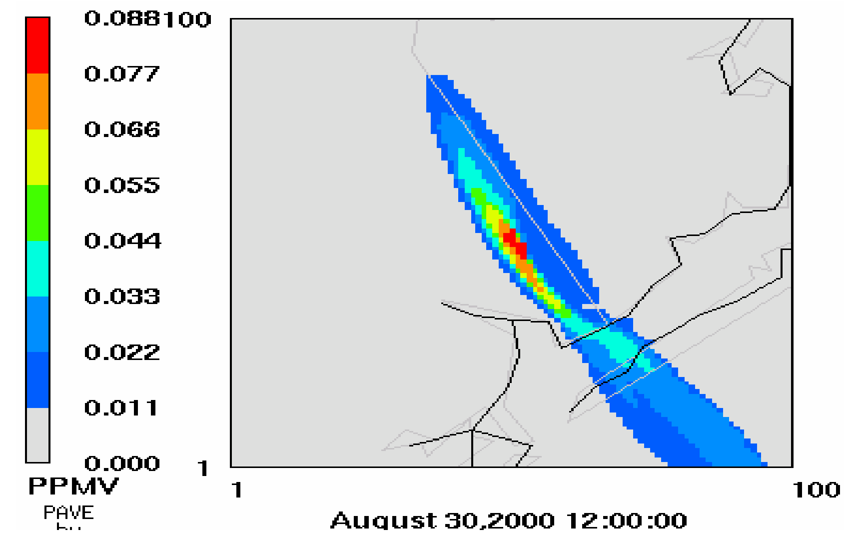


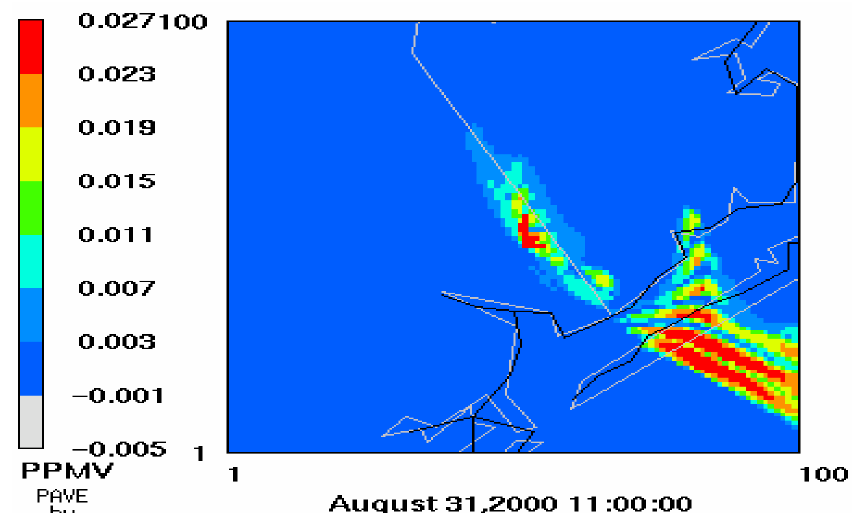
(H-G area)

UNC

Difference in Max. O_3: Upset – Base

- **Upset emission scenario (NO_x, VOC)**
- **Release time 1300-2200 UTC**
- **Differences in maximum surface ozone between the base and upset case**
- **Impact influenced by downwind chemical evolution and inter-actions with land-sea breeze dynamics**





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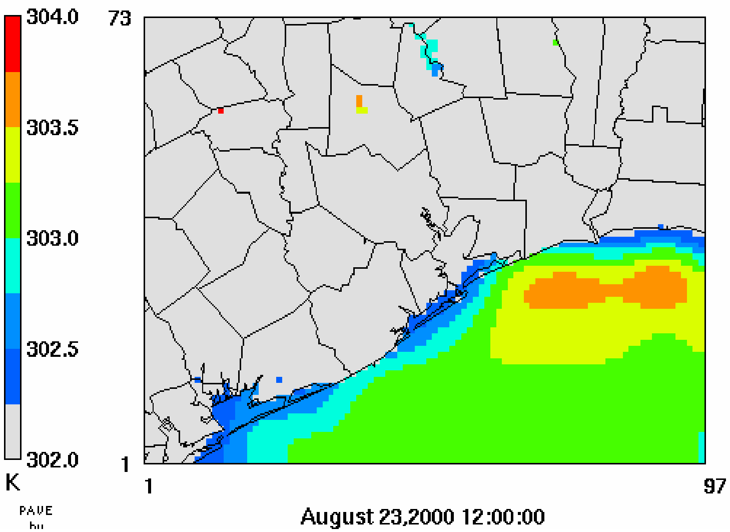
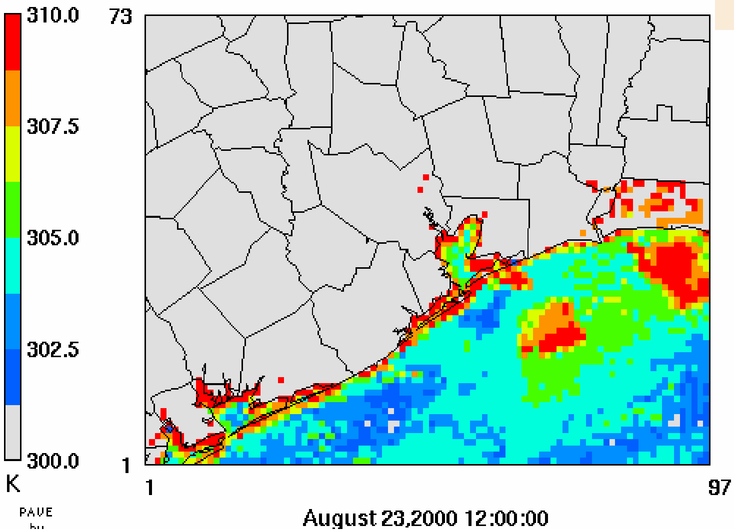
Sea Surface Temperature

- Traditional NCEP SST analysis
- Domain D03; 1200 UTC 23 August 2000
- Satellite-derived SST measurements

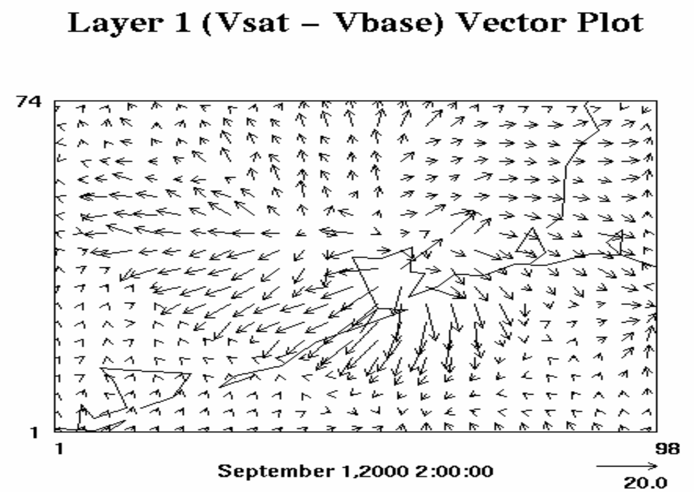


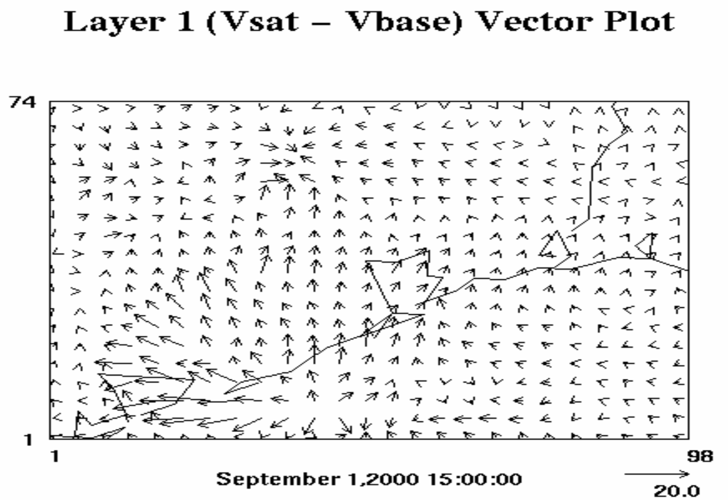


UNC

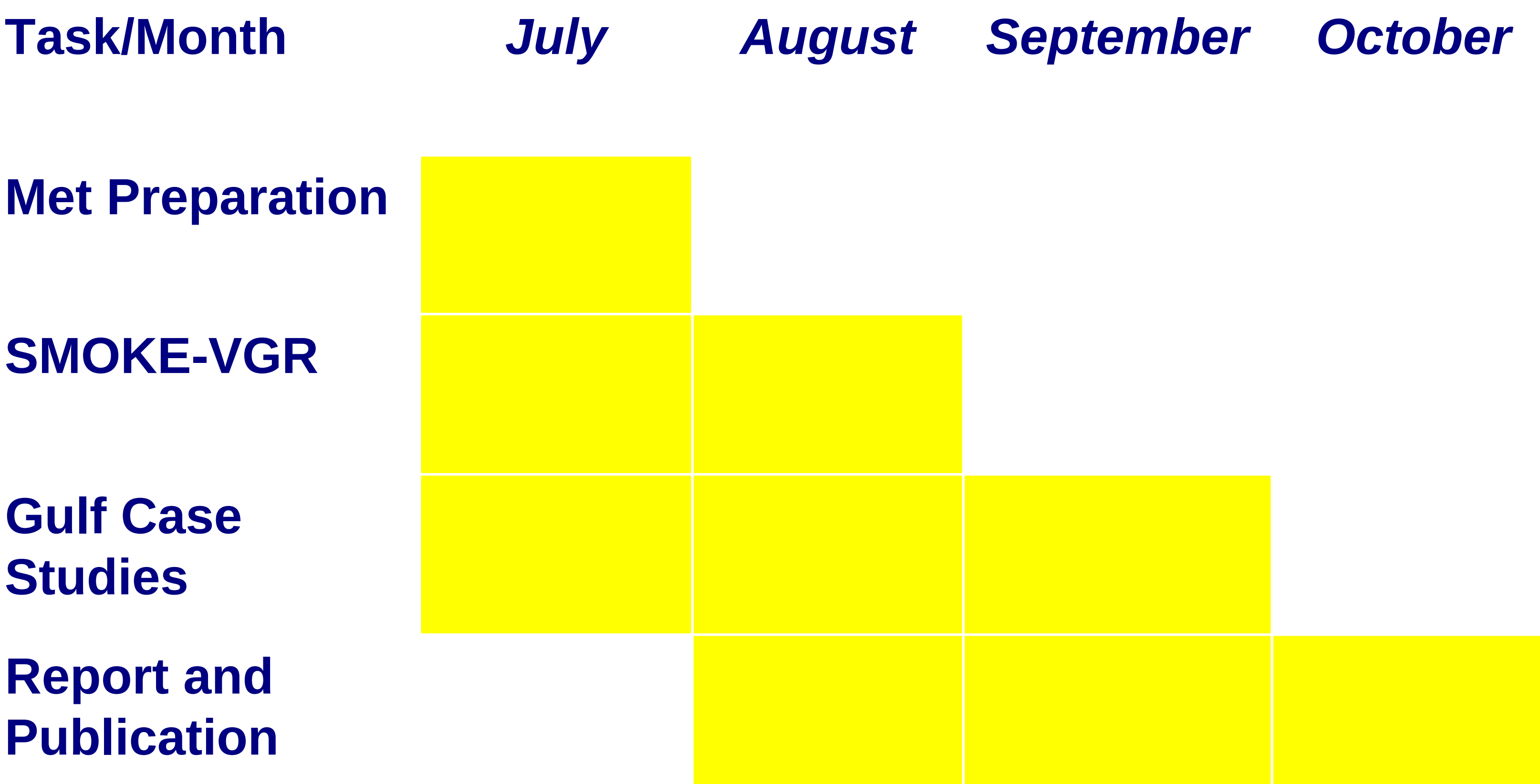
Vector Wind Simulations

- **September 1 at 0200 UTC (8:00 PM local) (above)**
- **Differences (Sat case – Base case) of MM5 layer 1 vector wind simulations**
- **September 1 at 1500 UTC (9:00 AM local) (below)**





Schedule



Task/Month
July
August
September
October
Met Preparation
SMOKE-VGR
Gulf Case Studies
Report and Publication

Benefit to Oil and Gas Industry

- A modeling tool to provide more accurate assessment of the impact of emissions related to oil and gas activities on local and regional air quality
- The modeling tool can help in designing field measurements and monitoring networks
- Could be used in examining potential impacts of future E&P activities

Transfer of Knowledge

- **Community Modeling and Analysis System (CMAS) Center (cmascenter.org)**
  - A community-based technology transfer platform
- **Training**
  - Training can be provided using the CMAS training program (CMAQ, SMOKE, WRF, MAQSIP-VGR)
- **Publications and Conference Presentations**
  - Hanna et al. (2008): "Application of a Variable-Grid Air Quality Model to Simulate On-shore/Off-shore Emissions Near Coastal Areas" (AMS 2008 annual meeting)
  - A journal article is being prepared (Alapaty et al.)

Relationship to Other Research

- Accidental releases
- Pollution transport
- Biochemical/hazardous releases
- Homeland Security research
- Alternate to plume-in-grid models
- States can do real-time simulations using

  VGR at fine scale without doing nested runs for real-time/SIP modeling
- Intercontinental transport
- Health impact studies

Funding

- DOE
  - 3-year program (award)
  - $532,365 (Balance Available: $90,000)
- Cost Share
  - $177,455 (Balance Available: $40,000)

Project Web Site

http://www.ie.unc.edu/cempd/projects/variable_grid/index.cfm

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