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Linkage between WRF/NMM and CMAQ Models

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1. INTRODUCTION

Recently, NOAA (National Oceanic and Atmospheric Administration) National Weather Service (NWS) and Office of Oceanic and Atmospheric Research (OAR) in collaboration with the U.S. EPA have been testing an initial capability for numerical air quality forecasting. The backbone of the initial capability was a computer modeling system based on the NWS Eta mesoscale meteorological forecast model and the NOAA/EPA Community Multiscale Air Quality (CMAQ) model (Byun and Ching, 1999; Byun and Schere, 2006). In 2006 the Eta model was replaced by the WRF/nmm model. An initial implementation linking the WRF/nmm and the CMAQ models was deployed in 2006. However there still exists a need to develop a more consistent coupling between the models wherein the chemistry/transport calculations in CMAQ are performed using the same grid and coordinate structure as the WRF/nmm. The fully compressible governing set of equations used in CMAQ can maintain the dynamic description of WRF just by replacing the Jacobian defining the vertical coordinate transformation and by carefully writing out dynamic and thermodynamic variables.

The goal of this research is to provide a linkage between the WRF/nmm and the CMAQ models while maintaining the dynamic description of the WRF/nmm meteorological model as closely as possible, minimizing meteorological data interpolation needs in vertical and horizontal directions.

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This document discusses issues involved in linking CMAQ to the dynamics and grid structure of WRF/nmm, such as model coupling paradigms, issues on the horizontal grid structure and the vertical coordinates, and experimental results of the horizontal advection schemes using WRF/nmm Arakawa E-Grid data in CMAQ.

2. COUPLING PARADIGMS

For consistent coupling, the governing equations, grid systems, and computational algorithms of the air quality models need to be compatible with the meteorological models. Many air quality models were designed, historically, with some limiting atmospheric dynamics assumptions. The CMAQ system, utilizing the fully compressible atmospheric descriptions in a generalized coordinate system described above, can adapt to the dynamics and coordinate system of the linked meteorological model consistently.

One of the key tasks of this project is modification of the Meteorology-Chemistry Interface Processor (MCIP) to handle the output of the WRF/nmm model to provide dynamically consistent and conservative meteorological inputs for CMAQ. Hereafter, the interface processor is called the WRF-CMAQ Interface Program (WCIP). Based on the CMAQ Preprocessor, PREMAQ code (Otte et al., 2005), the WRF/nmm-CMAQ Interface Program (WCIP/NMM) has been developed. The linkage paradigm used is a one-way “tight” (that is consistent and conservative) coupling method, as compared to the current forecasting system which is characterized as a “loose” coupling method, in which interpolations of meteorological data on different vertical and horizontal grids are involved.

3. COORDINATES AND GRID STRUCTURE

WRF/nmm uses the horizontal grid structure of the Arakawa E-grid with a rotated latitude-longitude coordinate system. In the rotated latitude-longitude coordinate system, the latitude and longitude of the center of the domain, (φ_o, λ_o), are placed at the rotated latitude 0^o and longitude 0^o, i.e., $(\Phi, \Lambda) = (0,0)$ and the equator and prime meridian intersect at the center of the WRF/nmm computational domain.

The rotated system has a significant advantage over a conformal mapping scheme. It reduces the meridian convergence and keeps the true horizontal scale relatively uniform over the domain (Black, 1988; Pyle et al., 2004). The scale factor of the map, based on the rotated latitude-longitude, is unity because the displacement on the earth would be invariant with the rotation of the coordinate. WRF/nmm uses the semi-staggered Arakawa E-grid (Arakawa and Lamb, 1977) as the horizontal grid structure.

WCIP needs to inherit the horizontal E-grid structure from the output of WRF/nmm, which uses the Arakawa E-grid horizontal domain. Vector quantities such as horizontal wind velocity (u, v) are at “dot” points. Vector quantities are point values. Scalar quantities such as density, concentration, and mixing ratio are at “cross” points. The grid size of an E-Grid is considered to be the distance between neighboring grid points of the same type.

The current PREMAQ for the model forecast system uses the Arakawa C-grid data that requires two different data structures for cross and dot files, respectively (Otte, et al., 2005). In contrast, the data structure for the Arakawa E-grid is distinctly different from that of the C-grid. For example, a pair of both a scalar point (H-point) and a vector point (V-point) exists at a specific index of grid point along the x-direction, while the H-point and the V-point appear alternately with their own different indices of grid point along the y-direction. Because of the characteristics of this structure, in terms of the assignment of the horizontal grid index within WCIP, there is no difference in the data structure between the ‘dot’ and ‘cross’ points. That is, ‘dot’ and ‘cross’ grid points are represented with the same dimensions and indices as each other. However, the dot and cross points correspond to different geographical locations, represented by the rotated longitude/latitude and the incremental distances in x- and y- directions respectively (see Figure 1). To generate the proper geographical information for this coordinate, additional codes were implemented in WCIP.

WRF/nmm uses the pressure-sigma hybrid vertical coordinate that replaces the abrupt changes in the altitudes of the terrain-following sigma coordinate present at upper layers with smooth surfaces. CMAQ uses the generalized vertical coordinate, which increases monotonically with height. We have investigated the mapping method of the hybrid vertical structure of WRF/nmm onto the generalized vertical coordinate of CMAQ.

A method proposed by UH uses predefined sigma values assigned in WCIP, whose definition should be consistent with that of WRF-NMM to construct the hybrid coordinates in the standard initialization (SI) of WRF-NMM. Another method proposed by NOAA/ARL uses two distinct vertical coordinates (hydrostatic pressure upper part and the sigma-p lower part) scaled independently across the discontinuous interface. One of the interesting features of this method is that the sigma surfaces are mapped onto the new vertical coordinate value below 0.5 and the pressure surfaces are assigned values above 0.5. One can demonstrate that the two methods are equivalent and, therefore, the vertical Jacobians for the two differ only by scale factors.

4. HORIZONTAL ADVECTION ON E-GRID IN CMAQ

The purpose of this section is to develop an approach to adapt the science process algorithms implemented in CMAQ, Byun and Ching (1999), to work directly with data from the WRF/nmm meteorological model, whose computed variables are on the Arakawa E-Grid (Arakawa and Lamb, 1977). Our goal is to develop a horizontal advection algorithm in CMAQ using the meteorological data on the Arakawa E-grid without requiring spatial interpolation such as that used in the current linkage between meteorology on an Arakawa B-Grid and CMAQ transport algorithms on an Arakawa C-Grid. Our focus is to describe a way to formulate the one-dimensional (1-D) finite-volume flux-form schemes that result when a 2-D horizontal advection operator is split into 1-D operators, with alternation between the x-direction and the y-direction.

We tested two different approaches:

(1) Advection with xy-cell E-grid: Split 2-D horizontal advection operator into 1-D operators and using current CMAQ 1-D schemes, such as PPM, alternating between appropriate x- and y-directions. Advantages of this approach are:

- E-grid wind velocity components are already at cell flux points – no interpolation needed
- Simpler book-keeping (but columns and row lengths can still vary by 1)
- Easier parallelization

However, the disadvantages are:

- Grid separation effect: The sub-grid with odd numbered columns and rows and the sub-grid with even numbered columns and rows form two separate C-grids that don't exchange mass by advection.
- Lower resolution (greater distance between cell centers) in the advection directions
- Need an extra E-grid column or row on each edge to get boundary conditions

Among other things, the grid separation effect is, in fact, a fatal flaw that makes this approach unusable. Also, the scheme is overly diffusive.

(2) Advection with rotated cell E-grid: Work directly with meteorological variables on the rotated E-grid (diagonal direction C-grid).

One way of laying out the neighborhoods of "cross" points is to assume that they are constant over the diamond-shaped grid cells. This cell layout makes the E-grid transport look like a B-Grid whose rows and columns are along orthogonal diagonals. With interpolation of the vector components to the flux data points (middle of the sides of the diamonds), scalar transport can be computed with C-grid algorithms.

Advantages of the rotated cell E-grid approach are:

- Makes the E-Grid look like a B-grid whose "rows" and "columns" are along diagonal SW→NE and SE→NW lines
- Can use 1-D algorithm, e.g. PPM, along these lines
- CMAQ (and preprocessors) are familiar with turning B-grid data into C-grid flux point data

Disadvantages are:

- Diagonal lines of cells have variable lengths, which requires non-trivial extra book-keeping (in EGRID_MODULE.F)
- Requires interpolation of wind velocities to get flux point values
- Jagged boundary effect
- Parallelization may be more difficult
- Book-keeping issues: Grid geometry changes depending on whether the number of columns or rows is even or odd.

In the WRF/nmm-CMAQ prototype, we utilize the rotated cell E-grid approach. Similarly, horizontal diffusion routine has been modified to accommodate the WRF/nmm Arakawa E-grid data for CMAQ explicit numerical diffusion algorithm.

5. COMPARISON OF ATMOSPHERIC TRANSPORT BETWEEN MM5-CMAQ AND WRF/NMM-CMAQ

We have tested the WRF/nmm-CMAQ prototype to verify the newly implemented code. Table 1 summarizes model system components used for the testing of the newly developed WRF-nmm-CMAQ on the E-grid and a comparative simulation with CMAQ driven by the MM5 meteorology model output on the C-GRID domain. A 12-km resolution domain and CB-4 chemical mechanism were used for the preliminary comparison study. Domain configurations used for both models are summarized in Table 2.

The initial condition for the simulation was obtained by a 12-km resolution C-GRID CMAQ simulation results at 00 UTC June 28, 2006. The boundary condition was provided by a 36-km resolution CMAQ simulation results for 00 UTC June 28-June 30, 2006.

This test is designed to verify the modifications to the transport and gas-phase reaction portions of the CMAQ code and hence no emissions inputs were provided. The extent of the modeling domains between the two sets is also different

First, the main wind flow patterns between the MM5 and WRF/nmm models were initialized using the same Eta forecast output, there are substantial differences in the wind and planetary boundary layer parameters predicted (not shown here). Subsequently, the overall transport and chemical reactions, albeit without emissions, result in differences in the ozone field (see Figures 1 and 2).

Table 1. Modeling system components used for the preliminary comparison test for model verification.

	C-GRID	E-GRID
Met. model	MM5 v3.6.1 with Eta forecast	WRF/NMM v2.1 with Eta forecast
MCIP	MCIP v3.0	WCIP/NMM v1.0
BCON	BCON Standard	BCON/E-grid v1.0
ICON	ICON Standard	ICON/ E-grid v1.0
CMAQ	CMAQ v4.4	CMAQ/ E-grid v1.0

Table 2. Domain configurations

	C-GRID	E-GRID
Met. model	MM5	WRF/NMM v2.1
NX (dx)	100 (12 km)	65 (0.0780^{o})
NY (dy)	100 (12 km)	135 (0.0724^{o})
NZ	43, fixed sigma-p	44, hybrid (sigma-p/p)
CMAQ		
NCOLS	89 90 for DOT point	57 59 for WCIP
NROWS	89 90 for DOT point	113 115 for WCIP
NZ	23	23

6. DISCUSSIONS

We have modified MCIP/PreMAQ to handle the output of the WRF/nmm model to provide dynamically consistent and conservative meteorological inputs for the CMAQ Chemistry Transport Model. The interface processor, named the WRF-CMAQ Interface Program (WCIP) inherits the horizontal coordinate and grid structure of the WRF/nmm, i.e., the Arakawa E-grid horizontal domain with rotated latitude/longitude coordinates.

We have developed an approach to adapt the science process algorithms implemented in CMAQ to work directly with data from the WRF/nmm meteorological model. We have tested different horizontal advection approaches and have decided to use the Advection with rotated cell E-grid. The difficulties are: (1) diagonal lines of cells have variable lengths, which requires non-trivial extra book-keeping of the grid geometry depending on whether the number of columns or rows is even or odd, (2) interpolation of wind velocities to get flux point values, (3) parallelization may be more difficult, and (4) the jagged boundary effect. We have developed code to handle most of these issues but a further study is necessary to minimize the jagged boundary effects.

ACKNOWLEDGMENTS

This work was in part supported by NOAA under project EA133R-04-RQ-0272. Also, the project is partially funded by the United States Environmental Protection Agency through Grant R-83037701 to the University of Houston. Contributions by co-authors (J.P, T.O, J.Y., and R.M) were performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views. Thanks are extended to Drs. Hsin-Mu Lin and David Wong for their help on the project.

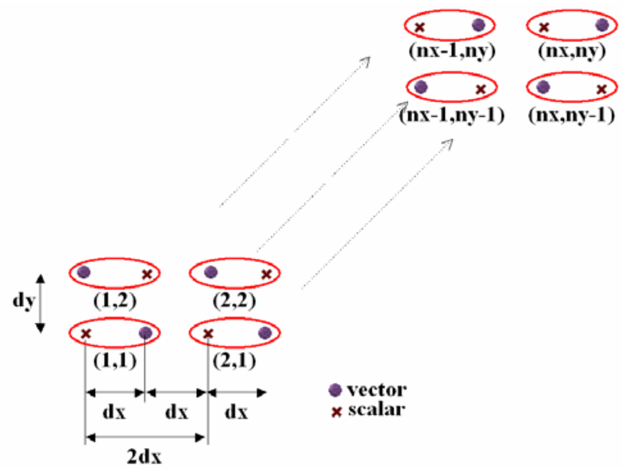

Figure 1. Dot and cross point data structure to represent vector and scalar quantities in the Arakawa E-grid.

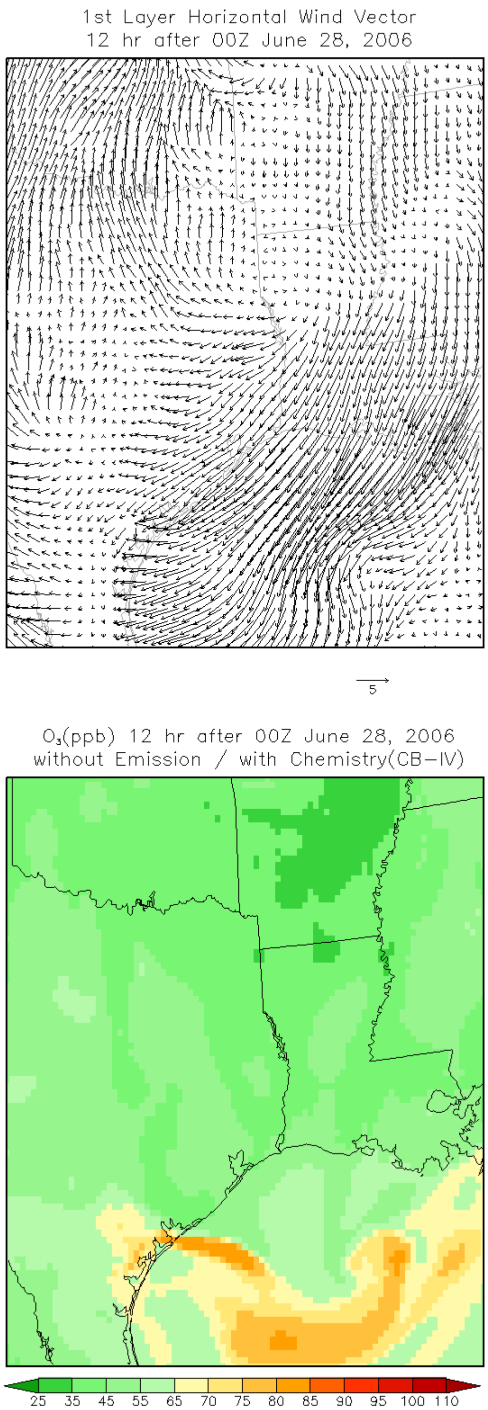

Figure 2. MM5 wind field and CMAQ result of ozone on C-grid after 12 hour transport and gas-phase reaction of initial and boundary conditions without emissions input.

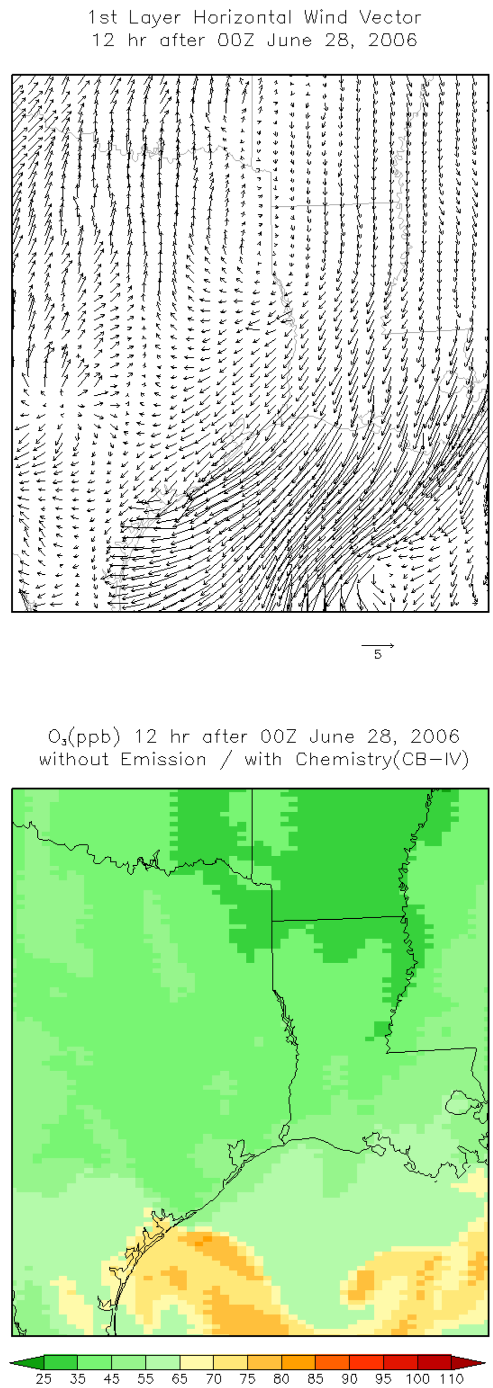

Figure 3. WRF/nmm wind field and CMAQ result of ozone on E-grid after 12 hour transport and gas-phase reaction of initial and boundary conditions without emissions input. Due to the jagged location of the E-grid cells, there are half cell shifts along the columns in the graphics.

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