Coupling of WRF/nmm with the Community Multiscale Air Quality (CMAQ) Model

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1. INTRODUCTION

The WRF models represent culmination of various atmospheric modeling efforts and has the potential to not only replace many of the current operational and research weather forecasting models, but also to provide meteorological inputs that allow simultaneous on-line/off-line air quality modeling paradigms. Byun (1999a; 1999b) presented the need to have dynamically consistent formulations in meteorological and air quality models for multi-scale air quality studies and addressed the mass conservation issues when linking the meteorological data for and air quality modeling.

Currently, two distinct versions of Weather Research and Forecasting (WRF) model are underdevelopment by NCEP and NCAR, respectively. Within the next couple of years, NOAA/NWS will be replacing the current Eta model with the version of WRF model that contains the dynamic core of the NWS non-hydrostatic mesoscale model (hereafter designated as WRF/nmm) (Janjic et al., 2004). Recent developments of NOAA (NWS and OAR) include implementation of the initial capability for numerical air quality forecasting. The backbone of this initial capability is a computer modeling system based on the NWS Eta mesoscale meteorological forecast model and the NOAA/EPA Community Multiscale Air Quality (CMAQ) model. Because the Eta model will be replaced by the WRF/nmm in near future, there is a need to build the air quality forecasting capability by linking CMAQ with WRF/nmm.

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The major goal of the present study is to build a linkage between the meteorological and air quality model while maintaining the dynamic description of the base meteorological model as closely as possible for the air pollutant transport and chemistry processing. The project requires building such a system to allow models to communicate in a manner that minimizes required data interpolations from the WRF/nmm to the CMAQ model. Here we propose to take advantage of CMAQ's generalized coordinates and fully compressible form of governing set of equations, described in Byun and Ching (1999), to build a dynamically consistent off-line modeling linkage.

2. DESIGN AND IMPLEMENTATION OF WRF-CMAQ COUPLING

As a first step, we have developed an off-line linkage between WRF and CMAQ through the WRF-CMAQ Interface Processor (WCIP), which is an outgrowth of the original MM5-Chemistry Interface Processor (MCIP) in the CMAQ modeling system. The details of the design and implementation plan are currently under development. We may utilize the initial coupled code to study: (1) spectral characteristics of the WRF-dynamics and physics module interactions, (2) dynamic and numerical consistency between the WRF and CMAQ modeling systems, and (3) real-time forecasting system with WRF-SMOKE-CMAQ.

The CMAQ system utilizes the fully compressible atmospheric descriptions in a generalized coordinate system to allow CMAQ to adapt to the dynamics and coordinate system of the linked meteorological model consistently. Multiscale air quality applications require strict mass conservation properties. Therefore, the prognostic equations for the thermodynamic variables need to be expressed in a conservative form.

One of the important benefits of using the common FCGSEs in both WRF and CMAQ is that the mass consistent characteristics simulated in WRF can be transferred into the mass conservation characteristics of the trace species in CMAQ. The results clearly demonstrated the benefit of using consistent fully compressible set of equations in both meteorology and air quality models (Kim and Byun, 2002).

3. REPRESENTATION OF VERTICAL COORDINATES

The CMAQ system is based on a fully compressible governing set of atmospheric dynamics and thermodynamics equations and utilizes a generalized coordinate system to allow representation of the dynamics and coordinate system of the meteorological model consistently (Byun and Ching, 1999). Multiscale air quality applications require strict mass conservation properties. Therefore, the prognostic equations for the thermodynamic variables and conservation equations for trace species transport need to be expressed in a conservative form. In Kim and Byun (2002), we demonstrated that both the height- and mass-coordinate dynamic cores of NCAR WRF could be directly derived from the CMAQ’s fully compressible governing set of equations (hereafter, FCGSEs). It was shown that the WRF Eulerian Mass (EM) core and Eulerian Height (EH) core formulations can be derived from CMAQ’s FCGSEs by just replacing the Jacobian, defining the vertical coordinate transformation.

NCEP WRF/nmm is a nonhydrostatic mesoscale model, which is based on a proven hydrodynamic numerical weather prediction (NWP) system. The hydrostatic approximation is relaxed to include nonhydrostatic motions while preserving its favorable features (Janjic et al., 2004). WRF/nmm utilizes a hybrid sigma p-p vertical coordinate and a rotated latitude-longitude map horizontal coordinate with Arakawa E-grid discretization. The WRF/nmm dynamics can be represented with the CMAQ's generalized FCGSE forms. We may represent the WRF/nmm hybrid vertical coordinate following Kar et al. (2004) in a general form:

$$\tilde{p}(x,y,\eta,t) = A(\eta)\,p_T + B(\eta)\,\tilde{p}_*(x,y,t) \qquad (1)$$

where η is the hybrid vertical coordinate, $\tilde{p}$ is hydrostatic pressure, and p_T and $\tilde{p}_*$ are constant pressures at model top and model bottom, respectively. The functions $A(\eta)$ and $B(\eta)$ are arbitrary, but must satisfy the following:

$$A(0)=0;\, B(0)=1;\, A(1)=1;\, B(1)=0 \qquad (2).$$

The earth's surface (η=0), the model top (η=1), and layers defined by η are assumed to be material surfaces. The hybrid vertical coordinate used in WRF/nmm can be represented by prescribing the *A* and *B* functions appropriately. Following Byun (1999), the vertical component of Jacobian J_η is obtained with

$$\frac{\partial\tilde{p}}{\partial\eta} = -g\tilde{\rho}J_\eta = \frac{\partial A(\eta)}{\partial\eta}p_T + \frac{\partial B(\eta)}{\partial\eta}\tilde{p}_* \qquad (3)$$

Once J_η is defined we can establish the consistent conservation equation for the trace species in CMAQ as follows:

$$\frac{\partial(\tilde{\rho}q_i J_\eta)}{\partial t} + m^2\nabla_\eta \bullet \left(\frac{\tilde{\rho}q_i J_\eta \hat{\mathbf{v}}_\eta}{m^2}\right) + \frac{\partial(\tilde{\rho}q_i J_\eta \hat{v}^3)}{\partial\eta} = J_\eta Q_{q_i} \qquad (4)$$

where $\hat{\mathbf{v}}_\eta$ and $\hat{v}^3$ are horizontal and vertical contravariant wind components, respectively, and q_i is mixing ratio of trace species *i*. Refer to the CMAQ science documentation (Byun and Ching, 1999) for the definition of various symbols.

As shown above, CMAQ can be used almost as is to use the same vertical layer coordinate (hybrid sigma p-p) as the WRF/nmm. However, we may need to utilize a customized vertical coordinate type to represent the hybrid vertical coordinate in CMAQ for the input/output processes.

4. MASS FLUX VARIABLES IN CMAQ

Lee *et al*. (2004) compared effects of mass consistency errors in meteorological data for air quality modeling using the hydrostatic and nonhydrostatic versions of MM5. They showed that the hydrostatic MM5 introduced much less errors in the trace species transport in air quality simulations than the nonhydrostatic MM5 because of the better mass conservative characteristics of the hydrostatic formulations.

WRF/nmm utilizes mass coordinate dynamics, which will inherit the benefit of the hydrostaic formulations. Byun and Kim (2003) showed that CMAQ linked with a mass coordinate WRF system conserves mass quite well due to the use of complete governing set of fully compressible atmosphere as well as the accurate numerical algorithms implemented in WRF. The result clearly demonstrated benefits of using dynamically consistent formulations between the meteorology and air quality models.

As part of the PREMAQ for WRF/nmm development, we will define wind and other dynamic variables coherent with the temporal interpolation scheme for winds proposed by Byun (1999b). In the scheme, the contravariant components of winds in the generalized vertical coordinate system at a time $t = (1-\alpha)t_n + \alpha t_{n+1}$ between the two consecutive meteorological output time steps t_n and t_{n+1} are determined by:

$$(\hat{\mathbf{v}}_\eta)_\alpha = \frac{(\tilde{\rho} J_\eta \hat{\mathbf{v}}_\eta)_\alpha}{(\tilde{\rho} J_\eta)_\alpha} \; ; \; (\hat{v}^3)_\alpha = \frac{(\tilde{\rho} J_\eta \hat{v}^3)_\alpha}{(\tilde{\rho} J_\eta)_\alpha} \qquad (5)$$

The Jacobian weighted density and wind components multiplied in the right hand side of Eq. (1) are interpolated linearly with the values at t_n and t_{n+1}. These are the mass flux variables responsible for maintaining the mass conservation characteristics of the off-line trace species transport.

One of the possibilities to suppress the mass inconsistency problems in the off-line modeling paradigm is to write out the averaged mass flux variables at each output time step. There are two possible ways to consider the averaged variables in Eq. (5). One is to separate the Jacobian weighted density from the contravariant wind components. In this case, the averaged contravariant wind provided by the meteorological model can be directly used for Eq. (4). Another method is to calculate both the contravariant wind multiplied with the Jacobian weighted density and the Jacobian weighted density separately in WRF and then divide the wind with the density in CMAQ. In addition, with the mass-coordinate dynamics core supported by WRF, the vertical coordinates are time-dependent following the change in the hydrostatic pressure field. In such a system, similar temporal averaging must be applied for the hydrostatic pressure variables for defining the coordinate system in air quality modeling.

5. HORIZONTAL GRID STRUCTURE

WRF/EM and CMAQ both utilizes the Arakawa C-grid and conformal map projections to represent the horizontal grid and coordinates, requiring no special interpolations between the two. However, WRF/nmm utilizes the Arakawa E-grid (Arakawa and Lamb, 1977; see Figure 1) with a rotated latitude-longitude map coordinate. Therefore it requires casting the scalar and vector quantities onto the CMAQ's horizontal structure, Arakawa C-grid and a conformal mapping. Utilization of the staggered Arakawa-E grid for air quality modeling poses some interesting challenges. First, we need to determine the relation between the scalar quantities and wind vector components. We can determine the grid definition for air quality corresponding to the meteorological scalar quantities, such as pressure, density, and humidity, etc. Then, the co-located horizontal wind components can be utilized to represent the flux-points.

Here, we outline an approach to adapting the science process algorithms implemented in CMAQ to work directly with data from a meteorological model, whose computed variables are on a uniformly spaced Arakawa E-Grid. Our goal is to use the meteorological data without requiring spatial interpolation such as is used in the current linkage between meteorology on an Arakawa B-Grid and CMAQ transport algorithms on an Arakawa C-Grid. The focus is on describing 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 (Byun and Ching, 1999).

Vector quantities such as horizontal wind velocity, (u, v), are at "+" points. The "+" is used here to indicate the directions of the two components of the vector. Vector quantities are point values. Scalar quantities such as density, concentration and mixing ratio are at "o" points. The "o" is to indicate that scalar quantities are constant over a neighborhood of the point. The grid size of an E-Grid is considered to be the distance, ds, between neighboring grid points of the same type.

One way of laying out the neighborhoods of "o" points for a scalar quantity is shown by the cells in Figure 2. This cell layout makes the E-Grid look like a B-Grid whose rows and columns are along orthogonal diagonals. Note that these rows and columns have variable lengths. Also, the wind speeds needed for horizontal advection in CMAQ's Chemical Transport Module (CTM) are the normal velocities to cell edges at edge midpoints, the "flux points". This requires interpolation of the corner values of wind velocities. It maps a B-Grid to a C-Grid. These disadvantages led us to develop an alternate approach that uses the E-Grid directly.

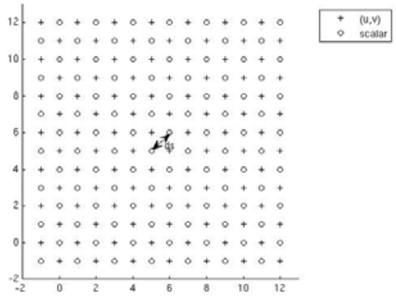

Figure 1. Spatial distribution of dependent variables for a uniformly spaced Arakawa E-Grid.

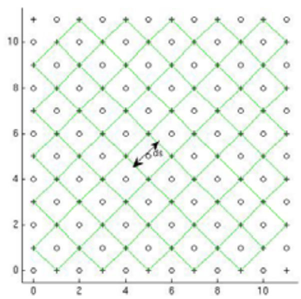

Figure 2. E-Grid with rotated square cells. Scalar variables are considered to be constant on each grid cell.

6. CONCLUSIVE REMARKS

In this paper, we discussed issues related with building linkage between the WRF models and CMAQ. We studied differences in the governing equations and coordinates, their interactions with transport algorithms in WRF and the CMAQ chemistry-transport model. Further we presented several methods to cast the WRF meteorological data on CMAQ grid and coordinate structures to represent transportation of pollutants. We contrasted the differences in dynamics descriptions between the WRF/nmm and WRF/EM and their implication on the development of the linking strategy. The distinct characteristics of the vertical coordinates and impacts of utilizing different map projections and grid systems were discussed.

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