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DEVELOPMENT OF THE WRF-CMAQ INTERFACE PROCESSOR

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1. INTRODUCTION

It is imperative that the governing equations and computational algorithms be consistent and compatible in each component of the air quality modeling system. Many air quality models, historically, were designed with limited atmospheric dynamics assumptions. The Community Multiscale Air Quality (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. Meteorology-Chemistry Interface Processor (MCIP) in the CMAQ system processes output parameters from MM5 to provide meteorological parameters for CMAQ Chemistry Transport Model (CCTM). MCIP interpolates the meteorological data, computes cloud parameters, and estimates surface and PBL parameters if needed, and finally transforms data in the generalized coordinate system for the CCTM. Because many mesoscale models were not designed specifically for air quality, and they do not output all the parameters necessary for air quality simulations, diagnostic routines implemented in MCIP are used to fill the data gap.

This paper addresses issues associated with developing a Weather Research and Forecasting (WRF) model and CCTM Interface Processor (WCIP). Here, we demonstrate that both the height- and mass-coordinate dynamic cores of WRF can be directly derived from the CMAQ's fully compressible governing set of equations. We identify necessary processing steps relating WRF meteorological parameters for use in CCTM.

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2.0 GOVERNING EQUATIONS FOR FULLY-COMPRESSIBLE ATMOSPHERE

Multiscale air quality applications require strict mass conservation, therefore the prognostic equations for the thermodynamic variables need to be expressed in a conservative form. In the following, we describe the fully compressible governing set of equations (hereafter, FCGSEs) on which the CMAQ system's formulations are based (Byun, 1999) and show that governing equations for WRF mass- and height-coordinate cores can be derived directly from the CMAQ's FCGSEs.

2.1 Equations in Generalized Coordinates

We can relate the generalized meteorological curvilinear coordinates $(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t})$ in a conformal map projection to the rotated earth-tangential coordinates (x, y, z, t) as:

$$\begin{cases} \hat{x}^1 = mx \\ \hat{x}^2 = my \\ \hat{x}^3 = s(x,y,z,t) \\ \hat{t} = t \end{cases} \qquad \begin{cases} x = m^{-1}\hat{x}^1 \\ y = m^{-1}\hat{x}^2 \\ z = h(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t}) \\ t = \hat{t} \end{cases} \qquad (1)$$

where *m* is the map scale factor, *s* is the generalized meteorological vertical coordinate, z_{sfc} is the topographic height. In the generalized coordinate system, the contravariant and covariant wind components are represented with $\hat{v}^j$ and $\hat{v}_k$.

The square root of the determinant of the metric (Jacobian hereafter) is composed of the map scale factor and vertical derivative $J_s = |\partial h / \partial s|$:

$$\sqrt{\hat{g}} \equiv \left|\hat{g}_{jk}\right|^{1/2} = \frac{1}{m^2}\left|\frac{\partial h}{\partial s}\right| = \frac{J_s}{m^2}, \qquad (2)$$

where $\hat{g}_{jk} = \frac{\partial x^i}{\partial \hat{x}^j}\frac{\partial x^i}{\partial \hat{x}^k}$. The horizontal momentum equation is given as:

$$\frac{\partial (\rho J_s \mathbf{V}_z)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s \mathbf{V}_z}{m}\right)\mathbf{V}_z + \frac{\partial \rho J_s \mathbf{V}_z \hat{v}^3}{\partial \sigma} + f\hat{\mathbf{k}}^3 \times \rho J_s \mathbf{V}_z$$

$$+ \rho J_s\left[\frac{m}{\rho}\nabla_s p - \frac{m}{\rho g}\left(\frac{\partial \sigma}{\partial z}\right)\frac{\partial p}{\partial \sigma}\nabla_s \Phi\right] = \rho J_s \hat{\mathbf{F}}_s \qquad (3)$$

where $\mathbf{V}_z = v_1\mathbf{i} + v_2\mathbf{j}$ is the horizontal wind vector on the reference earth-tangential Cartesian coordinates. The horizontal wind vector is represented in the conformal map coordinates as: $\hat{\mathbf{V}}_s = \hat{v}^1\mathbf{i} + \hat{v}^2\mathbf{j} = m\mathbf{V}_z$, $\nabla_s = \hat{\mathbf{i}}\partial / \partial \hat{x}^1\big|_s + \hat{\mathbf{j}}\partial / \partial \hat{x}^2\big|_s$, f is the Coriolis factor, $\hat{\mathbf{F}}_s$ is the horizontal forcing vector, *p* is atmospheric pressure, $\Phi = gh$ is the geopotential height, and ρ is air density. A prognostic equation for the vertical velocity component (*w*) in the Cartesian coordinates is given as:

$$\frac{\partial (\rho J_s w)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s w \mathbf{V}_z}{m}\right) + \frac{\partial (\rho J_s w \hat{v}^3)}{\partial \sigma}$$

$$+ \rho J_s\left(\frac{m}{\rho}\frac{\partial p}{\partial \sigma} + \frac{\partial \Phi}{\partial \sigma}\right)\left(\frac{\partial \sigma}{\partial z}\right) = \rho J_s\left(F_3 + \frac{wQ_\rho}{\rho}\right) \qquad (4)$$

where F_3 is the forcing term for the *w*-component. The contravariant vertical velocity component is related to the Cartesian vertical velocity with:

$$\hat{v}^3 = \frac{d\sigma}{dt} = \frac{\partial \sigma}{\partial t} + \mathbf{V}_z \bullet \nabla_z \sigma + w\left(\frac{\partial \sigma}{\partial z}\right)$$

$$= \frac{\partial \sigma}{\partial t} + \left(-\frac{1}{g}\hat{\mathbf{V}}_s \bullet \nabla_s \Phi + w\right)\left(\frac{\partial \sigma}{\partial z}\right), \qquad (5)$$

where $\nabla_z = \hat{\mathbf{i}}\partial / \partial x\big|_z + \hat{\mathbf{j}}\partial / \partial y\big|_z$.

Using the ideal gas law, the thermodynamic variables (i.e., temperature, entropy, pressure gradients, and density) are diagnostically related. The entropy per unit volume (entropy density), s, is defined as:

$$s = \rho C_{vd} \ln\left(\frac{T}{T_{oo}}\right) - \rho R_d \ln\left(\frac{\rho}{\rho_{oo}}\right), \qquad (6)$$

where *T* is temperature, C_{vd} is the specific heat capacity for dry air at constant volume, and R_d is the dry air gas constant. T_{oo} is temperature of the reference atmosphere at the reference pressure $p_{oo} = 10^5$ Pascal. The atmospheric pressure is treated as a thermodynamic variable that is fully defined by the density and entropy of the atmosphere. The conservation equations for air density, entropy density, and tracer concentrations are:

$$\frac{\partial (\rho J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s \hat{\mathbf{V}}_s}{m^2}\right) + \frac{\partial (\rho J_s \hat{v}^3)}{\partial \sigma} = J_s Q_\rho \qquad (7)$$

$$\frac{\partial (s J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{s J_s \hat{\mathbf{V}}_s}{m^2}\right) + \frac{\partial (s J_s \hat{v}^3)}{\partial \sigma} = J_s Q_s \qquad (8)$$

$$\frac{\partial (\varphi_i J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\varphi_i J_s \hat{\mathbf{V}}_s}{m^2}\right) + \frac{\partial (\varphi_i J_s \hat{v}^3)}{\partial \sigma} = J_s Q_{\varphi_i}, \qquad (9)$$

where φ_i is the trace species concentration (mass per unit volume), and the *Q*-terms represent sources and sinks of each conservative property. Although the source term for air density (Q_ρ) should be zero in an ideal case, it is retained here to capture the possible density error originating from numerical procedures in a meteorological model. Because the error influences computations of other parameters such as vertical velocity and mass conservation, it is important to minimize propagation of the error in the system. Eqs. (3), (4), (7), (8) and (9) with additional diagnostic relations form the FCGSEs. The generalized coordinate system allows transformations among various horizontal map projections (e.g., spherical, rectangular, Lambert, Mercator, and polar stereographic), and various vertical coordinates (e.g., pressure or geometric height). The dynamics used in meteorological models are often linked to the choice of the vertical coordinate. In those vertical coordinates that depend on atmospheric pressure, the coordinate values decrease with height. To simplify implementation of the generalized coordinate in CMAQ, without a loss of generality, we redefine the terrain-following vertical coordinate σ with a positive definite coordinate $\xi = \hat{x}^3$ as:

$$\hat{x}^3 = \xi = \begin{cases} \sigma & (\text{for } \sigma = 0 \text{ at bottom}, 1 \text{ at top}) \\ 1 - \sigma & (\text{for } \sigma = 1 \text{ at bottom}, 0 \text{ at top}) \end{cases} \qquad (10)$$

2.2 WRF Mass- and Height-Coordinate Cores

The dynamic framework of the Weather Research & Forecasting (WRF) modeling system is under development by scientists at NCAR, NOAA, Air Force. In this section, we will relate CMAQ's FCGSEs to the WRF's mass- and height-coordinate dynamic cores (Klemp et al., 2000). Although the Eulerian height-coordinate (EH) core was developed earlier than the Eulerian mass-coordinate (EM) core, NCAR has recently decided to support only the EM core exclusively. Note that for the simplicity of the presentation, we will only consider the dry atmosphere here. The governing set of equations for the EM-core can be derived from the CMAQ's FCGSEs. The WRF EM core utilizes the terrain following coordinate defined with the time-dependent hydrostatic pressure (π):

$$h = \frac{p - p_t}{m};\ m = p_s - p_t \tag{11}$$

In this coordinate, we find

$$J_s = m / rg \,. \tag{12}$$

The wind components are defined in the EM core as:

$$U = mv_1;\ V = mv_2;\ W = mv_3;\ \Omega = m\hat{v}^3 \,. \tag{13}$$

Then, Eq.(3) becomes

$$\frac{\P (m\mathbf{V}_z)}{\P t} + m^2 \nabla_s \bullet (\frac{m\mathbf{V}_z}{m})\mathbf{V}_z + \frac{\P \mathbf{V}_z \Omega}{\P h} + f\mathbf{f}^3 \times m\mathbf{V}_z$$

$$+ mma\nabla_h p + m\frac{\P p}{\P h}\nabla_h \Phi = m\hat{\mathbf{F}}_s \tag{14}$$

and Eq. (4) can be rewritten as (when RHS is assumed to vanish):

$$\frac{\P (mw)}{\P t} + m^2 \nabla_h \bullet \left(\frac{m\mathbf{V}_z w}{m}\right) + \frac{\P (\Omega w)}{\P h} + g\left[m - \frac{\partial p}{\partial h}\right] = 0 \tag{15}$$

Further, one can readily show that the thermodynamic variable $\Theta = mq$ in WRF is related to the entropy density for dry atmosphere with $s = r \ln q$. The continuity equation is written as:

$$\frac{\P m}{\P t} + m^2 \nabla_s \bullet \left(\frac{m\mathbf{V}_z}{m}\right) + \frac{\P \Omega}{\P h} = mQ_r / r \tag{16}$$

$$\frac{\P q}{\P t} + m^2 \nabla_s \bullet \left(\frac{m\mathbf{V}_z q}{m}\right) + \frac{\P (\Omega q)}{\P h} = J_s Q_q \tag{17}$$

$$\frac{\P (mq_i)}{\P t} + m^2 \nabla_h \bullet \left(\frac{m\mathbf{V}_z q_i}{m}\right) + \frac{\P (q_i \Omega)}{\P h} = mQ_{j_i} / r \tag{18}$$

Note that the only difference is that q is used instead of $\ln q$. This verifies that the WRF EM formulation can be derived from CMAQ's FCGSEs just by replacing J_s. Similarly, one can show the FCGSEs is equivalent to the governing set of equations of the WRF EH core with its vertical coordinate defined by:

$$V = \frac{z - h_s(x,y)}{H - h_s(x,y)} \tag{19}$$

and its Jacobian component is given as:

$$J_s = H - h_s(x,y)\,, \tag{20}$$

where $h_s(x,y)$ is the terrain height.

3.0 METEOROLGICAL PARAMETERS FOR CCTM GENERALIZED COORDINATE SYSTEM

One distinct feature of the CMAQ system from other AQMs is the ability to adapt the various different coordinates and dynamics in the linked meteorological model. This functionality is achieved by recasting meteorological parameters in terms of variables in the fully-compressible form. The consistency is maintained in the CCTM with appropriate interpolation methods.

3.1 Thermodynamic variables: Pressure, Density, and Entropy

In the WRF model, like in the CMAQ's FCGSEs, the pressure is treated as a diagnostic variable, which is computed with:

$$p = p_o\left(\frac{R_d \Theta}{p_o}\right)^g \tag{21}$$

where $g = (1 + R_d / C_{vd})$. Density is directly passed through from WRF. Entropy can be computed using Eq. (6).

3.2 Jacobian and layer height

The trace species concentrations are coupled with the Jacobian Eq. (2) in the CCTM. It is computed with Eq. (12) for the EM core and Eq. (20) for the EH core, respectively. For use in the mass-conserving temporal interpolation, both the Jacobian weighted densities and Jacobian weighted entropy are computed and stored in the WCIP output.

The layer height can be computed using the basic definition of the geopotential height in terms of the Jacobian instead of the coordinate-specific analytical equation for the generality with:

$$h = \Phi / g = h_s + \int_{x_s}^{x} J_x \, dx \tag{22}$$

To obtain the height above the ground level, $(h - h_s)$ is used.

3.3 Contravariant velocity components

The generalized CCTM requires a set of contravariant velocity components (i.e., $\hat{v}^1, \hat{v}^2, \hat{v}^3$). Contravariant velocity components are scaled components of the wind vectors for the transformed map-projection coordinates. In addition, to maintain the mass consistency during the numerical transport processes, we generated the Jacobian-mass-weighted contravariant wind components.

For WRF EM-core, the covariant wind components ($\mathbf{V}_z$) are provided. Therefore, we need to compute the horizontal wind components with:

$$\frac{rJ_x}{m^2}\hat{\mathbf{V}}_x = \frac{rJ_h}{m^2}\hat{\mathbf{V}}_h = \frac{m}{mg}\mathbf{V}_z \tag{23}$$

For the vertical wind component, the Jacobian weighted contravariant wind is available ($\Omega = m\hat{v}^3$) in the WRF output. Therefore we compute

$$\frac{\rho J_\xi}{m^2}\dot{\xi} = \frac{-\Omega}{m^2 g}. \quad (24)$$

Note that the negative sign is needed because the CMAQ's vertical coordinate increase with height as defined in Eq. (10).

For the WRF EH-core, the horizontal covariant wind components coupled with the density ($\rho \mathbf{V}_z$) are provided. Therefore, we need to compute

$$\frac{\rho J_\xi}{m^2}\hat{\mathbf{V}}_s = \frac{(H-h_s)}{m}(\rho \mathbf{V}_z). \quad (25)$$

Because only the covariant vertical wind component coupled with the density is available, we compute the contravariant vertical wind component with Eq. (5) as:

$$\hat{v}^3 = \frac{\partial \xi}{\partial t} + (-m\hat{\mathbf{V}}_\xi \bullet \nabla_\xi h + w)\left(\frac{\partial \xi}{\partial z}\right) = \frac{(-m\mathbf{V}_z \bullet \nabla_\xi h + w)}{H-h_s} \quad (26)$$

where $\frac{\partial \xi}{\partial t} = 0$ is used because the terrain-following height coordinate is independent of time. Finally, we compute

$$\frac{\rho J_\xi}{m^2}\hat{v}^3 = \frac{\rho (H-h_s)}{m^2}\hat{v}^3. \quad (27)$$

4.0 VERIFICATION OF IMPLEMENTATION

To verify the WCIP implementation, we have set up the comparable simulations for the MM5 and WRF for the Houston-Galveston area at 4-km resolution. Simulation period is from August 26-September 2, 2000. Horizontal domains include 161x146 cells. For the WRF EM core, we have used 44 vertical layers. However, because of the "top too high" error message from the WRF standard initialization (SI) processor, we are forced to use 43 layers for the WRF EH core. We set up the MM5 (with nonhydrostatic sigma-P_0 coordinate) following the WRF EH core.

In Figure 1, we show the Jacobian-mass-weighted contravariant vertical wind components for the MM5 and WRF EM and EH dynamic core simulations. Although there are noticeable differences among the simulations, the signs and general patterns of the computed fields are consistent.

5.0 CONCLUSIVE REMARKS

There have been a few operational problems with the WRF. For example, nesting capability is still not implemented in the WRF version we tested. Because the WCIP code is just implemented, we must scrutinize all the parameters in the WCIP output files. Once the WCIP code implementation is fully verified, we will simulate CMAQ to test validity of the WCIP generated meteorology data.

6.0 REFERENCES

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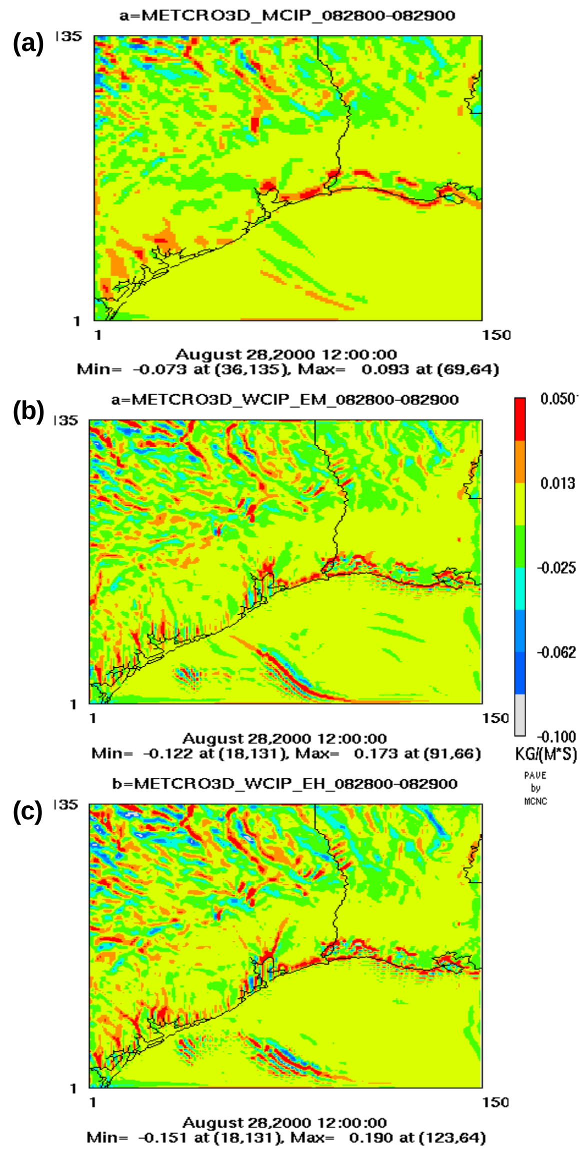

Figure 1. Jacobian-mass weighted contravariant vertical wind component at K=3 for 12 UTC 28 August, 2000: (a) MCIP, (b) WCIP EM and (c) WCIP EH results, respectively.