Coupling of WRF with the EPA's Community Multiscale Air Quality (CMAQ) Model

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and many others...

Goal: Build Dynamically Consistent Coupled WRF/nmm & CMAQ Air Quality Forecasting System

- build a linkage between the meteorological and air quality model while maintaining the dynamic description of the base model as closely as possible
- Use meteorological data (state variable definitions) that minimize errors during the temporal interpolations in air quality model.

Development objectives

1) One-way coupling:
   Loose coupling (NOAA & EPA RTP group)
   Tight coupling (University of Houston & EPA)

2) Provide algorithms for the coupling

3) Verification of coupling

Brief History of Atmospheric Models

Numerical Weather Prediction (NWP)

~ 1950s with the advent of modern computer

Simplified Dynamics Models

- barotropic models
- baroclinic models
- hydrostatic models
- incompressible atm. assumption.
- compressible atm. assumption
- pseudo nonhydrostatic model

Fully-compressible atm. models

Air Quality Models (AQMs) (USA only...)

~ 1970s started by chemical engineers

Simulates pollutant transport only.

Meteorological data as external inputs

Objective analyzed winds

•UAM & ROM utilize Implicit/Explicit assumption of

hydrostatic & incompressible atmosphere

NWP output

•RADM (late 1980s) is the first (?) model linked with an NWP model (e.g., MM4)

•SAQM – linked with MM5 (pseudo nonhydrostatic)

•CMAQ - fully compressible & generalized coordinate formulation (linked with MM4, MM5, RAMS, CALMET, WRF/EM, WRF/EH, etc...)

Brief Introduction of CMAQ

Science Characteristics of EPA's Community Multiscale Air Quality Model (CMAQ)

- "First principles" description of atmospheric system
  - Conservation laws – mass, energy, momentum, …
- Multiple scale atmospheric dynamics
  - Meso-gamma, urban, regional, global scales
  - Daily, episodic, seasonal, annual time scales
- Multiple atmospheric pollutants
  - Ozone, acid deposition, eutrophication
  - Fine particles, visibility
  - Tracer transport
  - Toxics

References; Byun & Ching (1999), Byun & Schere (2005) & papers by many others….

Degree of Comprehensiveness in science process representation

- Aerosol thermodynamics codes:
- equilibrium model, hybrid model, dynamic model
- Aerosol distribution: modal & sectional
- Advection: finite volume methods (Botts, PPM, YAM, etc..)
- Diffusion: K-theory & Asymmtric Convective Model (Pleim & Chang)
- Deposition: RADM-scheme (Weseley et al, 1989), M3DRY (Pleim)
- Gas-phase: CB-4, RADM, SAPRC99, Air Toxics, Hg, etc...

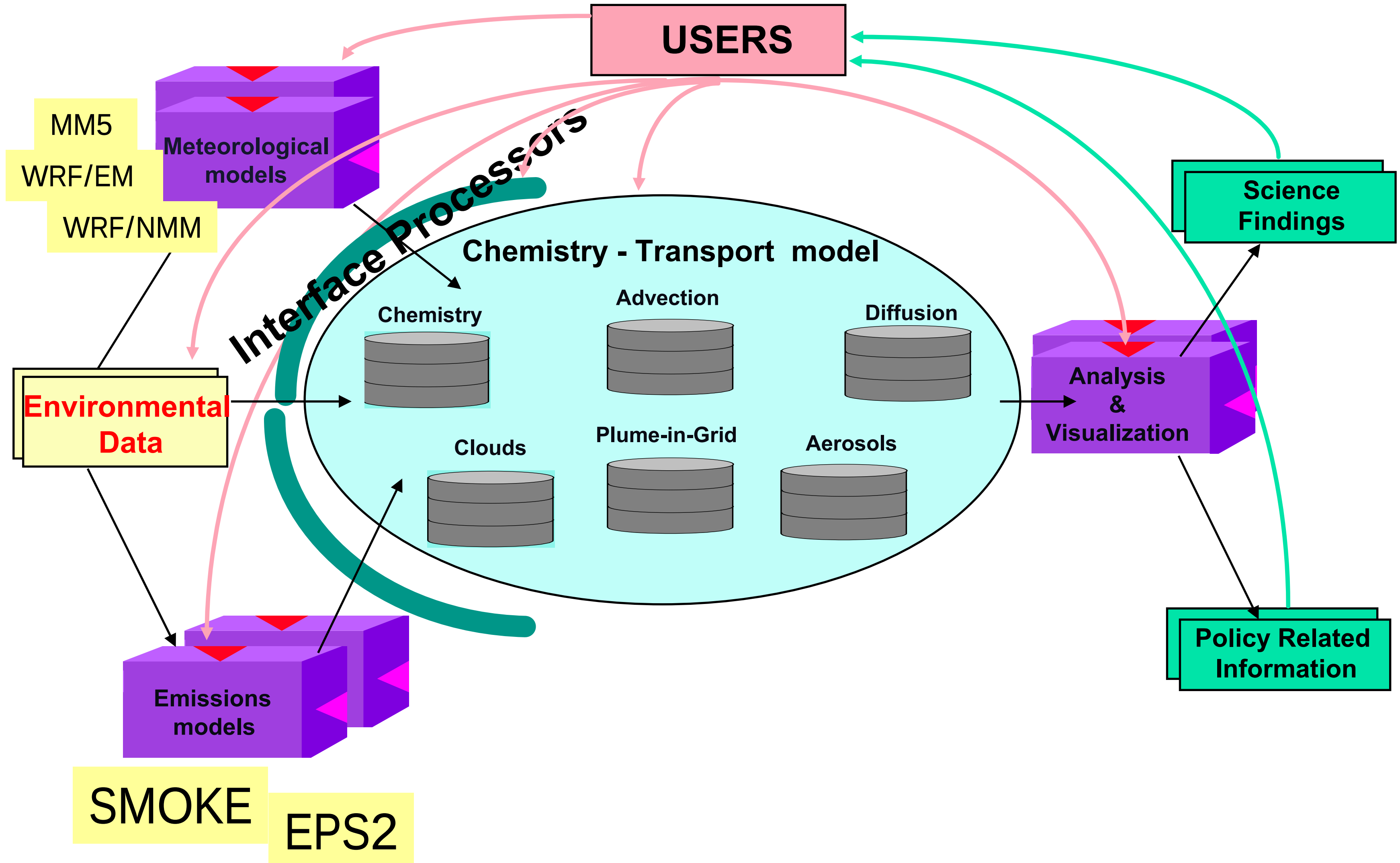
Degree of Generality in the governing equations

- Example for the atmospheric dynamics and thermodynamics: fully compressible nonhydrostatic formulation vs. hydrostatic, nondivergent flow assumption

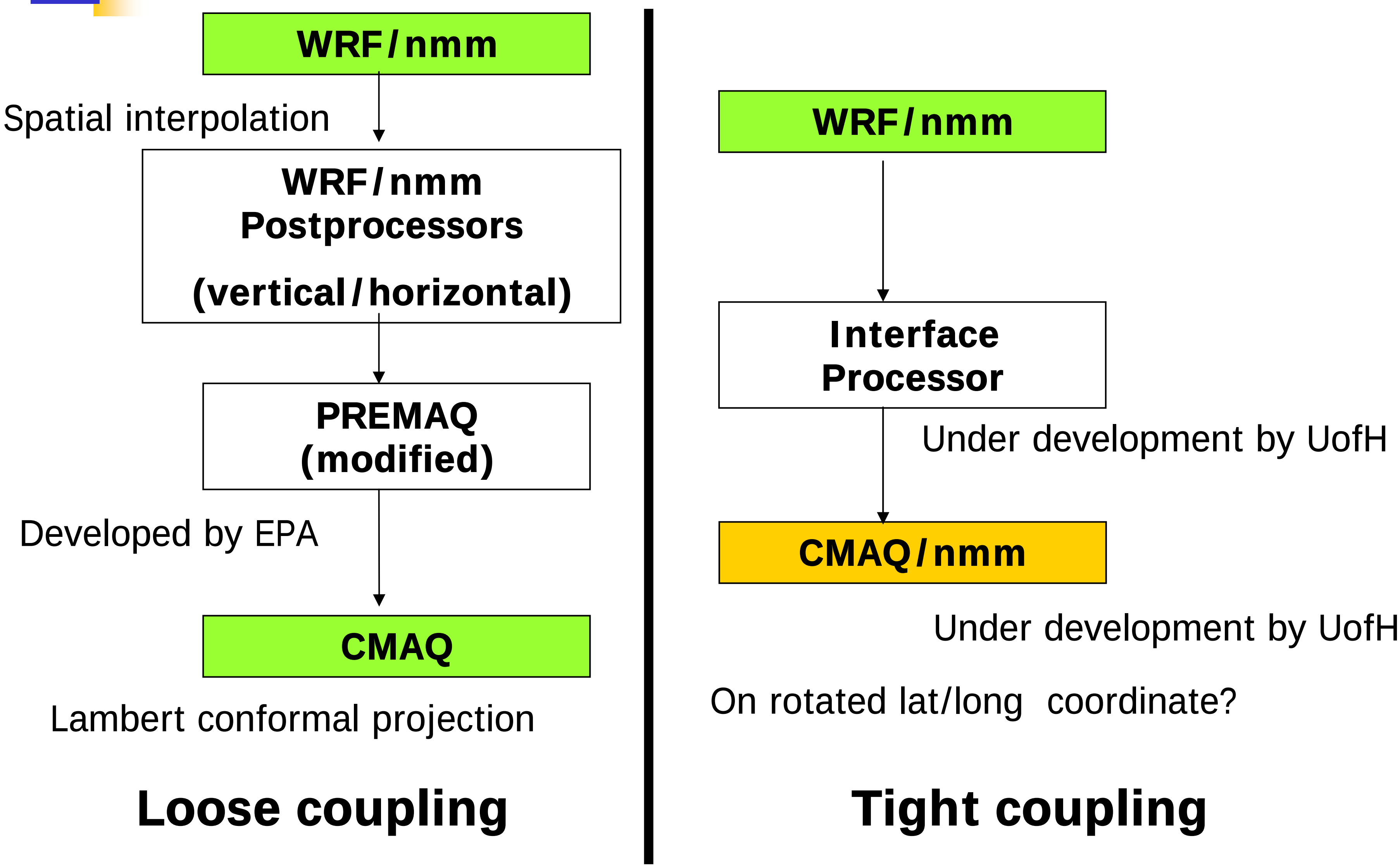
Note: More general and comprehensive formulations do not necessarily increase numerical complexity

- Generalized coordinate system expands model application domain with minimal increase in the computational cost

Communty Multiscale Air Quality (CMAQ) System



Components of Coupled system



What are the main science issues of the NWP & AQM coupling?

- Consistent governing set of equations & state variables
- Consistent coordinates and grid structures

- Consistent numerics & physics, and parameterizations
- Consistent use of basic input data (e.g., Land Use/Land Cover, topography)
- Flexibility: ability to help diverse stake holders (research – regulatory application)

Fully Compressible Atmosphere (OOyama, 1990) used for CMAQ

$$\frac{\partial(\rho J_s \mathbf{V}_z)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s \mathbf{V}_z}{m}\right)\mathbf{V}_z + \frac{\partial \rho J_s \mathbf{V}_z \hat{v}^3}{\partial s} + f\hat{\boldsymbol{\tau}}^3 \times \rho J_s \mathbf{V}_z + \rho J_s \left[\frac{m}{\rho}\nabla_s p - \frac{mJ_s}{\rho g}\left(\frac{\partial s}{\partial z}\right)\frac{\partial p}{\partial s}\nabla_s \Phi\right] = \rho J_s \hat{\mathbf{F}}_s$$

$$\frac{\partial(\rho J_s w)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s w \mathbf{V}_z}{m}\right) + \frac{\partial(\rho J_s w \hat{v}^3)}{\partial s} + \rho J_s \left(\frac{m}{\rho}\frac{\partial p}{\partial s} + \frac{\partial \Phi}{\partial s}\right)\left(\frac{\partial s}{\partial z}\right) = \rho J_s \left(F_3 + \frac{wQ_\rho}{\rho}\right)$$

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

$$\frac{\partial(\varphi_i J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\varphi_i J_s \hat{\mathbf{V}}_s}{m^2}\right) + \frac{\partial(\varphi_i J_s \hat{v}^3)}{\partial s} = J_s Q_{\varphi_i} \qquad p = p_o\left(\frac{R_d \Theta}{p_o}\right)^\gamma \qquad \sigma = \rho C_{vd} \ln\left(\frac{T}{T_{oo}}\right) - \rho R_d \ln\left(\frac{\rho}{\rho_{oo}}\right)$$

Horizontal grid : Arakawa C grid (Lambert Conformal)

WRF (EM core)

$$\frac{\partial U}{\partial t} + \mu\alpha \frac{\partial p}{\partial x} + \frac{\partial p}{\partial \eta}\frac{\partial \phi}{\partial x} = -\frac{\partial U u}{\partial x} - \frac{\partial \Omega u}{\partial \eta}$$

$$\frac{\partial W}{\partial t} + g\left(\mu - \frac{\partial p}{\partial \eta}\right) = -\frac{\partial U w}{\partial x} - \frac{\partial \Omega w}{\partial \eta}$$

$$\frac{\partial \Theta}{\partial t} + \frac{\partial U\theta}{\partial x} + \frac{\partial \Omega\theta}{\partial \eta} = \mu Q$$

$$\frac{\partial \mu}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial \Omega}{\partial \eta} = 0$$

$$\frac{d\phi}{dt} = gw, \qquad \frac{\partial \phi}{\partial \eta} = -\mu\alpha, \qquad p = \left(\frac{R\theta}{p_0 \alpha}\right)^\gamma$$

$$\eta = (\pi - \pi_t)/\mu, \qquad \mu = \pi_s - \pi_t$$

$$U = \mu u, \quad W = \mu w, \quad \Theta = \mu\theta, \quad \Omega = \mu\dot{\eta}$$

Governing Eq. Formulation : Flux form
Prognostic variable :
 Momentum, Dry entropy, Geopotential, Column mass
Horizontal grid : Arakawa C grid (Lambert Conformal)
Vertical coordinate : Terrain following sigma

WRF (NMM core)

$$\frac{d\mathbf{v}}{dt} = -(1+\varepsilon)\nabla_\sigma \Phi - \alpha \nabla_\sigma p + f\,\mathbf{k} \times \mathbf{v}$$

$$\frac{\partial T}{\partial t} = -\mathbf{v} \bullet \nabla_\sigma T - \dot{\sigma}\frac{\partial T}{\partial \sigma} + \frac{\alpha}{c_p}\left(\frac{\partial p}{\partial t} + \mathbf{v} \bullet \nabla_\sigma p + \dot{\sigma}\frac{\partial p}{\partial \sigma}\right)$$

$$\sigma \frac{\partial \mu}{\partial t} = -\int_0^\sigma \left[\nabla_\sigma \cdot (\mu \mathbf{v}) + \frac{\partial(\mu\dot{\sigma})}{\partial \sigma}\right] d\sigma'$$

$$p\alpha = RT \qquad \frac{1}{\mu}\frac{\partial \Phi}{\partial \sigma} = -\alpha \qquad \varepsilon \equiv \frac{1}{g}\frac{dw}{dt} \qquad \frac{\partial p}{\partial \pi} = 1 + \varepsilon$$

$$w = \frac{1}{g}\left(\frac{\partial \Phi}{\partial t} + \mathbf{v} \bullet \nabla_\sigma \Phi + \dot{\sigma}\frac{\partial \Phi}{\partial \sigma}\right)$$

Governing Eq. Formulation : Advective form
Prognostic variable :
 Velocity, Temperature, Pressure, Column mass
Horizontal grid : Arakawa E grid (Rotated Lat./Lon.)
Vertical coordinate : Hybrid(Terrain following sigma/Pressure)

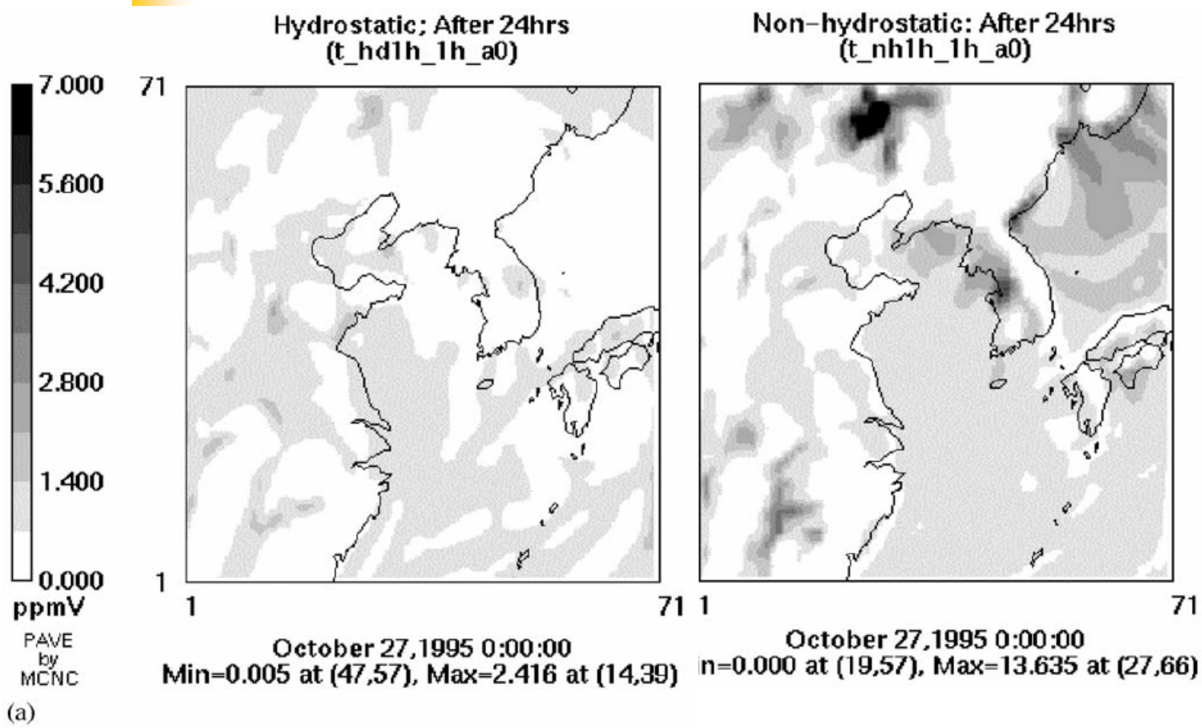
Generalized Vertical Coordinate Forms

	Vertical Coordinate, s	Vertical Jacobian, J_s
For MM5 (MCIP)	$s = 1 - \sigma_{po}$ $\quad \sigma_{po} = \frac{(p - p_T)}{(p_s - p_T)}$	$J_s = \frac{(p - p_T)}{\rho g}$
For WRF/EM (WCIP)	$s = 1 - \eta$ $\quad \eta = \frac{(\pi - \pi_T)}{(\pi_s - \pi_T)}$	$J_s = \frac{\mu}{\rho g}$ $\quad \mu = \pi_s - \pi_T$
For WRF/NMM	$\tilde{p}(x, y, \eta, t) = A(\eta) p_T + B(\eta) \tilde{p}_*(x, y, t)$	$\frac{\partial \tilde{p}}{\partial \eta} = -g \tilde{\rho} J_\eta = \frac{\partial A(\eta)}{\partial \eta} p_T + \frac{\partial B(\eta)}{\partial \eta} \tilde{p}_*$

Map Factor & Grid Resolution

	ID in Models-3 IOAPI	Map Scale (m)	Note
For MM5 (MCIP) [Lambert Conformal]	LATGRD3=2	$m = \frac{\sin(\pi/2 - \phi_1)}{\sin(\pi/2 - \phi)} \left[\frac{\tan(\pi/4 - \phi)}{\tan(\pi/4 - \phi_1)} \right]^n$ $n = \ln\left[\frac{\sin(\pi/2 - \phi_2)}{\sin(\pi/2 - \phi_1)} \right] \left[\ln\left(\frac{\tan(\pi/4 - \phi_2)}{\tan(\pi/4 - \phi_1)} \right) \right]^{-1}$	$(\hat{x}^1_{cent}, \hat{x}^2_{cent}) = (\lambda_0, \phi_0)$ $dx = dy$
For WRF/EM (WCIP) [Lambert Conformal]	LATGRD3=2	$m = \frac{\sin(\pi/2 - \phi_1)}{\sin(\pi/2 - \phi)} \left[\frac{\tan(\pi/4 - \phi)}{\tan(\pi/4 - \phi_1)} \right]^n$ $n = \ln\left[\frac{\sin(\pi/2 - \phi_2)}{\sin(\pi/2 - \phi_1)} \right] \left[\ln\left(\frac{\tan(\pi/4 - \phi_2)}{\tan(\pi/4 - \phi_1)} \right) \right]^{-1}$	$(\hat{x}^1_{cent}, \hat{x}^2_{cent}) = (\lambda_0, \phi_0)$ $dx = dy$
For WRF/NMM [Rotated Lat./Lon.]	LATGRD3=1	m = n = 1	$(\hat{x}^1, \hat{x}^2) = (Lon._{rotated}, Lat._{rotated})$ $dx = f(Lat._{rotated}),\ dy = const.$

Effects of Dynamic Descriptions: Mass consistency (ability to maintain constant mixing ratio during transport process)



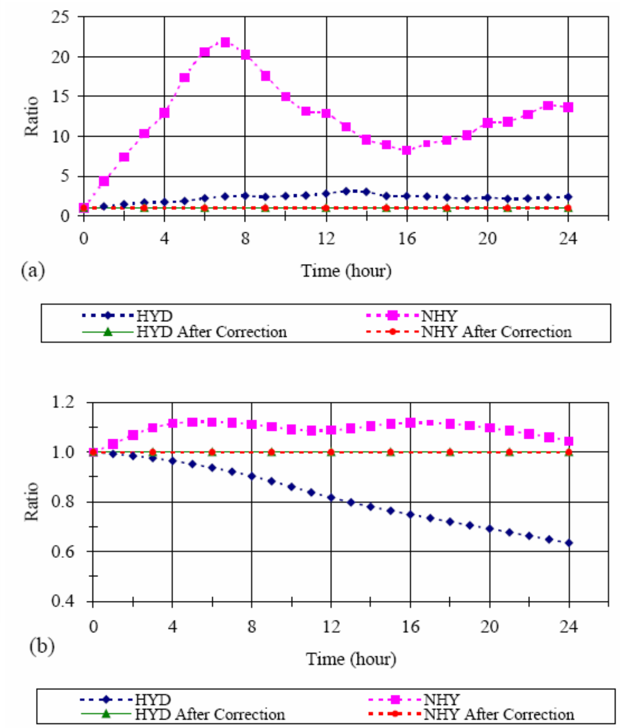


Fig. 9. Performance measures before and after a correction for mass inconsistency at the lowest computational layer: (a) represents peak ratio and (b) mass ratio.

- Hydrostatic (defunct) and Nonhydrostatic MM5 met. input used for CMAQ, no mass correction (S.M. Lee, S. C. Yoon & D.W. Byun, 2004)

How to link dynamics between WRF & CMAQ?

WRF EM coordinate information

$$\eta = \frac{\pi - \pi_t}{\mu} \qquad \mu = \pi_s - \pi_t \qquad J_s = \mu / \rho g$$

WRF EM dynamic variables

$$U = \mu \hat{v}_1 \qquad V = \mu \hat{v}_2 \qquad W = \mu w \qquad \Omega = \mu \hat{v}^3$$

CMAQ $$\frac{\partial(\rho q_i J_s)}{\partial t^{<\hat{\mathbf{v}}_s>}} + m^2 \nabla_s \bullet \left(\frac{\rho q_i J_s \hat{\mathbf{v}}_s}{m^2} \right) + \frac{\partial(\rho q_i J_s \hat{v}^3)}{\partial s} = J_s Q_{q_i}$$

On-line model: All the state variables available at integration time step

Off-line model: What temporal averaging schemes should be used?

Possibilities

CMAQ	$<\rho J_s \hat{\mathbf{v}}_s>$		$<\rho J_s>$		$<\hat{\mathbf{v}}_s>$	
WRF/EM	$\hat{\mathbf{v}}_s$	ρJ_s	$\rho J_s \hat{\mathbf{v}}_s$	$\overline{\hat{\mathbf{v}}_s}$	$\overline{\rho J_s}$	$\overline{\rho J_s \hat{\mathbf{v}}_s}$

For WRF/EM Core, consider how to apply temporal averaging for all the components in the conservation eq.

Previous Study: Use of instantaneous WRF output

- **Instantaneous Mass-Jacobian for coordinate**
- **Instantaneous Mass-Jacobian weighted Contravariant wind**

$$\frac{\rho J_\xi}{m^2}\hat{\mathbf{v}}_\xi = \frac{\rho J_\eta}{m^2}\hat{\mathbf{v}}_\eta = \frac{\mu}{mg}\hat{\mathbf{v}}_z \qquad \frac{\rho J_\xi}{m^2}\dot{\xi} = \frac{-\Omega}{m^2 g}$$

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

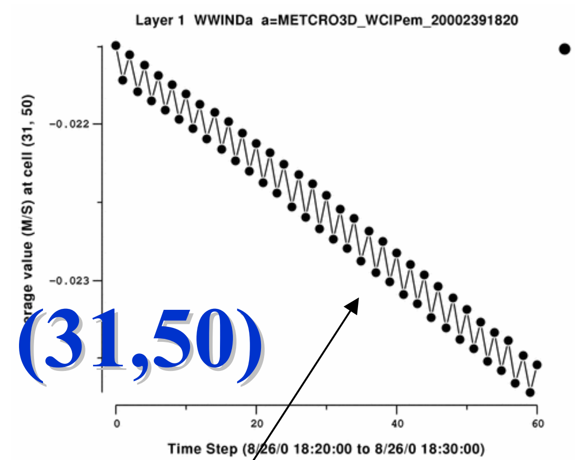
Cf: for EH Dynamic Core – vertical coordinate "fixed" (NCAR dropped EH)

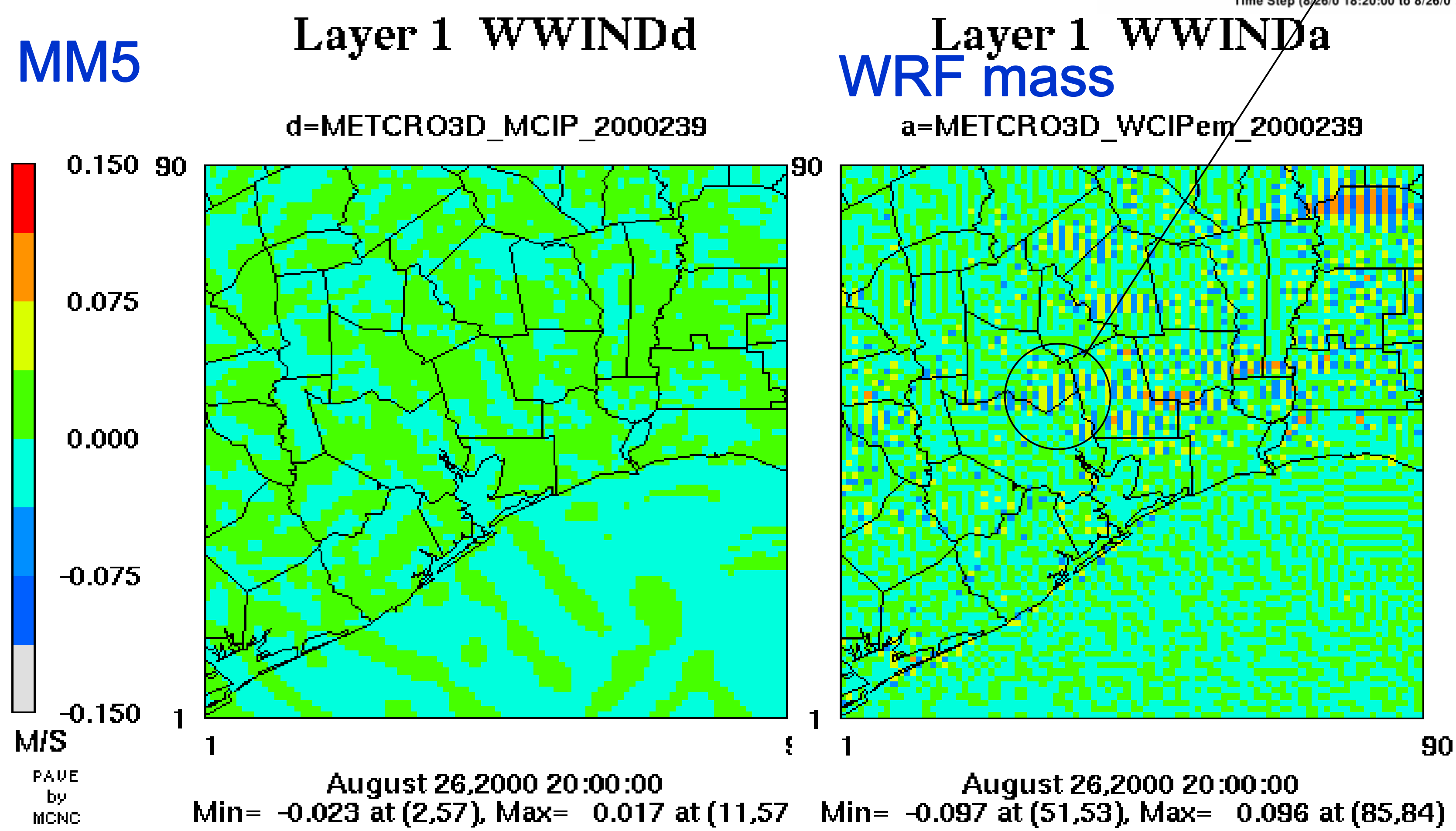
$$\frac{\rho J_\xi}{m^2}\hat{\mathbf{v}}_\xi = \frac{(H - h_s)}{m}(\rho\hat{\mathbf{v}}_z)$$

$$\frac{\rho J_\varsigma}{m^2}\hat{v}^3 = \frac{\rho(H - h_s)}{m^2}\hat{v}^3 \qquad \hat{v}^3 = \frac{\partial\varsigma}{\partial t} + (-m\hat{\mathbf{v}}_\varsigma \bullet \nabla_\varsigma h + w)\left(\frac{\partial\varsigma}{\partial z}\right)$$

Instantaneous Vertical Velocity at layer 1

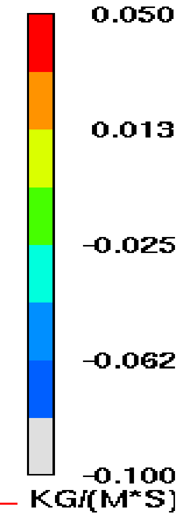
2000/08/26 20UTC (14LST)

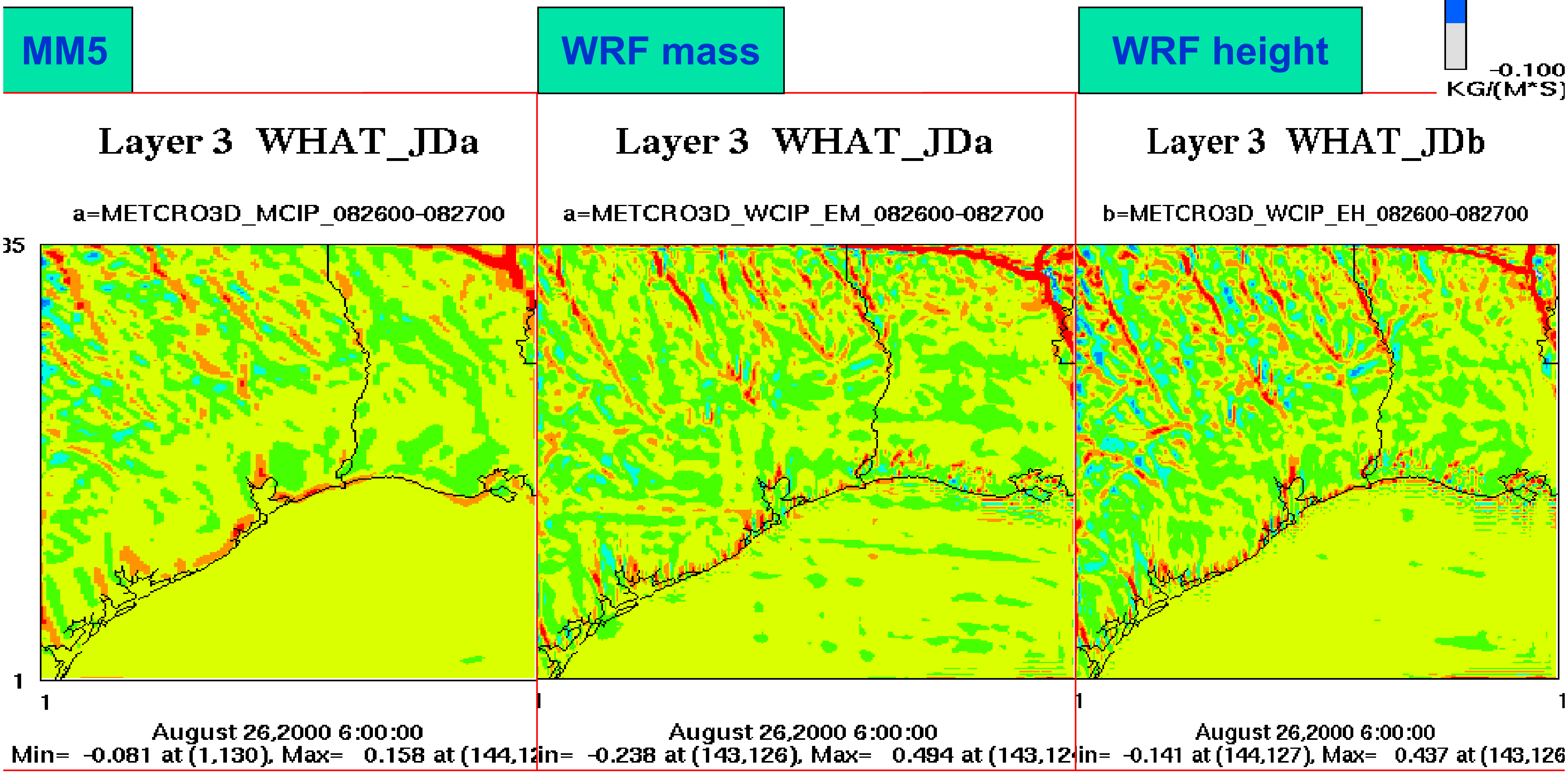




Vertical velocity multiplied with Jacobian-weighted density (instantaneous)

2000/08/26/06UTC





Mass conservative temporal interpolation of wind in CMAQ (*CMAQ method)

The Jacobian and density at a time $t_\alpha = (1-\alpha)t_n + \alpha t_{n+1}$

$$(J_s)_\alpha = (1-\alpha)(J_s)_n + \alpha(J_s)_{n+1}$$

$$(\rho J_s)_\alpha = (1-\alpha)(\rho J_s)_n + \alpha(\rho J_s)_{n+1}$$

$$\frac{\partial(\rho J_s)}{\partial t}$$

Contravariant wind components multiplied with Jacobian-weight density are interpolated linearly,

$$(\rho J_s \hat{V}_s)_\alpha = (1-\alpha)(\rho J_s \hat{V}_s)_n + \alpha(\rho J_s \hat{V}_s)_{n+1}$$

$$(\rho J_s \hat{v}^3)_\alpha = (1-\alpha)(\rho J_s \hat{v}^3)_n + \alpha(\rho J_s \hat{v}^3)_{n+1}$$

Finally, interpolated wind components are derived with:

$$<\hat{V}_s>_\alpha = <\rho J_s \hat{V}_s>_\alpha / <\rho J_s>_\alpha = (\rho J_s \hat{V}_s)_\alpha / (\rho J_s)_\alpha$$

$$<\hat{v}^3>_\alpha = <\rho J_s \hat{v}^3>_\alpha / <\rho J_s>_\alpha = (\rho J_s \hat{v}^3)_\alpha / (\rho J_s)_\alpha$$

Test of other temporal interpolation methods

Note: Current tests use instantaneous Mass*Jacobian as the vertical coordinate in CMAQ $\rho J_s g = \mu$

- Method 1 (both averaged coordinate and wind components)

$$< \hat{V}_s >_\alpha = \frac{\overline{(\rho J_s \hat{V}_s)}_\alpha}{\overline{(\rho J_s)}_\alpha} \qquad < \hat{v}^3 >_\alpha = \frac{\overline{(\rho J_s \hat{v}^3)}_\alpha}{\overline{(\rho J_s)}_\alpha}$$

- Method1.5 (instantaneous μ and averaged wind component)

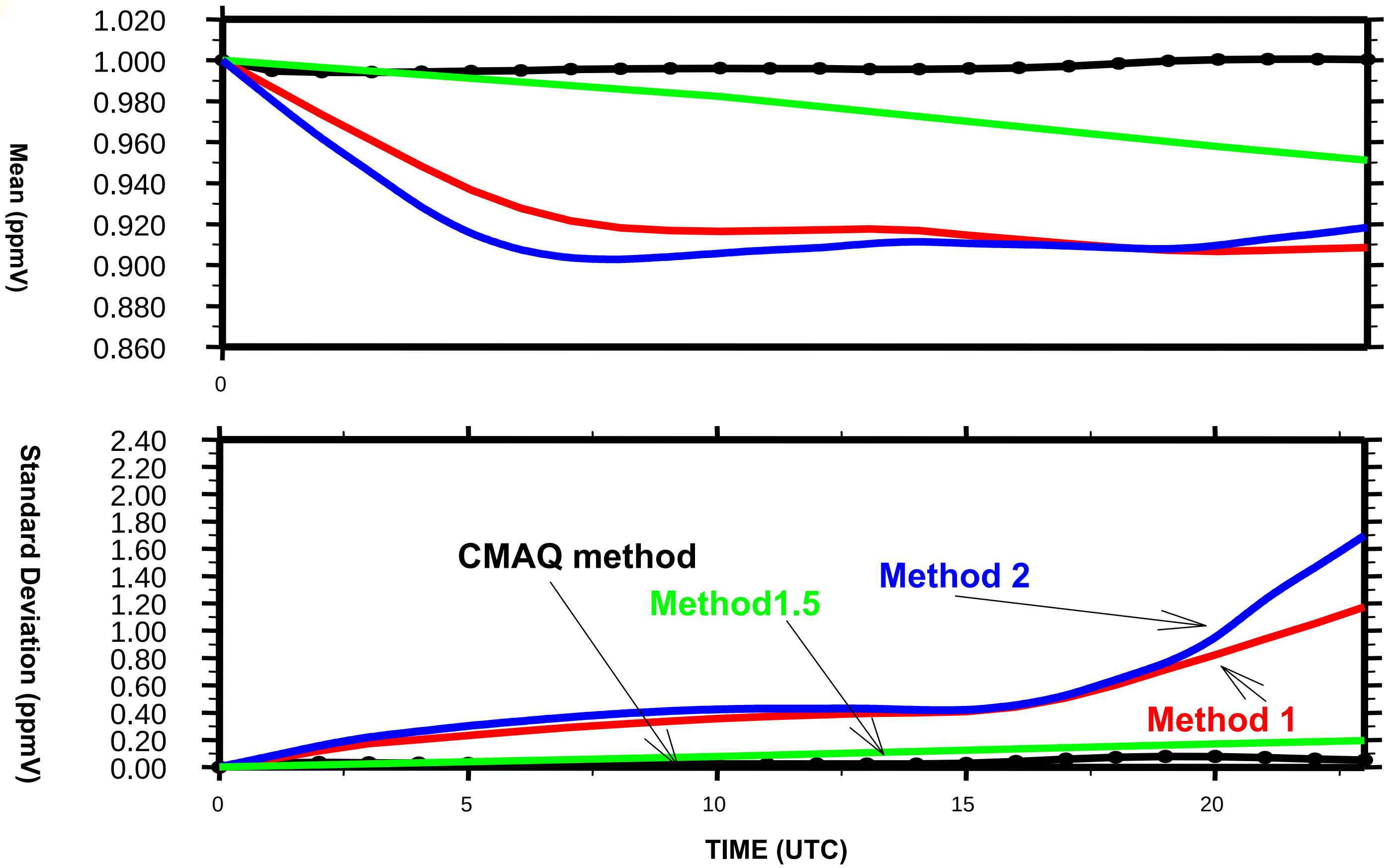
$$< \hat{V}_s >_\alpha = \frac{\overline{(\rho J_s \hat{V}_s)}_\alpha}{(\rho J_s)_\alpha} \qquad < \hat{v}^3 >_\alpha = \frac{\overline{(\rho J_s \hat{v}^3)}_\alpha}{(\rho J_s)_\alpha}$$

- Method 2 (use interpolated wind but no density interpolation)

$$< \hat{V}_s >_\alpha = \overline{(\hat{V}_s)}_\alpha \qquad < \hat{v}^3 >_\alpha = \overline{(\hat{v}^3)}_\alpha$$

1 day simulation with 1hrly met. data from WRF/EM-CMAQ coupling

NWP models can conserve air mass well! ~ 0.05 %/hr



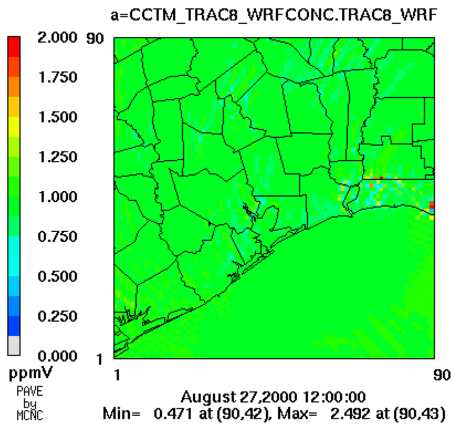
1. Except CMAQ method, mass is decreasing with time for other methods. No strong diurnal variation
2. CMAQ> M1.5: the variation of coordinate variables in 24 hrs is larger than that in 1hr. Thus, in linkage methods which use averaged values, it is also needed to consider time-averaged coordinate variables for building model coordinate.
3. ➔ to maintain mass conservation, there is no need to feed met data at the

Diurnal behavior of error growth (without correction)

Nighttime

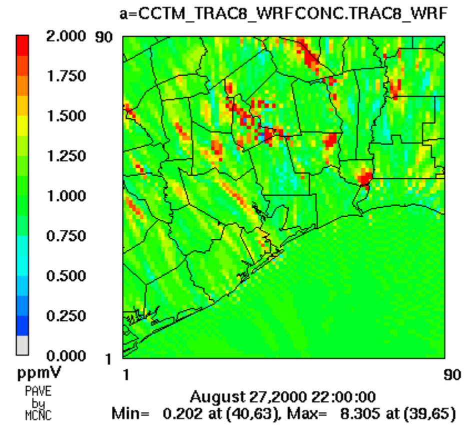
Daytime

Layer 1 IC1_BC1a



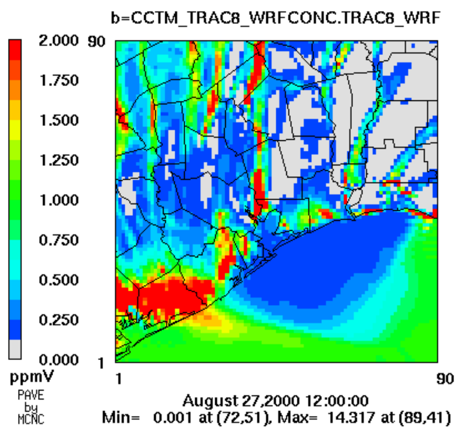
CMAQ interpolation method

Layer 1 IC1_BC1a



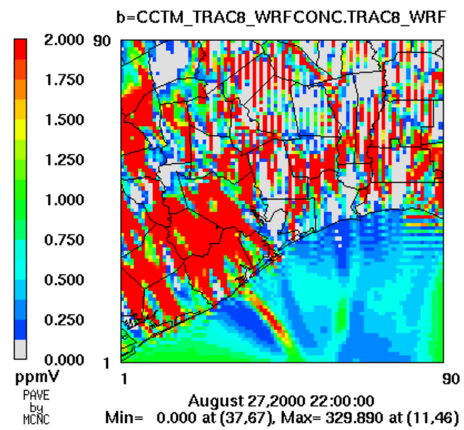
Error growth in the CMAQ method is due to the convective cells from NWP

Layer 1 IC1_BC1b



Method1.5

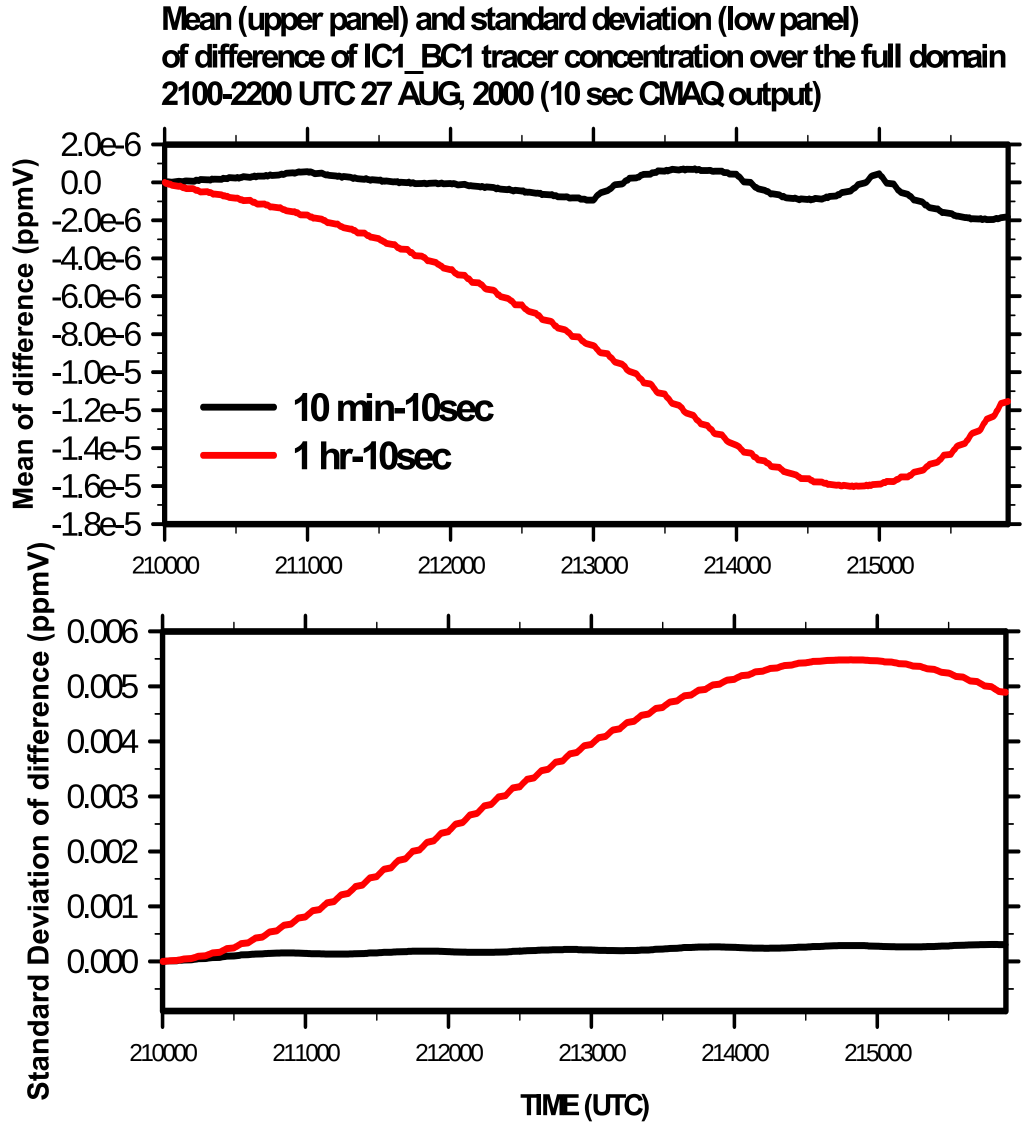
Layer 1 IC1_BC1b



In other methods, error growth is too fast!

Deviation of each experiment from the 10 sec experiment with the CMAQ interpolation method (I)

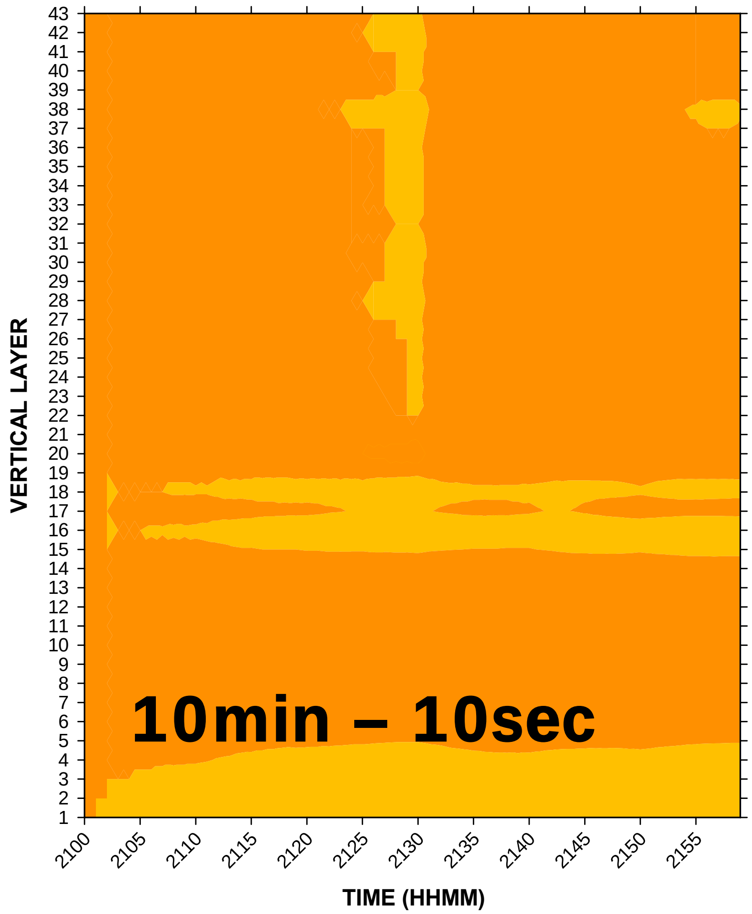
How critical to have high frequency output?



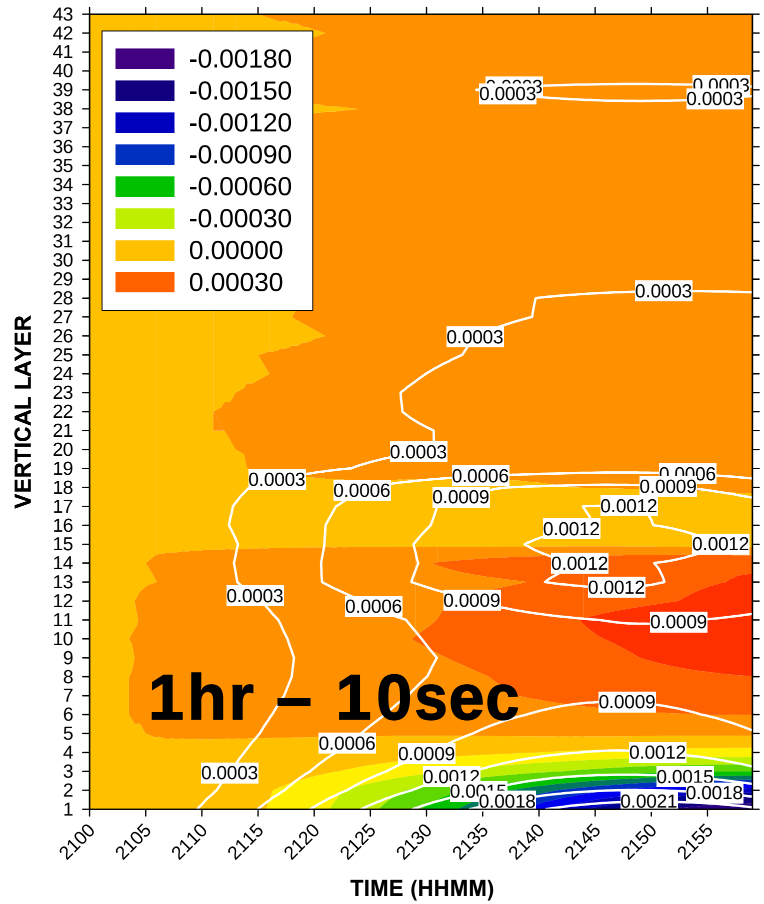
1. **Statistical properties are similar, but each experiment has different signal**
2. **Small fluctuations in both mean and SD, but 10min ~ 10sec**
3. **The difference of 1hr and 10sec is larger than that of 10min and 10sec.**

Deviation of each experiment from the 10 sec experiment with the CMAQ interpolation method (II)

Layer mean(shaded) and standard deviation (white line of difference of IC1_BC1 tracer concentration between 10min experiment and 10sec experiment

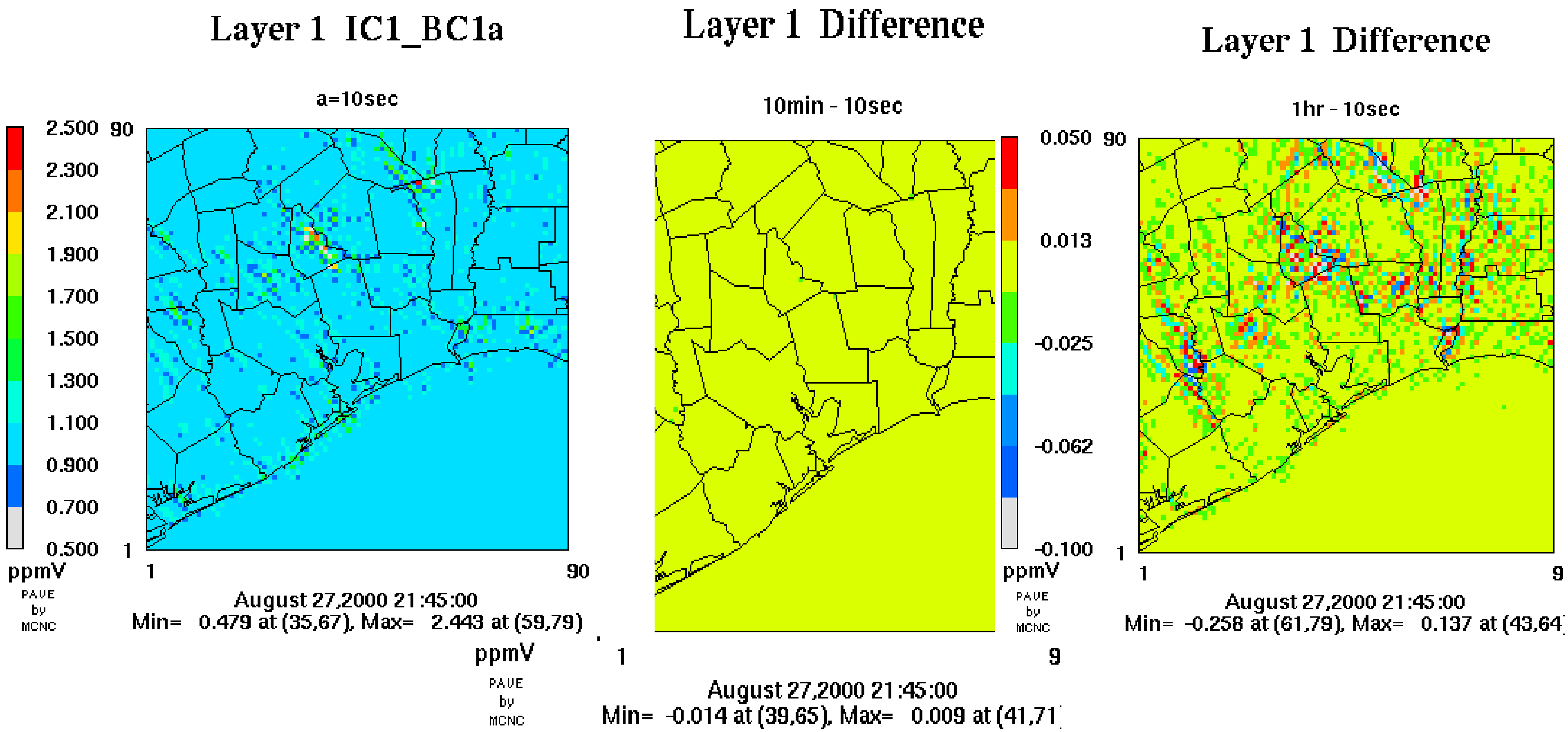


Layer mean(shaded) and standard deviation (white line) of difference of IC1_BC1 tracer concentration between 1hr experiment and 10sec experiment



1. **Layer mean difference in time-vertical cross-section**
2. **Large difference near surface → due to surface forcing**
3. **Same message (The difference of 1hr and 10sec is larger than that of 10min and 10sec)**

Deviation of each experiment from the 10 sec output experiment with the CMAQ interpolation method (III): Layer 1 at 21:45 UTC, August 27, 2000



1. **In this case, the dynamical variation in less 10min are not well represented in the WRF simulation → Related with Dr. Bill Skaramock's KE spectra analysis result**
2. **Possible to use a larger time step than meteorological integration time step without losing mass consistency of wind fields.**

- We have revealed that the wind from the WRF mass core is very mass-consistent most of the time
- Even without mass adjustment, the off-line WRF-CMAQ system has conserved the mass of pollutants well by using the mass conservative temporal interpolation of wind in CMAQ except for the convective cells.
- Higher met. data transfer frequency makes the off-line CMAQ model results closer to the on-line model.
- Also, this study clearly indicates that the mass-consistency of wind fields can be maintained with an output time step larger than met. time step because the WRF mass provides the mass-consistent wind field.

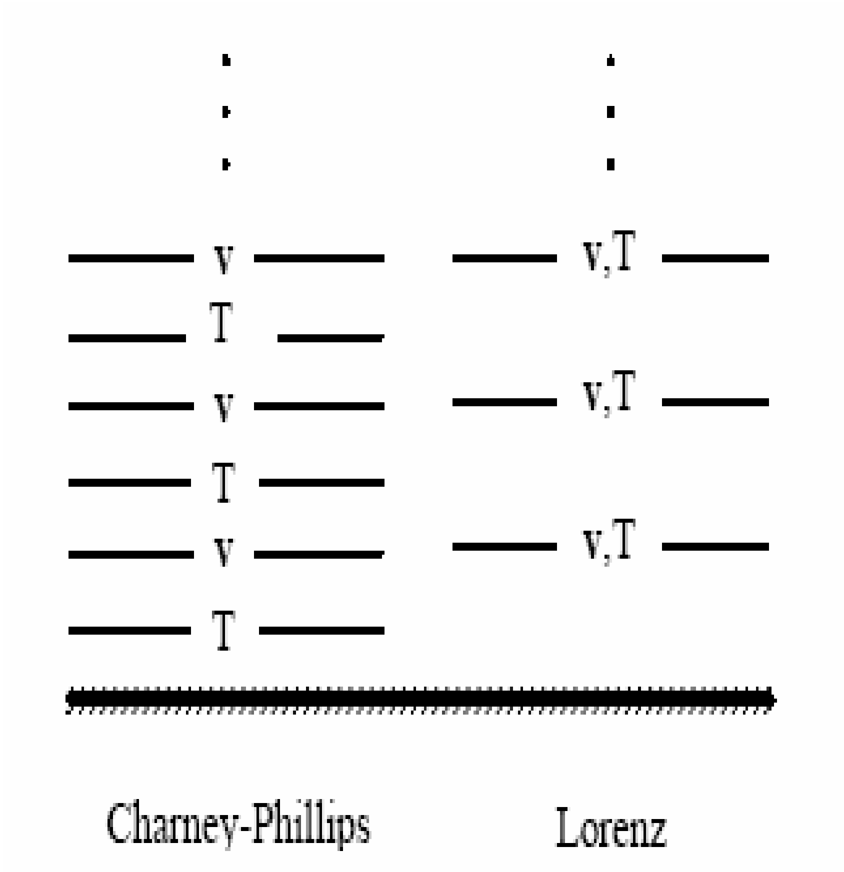
Consistent coordinates and grid structures

Vertical grid system of WRF/nmm

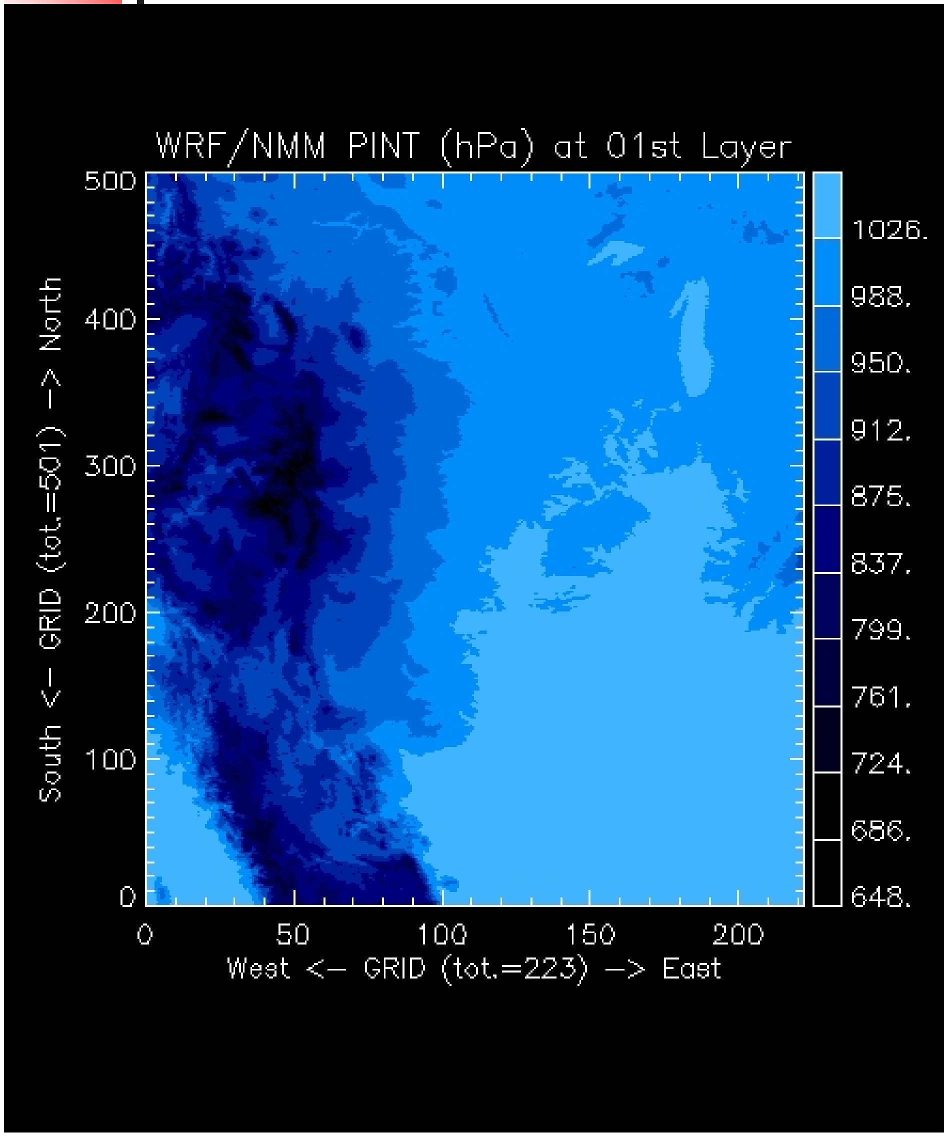
- Terrain-following hybrid pressure-sigma coordinate (Arakawa and Lamb, 1977)

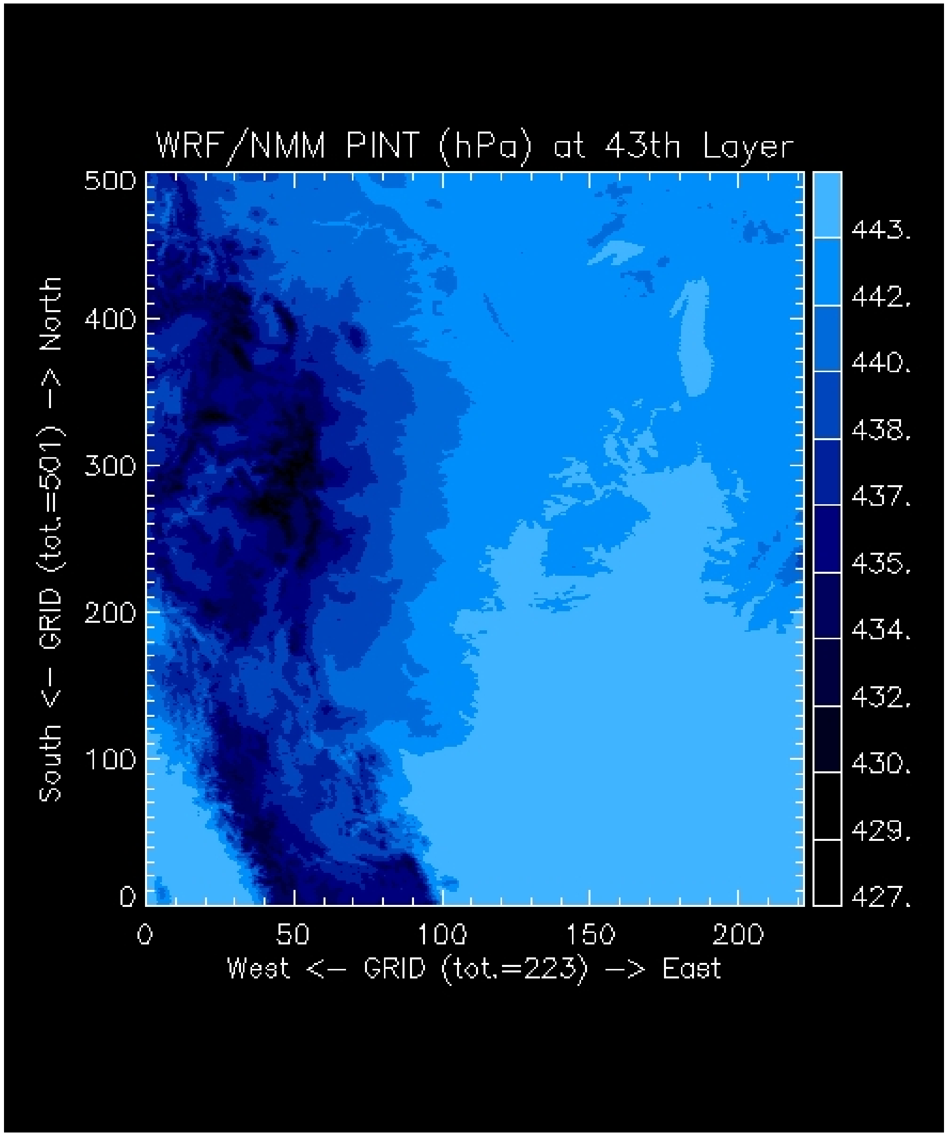
- Lorenz vertical staggering
  - Geopotential and nonhydrastatic pressure are on the interfaces

  - 3-D velocity components and temperature are on the middle layers



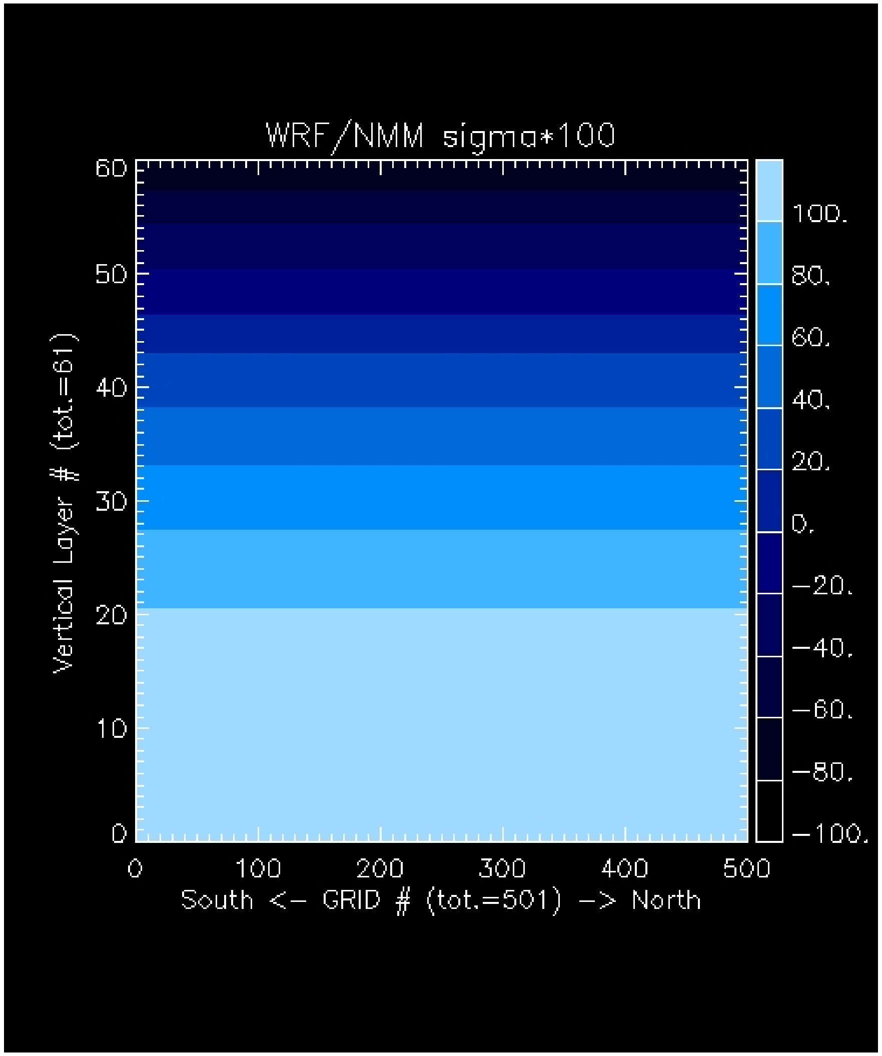
From Janjic (2003)


WRF/NMM PINT (hPa) at 01st Layer
South <-- GRID (tot.=501) --> North
West <-- GRID (tot.=223) --> East
0
100
200
300
400
500
0
50
100
150
200
1026.
988.
950.
912.
875.
837.
799.
761.
724.
686.
648.


WRF/NMM PINT (hPa) at 43th Layer
South <-- GRID (tot.=501) --> North
West <-- GRID (tot.=223) --> East
0
100
200
300
400
500
0
50
100
150
200
443.
442.
440.
438.
437.
435.
434.
432.
430.
429.
427.

sigma values for each levels of WRF/NMM

Level	sigma	Level	sigma
1	1.000	32	0.480
2	0.996	33	0.443
3	0.991	34	0.406
4	0.987	35	0.367
5	0.981	36	0.328
6	0.976	37	0.288
7	0.970	38	0.248
8	0.965	39	0.207
9	0.959	40	0.166
10	0.952	41	0.125
11	0.946	42	0.084
12	0.939	43	0.042
13	0.931	44	0.000
14	0.922	45	-0.061
15	0.912	46	-0.121
16	0.901	47	-0.181
17	0.889	48	-0.238
18	0.874	49	-0.292
19	0.856	50	-0.342
20	0.835	51	-0.387
21	0.812	52	-0.431
22	0.787	53	-0.475
23	0.761	54	-0.524
24	0.734	55	-0.581
25	0.705	56	-0.645
26	0.676	57	-0.715
27	0.646	58	-0.788
28	0.615	59	-0.860
29	0.582	60	-0.931
30	0.549	61	-1.000
31	0.515		



Hybrid terrain following pressure-sigma coord. & Lorenz staggering [Arakawa and Lamb, 1977; Janjic, 2003]

$$\sigma \equiv \frac{p - p_c}{\pi}$$

$$\pi \equiv \begin{cases} \pi_U = p_c - p_T & \text{for upper levels } (p_T \le p < p_c) \\ \pi_L = p_s - p_c & \text{for lower levels } (p_c < p \le p_s) \end{cases}$$

$p_T(const.)$: the pressure at the top of the atmosphere $(50\,hPa)$
$p_c(const.)$: the chosen pressure $(420\,hPa)$
$p_s(x_0, y_0, t)$: the pressure at the earth surface

$$J_\sigma = \left|\frac{\partial h}{\partial \sigma}\right| = \frac{1}{\rho_{hydro} g}\left|\frac{\partial p}{\partial \sigma}\right|$$

For lower levels : $p = (p_s - p_c)\sigma + p_c = (1-\sigma)p_c + \sigma p_s$

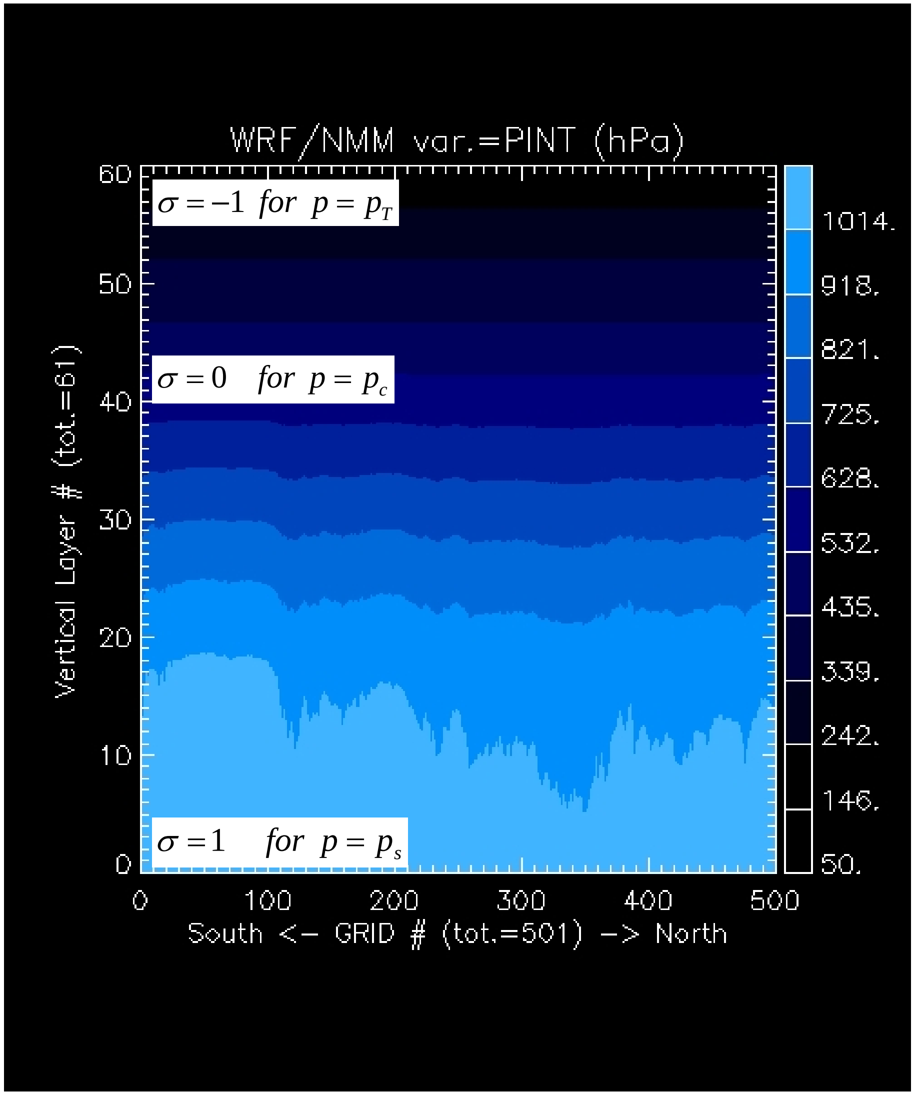
$$J_\sigma = \frac{p_s - p_c}{\rho_{hydro} g} = \frac{\pi_L}{\rho_{hydro} g}$$

*) $p \equiv A(\sigma_L)p_c + B(\sigma_L)p_s$
=> $A(\sigma_L) = (1-\sigma_L), B(\sigma_L) = \sigma_L$
$if\ \sigma = 0, then\ A = 1, B = 0\ and\ p = p_c$

For upper levels : $p = (p_c - p_T)\sigma + p_c = -\sigma p_T + (1+\sigma)p_c$

$$J_\sigma = \frac{p_c - p_T}{\rho_{hydro} g} = \frac{\pi_U}{\rho_{hydro} g}$$

*) $p \equiv A(\sigma_U)p_T + B(\sigma_U)p_c$
=> $A(\sigma_U) = -\sigma_U, B(\sigma_U) = (1+\sigma_U)$
$if\ \sigma = 0, then\ A = 0, B = 1\ and\ p = p_c$



$$J_\sigma = abs\left[(\rho g)^{-1}\left(\frac{\partial A(\sigma)}{\partial \sigma} p_T + \frac{\partial B(\sigma)}{\partial \sigma} \tilde{p}_*\right)\right]$$

WRF/nmm Utilizes Rotated Latitude/Longitude Coordinate

$$\Lambda = arctg \frac{\cos\varphi \sin(\lambda - \lambda_0)}{\cos\varphi_0 \cos\varphi \cos(\lambda - \lambda_0) + \sin\varphi_0 \sin\varphi}$$

$$\Phi = \arcsin\left(\cos\varphi_0 \sin\varphi - \sin\varphi_0 \cos\varphi \cos(\lambda - \lambda_0)\right)$$

(Λ, Φ) :*rotated coordinate sytem*

(φ_0, λ_0):*center of domain*

(φ, λ) :*natural coordinate sytem*

$$U = \frac{u[\cos\varphi_0 \cos\varphi + \sin\varphi_0 \sin\varphi \cos(\lambda - \lambda_0)] - v \sin\varphi_0 \sin(\lambda - \lambda_0)}{\sqrt{1 - [\cos\varphi_0 \sin\varphi - \sin\varphi_0 \cos\varphi \cos(\lambda - \lambda_0)]^2}}$$

$$V = \frac{u \sin\varphi_0 \sin(\lambda - \lambda_0) + v[\cos\varphi_0 \cos\varphi + \sin\varphi_0 \sin\varphi \cos(\lambda - \lambda_0)]}{\sqrt{1 - [\cos\varphi_0 \sin\varphi - \sin\varphi_0 \cos\varphi \cos(\lambda - \lambda_0)]^2}}$$

The horizontal wind in the rotated system

$$\mathbf{V} = (U, V)$$

$$u = \frac{U(\cos\varphi_0 \cos\Phi - \sin\varphi_0 \sin\Phi \cos\Lambda) + V \sin\varphi_0 \sin\Lambda}{\sqrt{1 - (\cos\varphi_0 \sin\Phi + \sin\varphi_0 \cos\Lambda \cos\Phi)^2}}$$

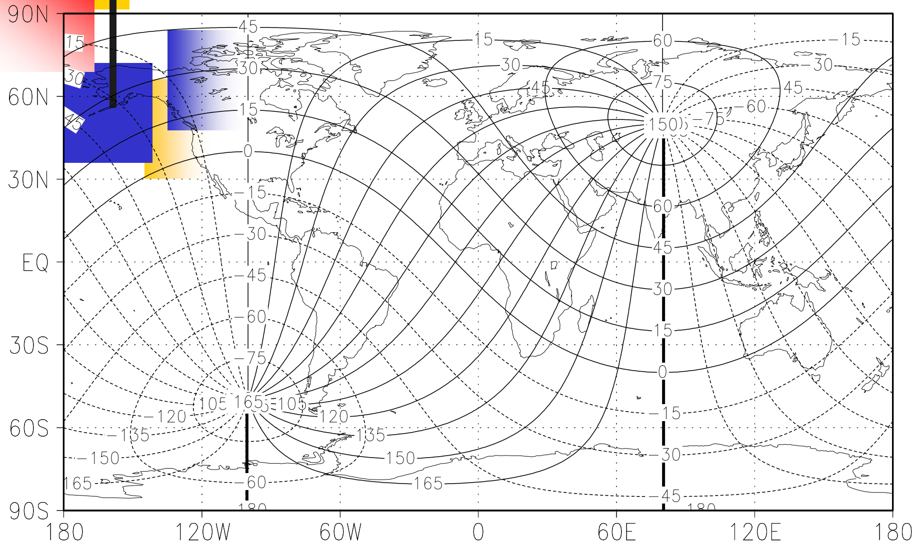
$$v = \frac{-U \sin\varphi_0 \sin\Lambda + V(\cos\varphi_0 \cos\Phi - \sin\varphi_0 \sin\Phi \cos\Lambda)}{\sqrt{1 - (\cos\varphi_0 \sin\Phi + \sin\varphi_0 \cos\Lambda \cos\Phi)^2}}$$

The horizontal wind in the natural latitude/longitude system

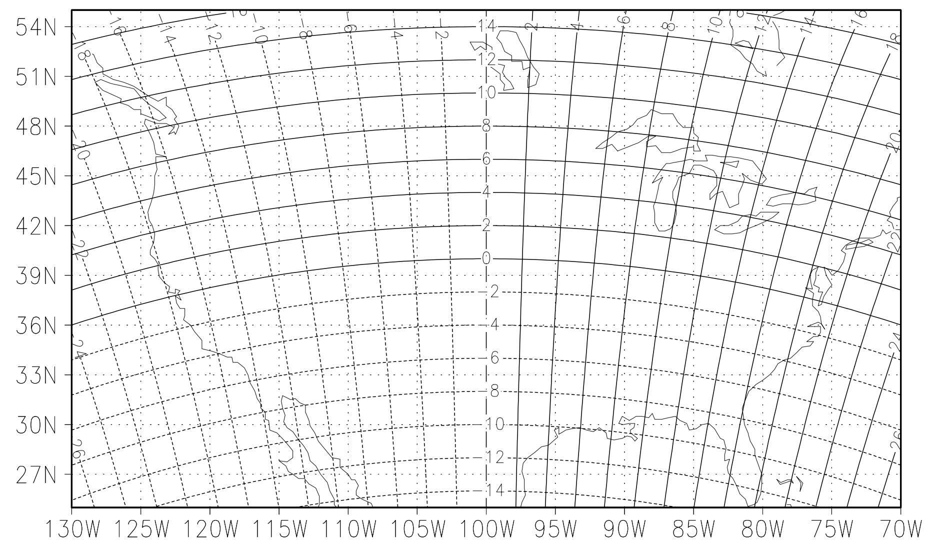
$$\mathbf{v} = (u, v)$$

- "The simplicity of a lat-lon grid is made applicable over the entire globe by rotating the earth's lat-lon grid such that the equator and prime meridian intersect at the center of the WRF/nmm computational grid. This rotation minimizes the convergence of meridians, keeping the true horizontal scale relatively uniform over the domain" (Tom Black, 1988; Pyle et al.,2004)

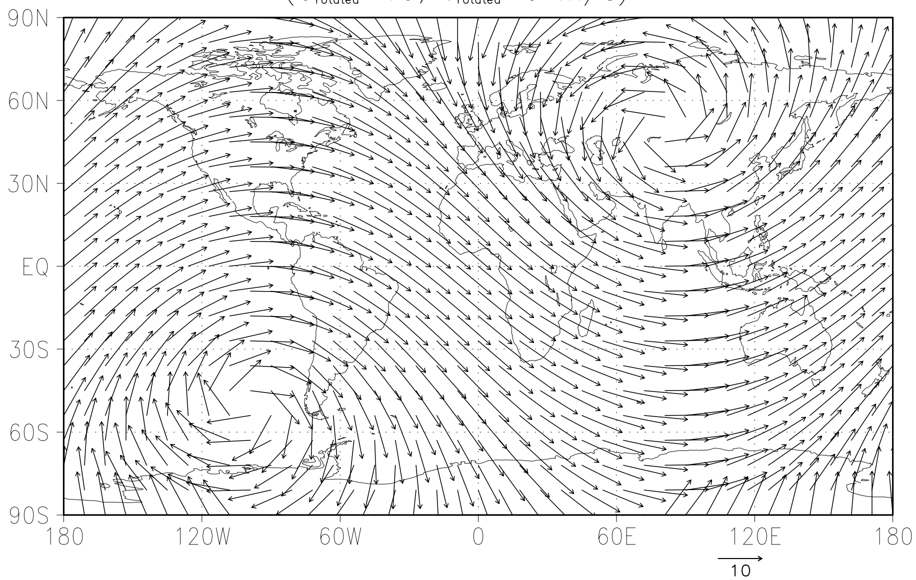
Rotated Lon./Lat.
O(0,0) -> O'(100W,40N)



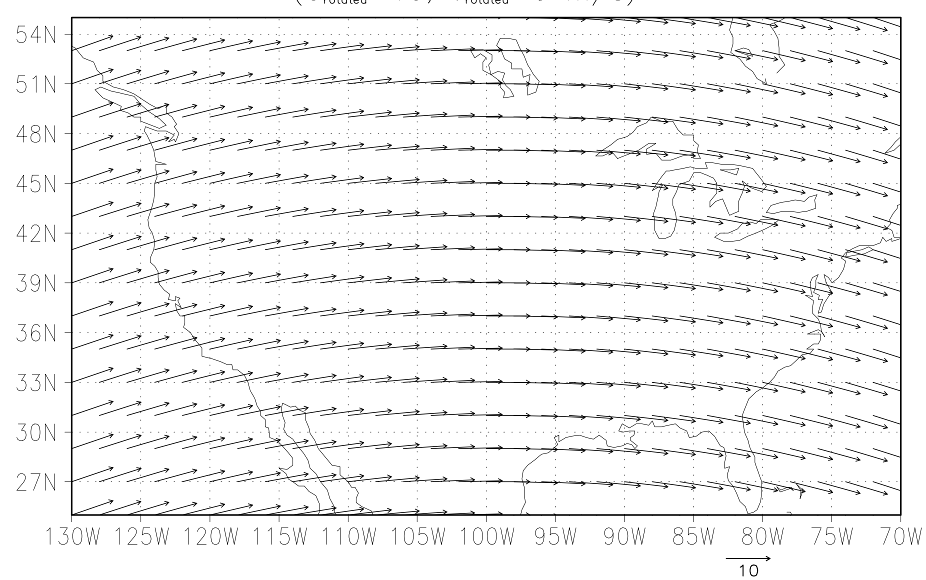
Lotated Lon./Lat.
O(0,0) -> O'(100W,40N)



Composite wind$_{rotated}$ into wind$_{origin}$
(U$_{rotated}$=10, V$_{rotated}$=0 m/s)



Composite wind$_{rotated}$ into wind$_{origin}$
(U$_{rotated}$=10, V$_{rotated}$=0 m/s)



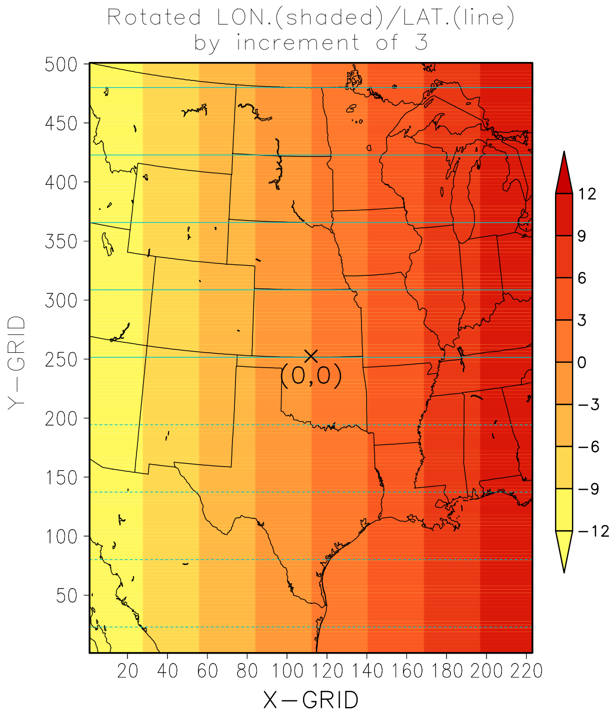
Grid definition <griddef_08central> for the model domain of (223x502)

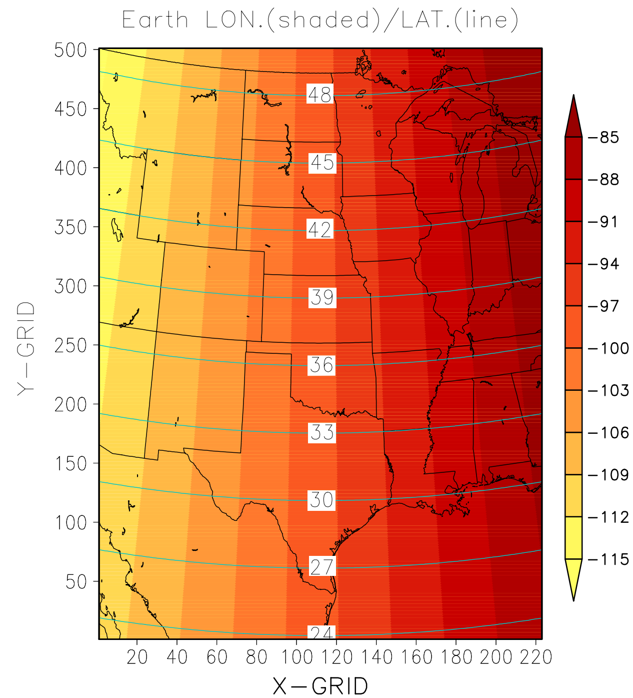
DATA TLM0D/-98.0/, TPH0D/37.0/, WBD/-11.866370/, SBD/-13.157894/, DLMD/.053452115/, DPHD/.052631578/

Earth Lon./Lat. of Center **Rotated Lon./Lat. of Left and Lower** **$dX_{rotated}/dX_{rotated}$ (degree)**

Calculate some information from <griddef_08central>

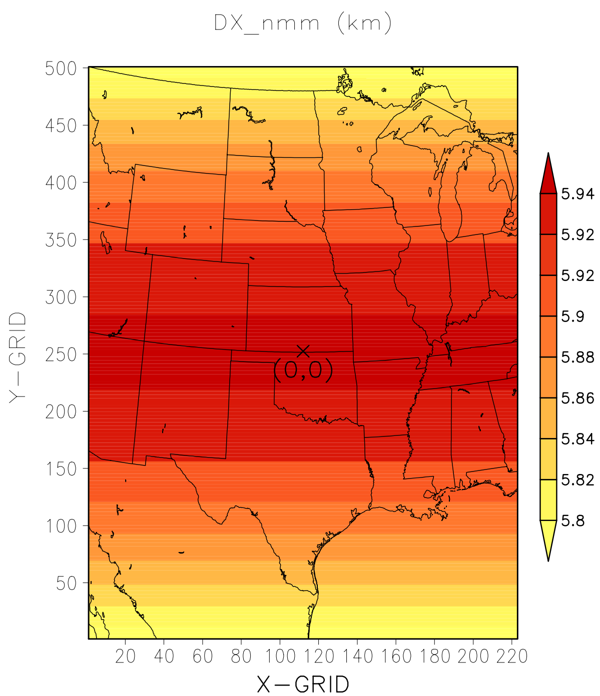
- $LON_{rotated}$ (i,j) & $LAT_{rotated}$ (i,j) (radian)
- LON_{earth} (i,j) & LAT_{earth} (i,j) (radian)





Finally, find out dX_{nmm} and dX_{nmm} which are invariant with the rotation of coordinate

$dX_{nmm}(i,j)$ (meter) = $dX_{rotated}$ (radian) * cos ($LAT_{rotated}(i,j)$) * Radius_Earth : **Variable according to Lat.**
$dY_{nmm}(i,j)$ (meter) = $dY_{rotated}$ (radian) * Radius_Earth : **Constant**



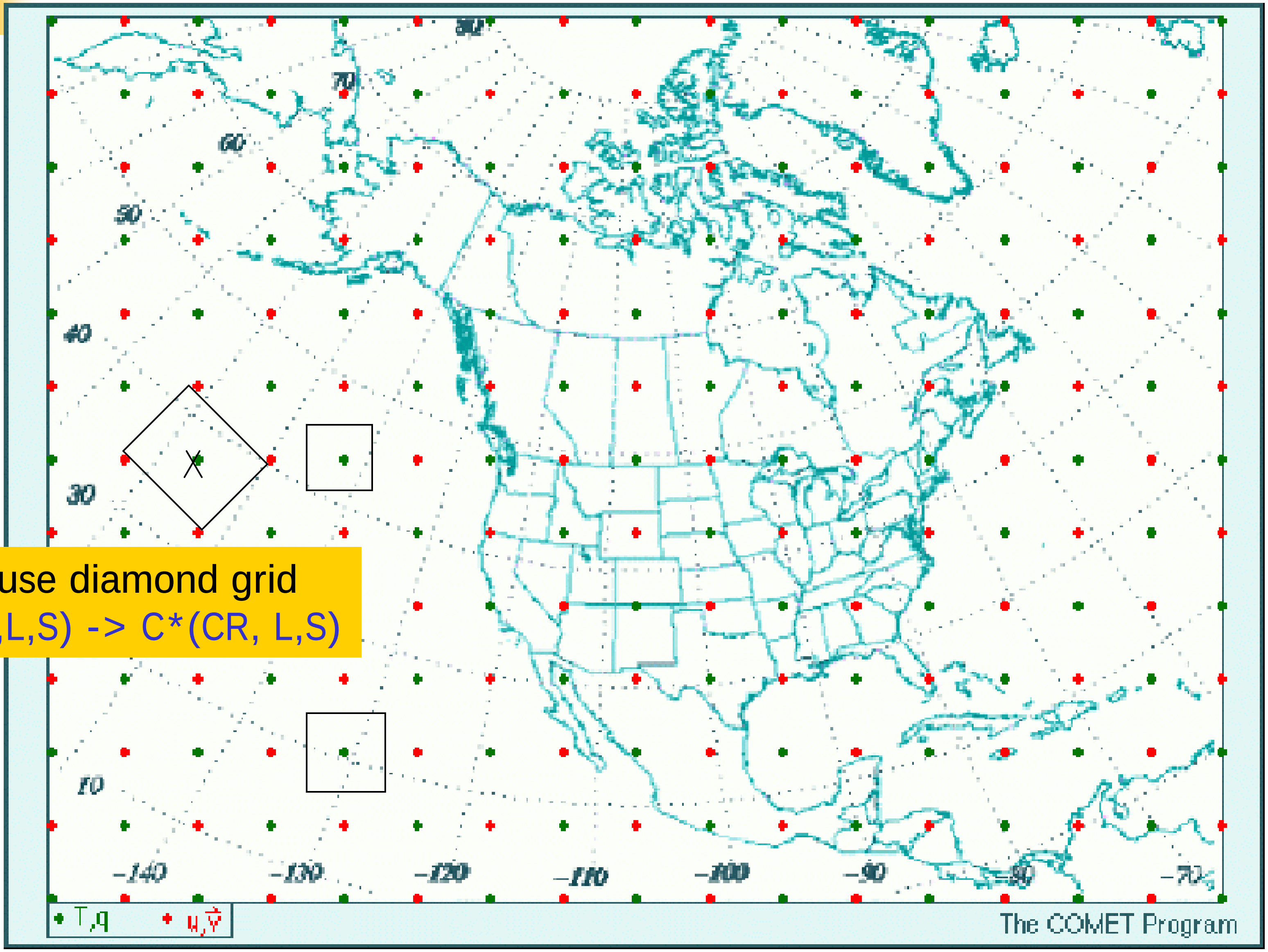
5.8 km < $dX_{nmm}(i,j)$ < 5.94 km
while, $dY_{nmm}(i,j)$ = 5.85 km

That means;

1) The displacement is invariant with the rotation of coordinate.
2) So, the map scale factor for domain of WRF-NMM has a value of unit (m=1).
3) However, dX_{nmm} is not the same as dY_{nmm} (non-conformality).

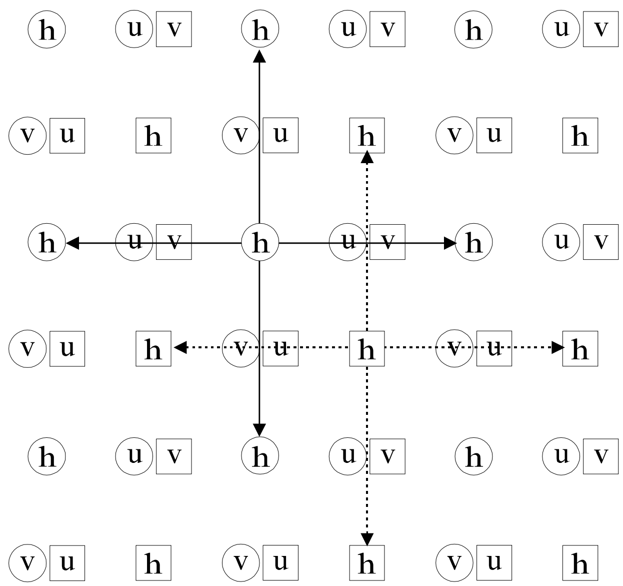
Horizontal Grid System of WRF/nmm:

Rotated lat./long & Arakawa-E grid -> C-grid for CMAQ

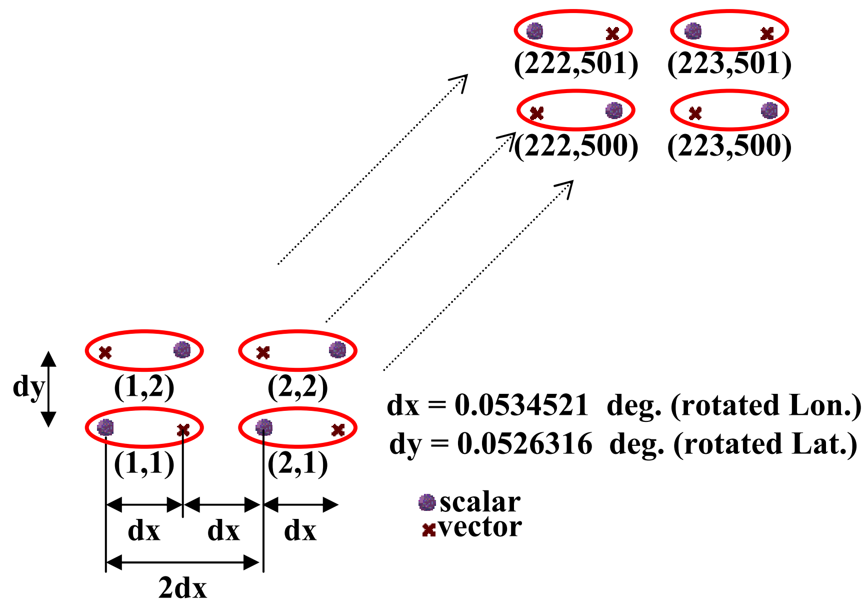


If we use diamond grid
C(C,R,L,S) -> C*(CR, L,S)

Dynamics at Semi-Staggered Arakawa E grid



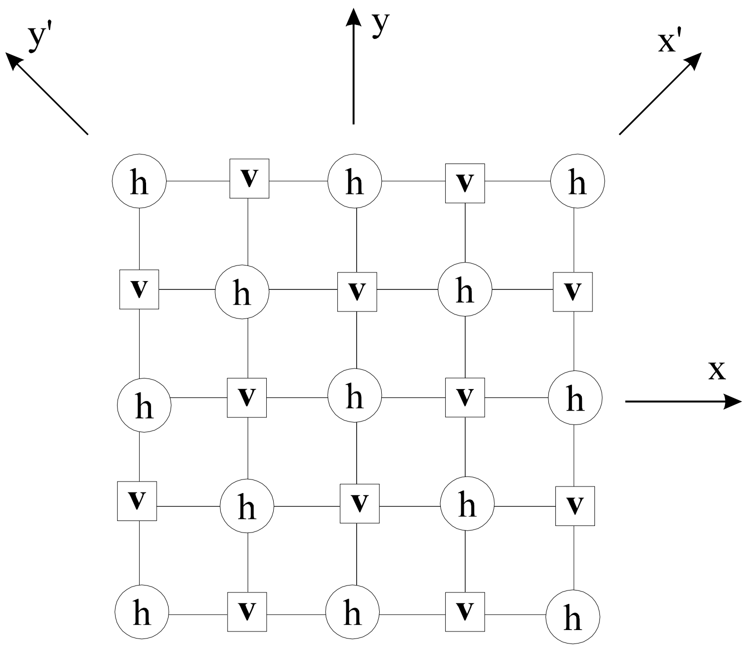
The E grid is essentially a superposition of two C grids.



✓When only the adjustment terms in the equations of motion and continuity are considered, it may be shown that two large-scale solutions from each C grid may exist independently, and a noisy total solution results.

✓So, to employ the forward-backward time differencing scheme in a way that prevents gravity wave separation and thereby precludes the need for explicit filtering (Mesinger 1973: Mesingerand Arakawa 1976; Janji´c 1979).

Semi-Staggered Arakawa E grid on the Rotated Lon./Lat. System



✓ The momentum field (u-wind and v-wind) is computed on different points than the mass or scalar field (temperature, moisture, TKE, vertical wind, pressure and passive substants)

✓ In order to achieve higher computational efficiency of the model code, the grid is rotated relative to other grid configurations (two horizontal coordinate systems in plane geometry, the main *(x,y)* and the auxiliary *(x',y')* system, both will be used in order to perform horizontal differencing)

Dynamics at Semi-Staggered Arakawa E grid

✓The horizontal advection scheme was developed by Janji´c (1984) by transforming the Arakawa-Lamb scheme in the E grid frame specifically for the E grid and controls the cascade of energy toward smaller scales.

The Arakawa Jacobian rewritten by Janji´c (1984)

$$J_A(p,q) =$$
$$\frac{1}{3}\left\{\delta_x\left[\left(-\delta_y p\right)\overline{q}^{x}\right] + \delta_y\left[\left(\delta_x p\right)\overline{q}^{y}\right]\right\} +$$
$$\frac{2}{3}\left\{\delta_{x'}\left[\frac{\sqrt{2}}{2}\left(\overline{-\delta_x p + \delta_y p}^{y'}\right)\overline{q}^{x'}\right] + \delta_{y'}\left[\frac{\sqrt{2}}{2}\left(\overline{\delta_x p + \delta_y p}^{x'}\right)\overline{q}^{y'}\right]\right\}$$

✓It is used in conjunction with a modified Euler-backward timedifferencing scheme that results in significantly less damping than occurs in the standard Euler-backward scheme for nonmomentum quantities and no damping of the wind components.

✓After each adjustment time step, a second-order nonlinear horizontal diffusion is applied to each of the primary prognostic variables (Janji´c 1990)

Dynamics at Semi-Staggered Arakawa E grid

Conservation properties

The conservation of the momentum

$$\frac{\partial}{\partial t}\left(h_u u\right) = -\left\{\frac{1}{3}\left[\delta_x\left(\overline{U}^x\,\overline{u}^x\right) + \delta_y\left(\overline{V}^x\,\overline{u}^y\right)\right] + \frac{2}{3}\left[\delta_{x'}\left(\overline{U}^x\,\overline{u}^{x'}\right) + \delta_{y'}\left(\overline{V}^x\,\overline{u}^{y''}\right)\right]\right\} + \ldots$$

The conservation the kinetic energy

$$\frac{\partial}{\partial}\left(\overline{h}^x\,\frac{1}{2}u^2\right) = -\left\{\frac{1}{3}\left[\delta_x\left(\overline{U}^x\,\frac{1}{2}\overline{\overline{uu}}^x\right) + \delta_y\left(\overline{V}^x\,\frac{1}{2}\overline{\overline{uu}}^y\right)\right]\frac{2}{3}\left[\delta_{x'}\left(\overline{U}^x\,\frac{1}{2}\overline{\overline{uu}}^{x'}\right) + \delta_{y'}\left(\overline{V}^x\,\frac{1}{2}\overline{\overline{uu}}^{y'}\right)\right]\right\} + \ldots$$

$$\frac{\partial}{\partial}\left(\overline{h}^x\,\frac{1}{2}v^2\right) = -\left\{\frac{1}{3}\left[\delta_x\left(\overline{U}^x\,\frac{1}{2}\overline{\overline{w}}^x\right) + \delta_y\left(\overline{V}^x\,\frac{1}{2}\overline{\overline{w}}^y\right)\right]\frac{2}{3}\left[\delta_{x'}\left(\overline{U}^x\,\frac{1}{2}\overline{\overline{w}}^{x'}\right) + \delta_{y'}\left(\overline{V}^x\,\frac{1}{2}\overline{\overline{w}}^{y'}\right)\right]\right\} + \ldots$$

After summation over a domain with cyclic boundary conditions, the right hand side of each equation vanishes, and thus, the properties are conserved.

Consistent coordinates and grid structures

WRF/EM & CMAQ utilize Arakawa-C Grid

Arakawa-B Grid (MM5) is linearly interpolated onto Arakawa-C Grid (CMAQ)

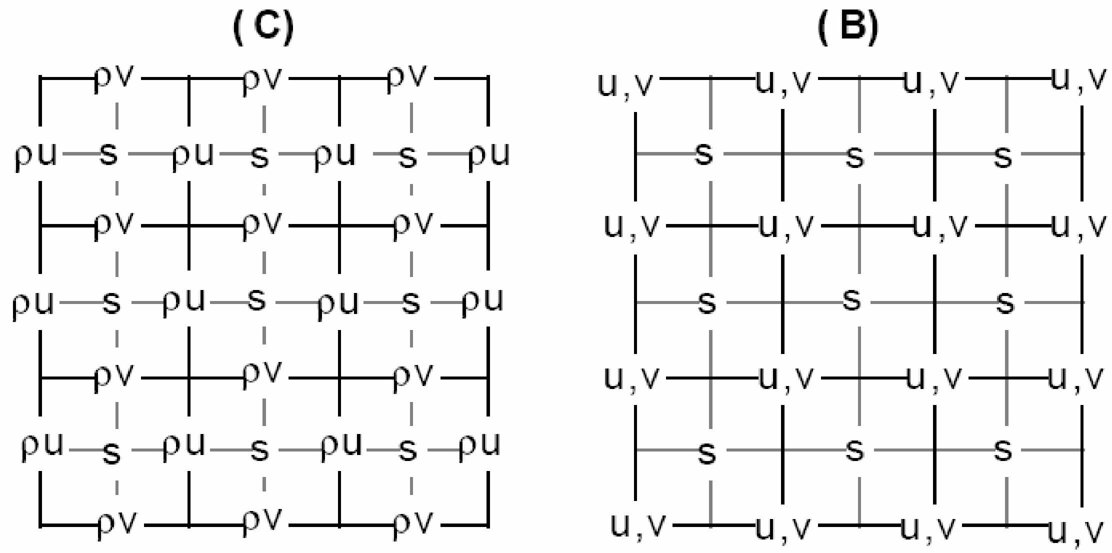


Figure 12-3. Two Different Grid Point Definitions, Arakawa *C*- and *B*-grids, Used in MCIP. *u* and *v* are horizontal wind components, *s* represents a scalar quantity, and ρ is density of air. For MM5, p^* is used instead of ρ.

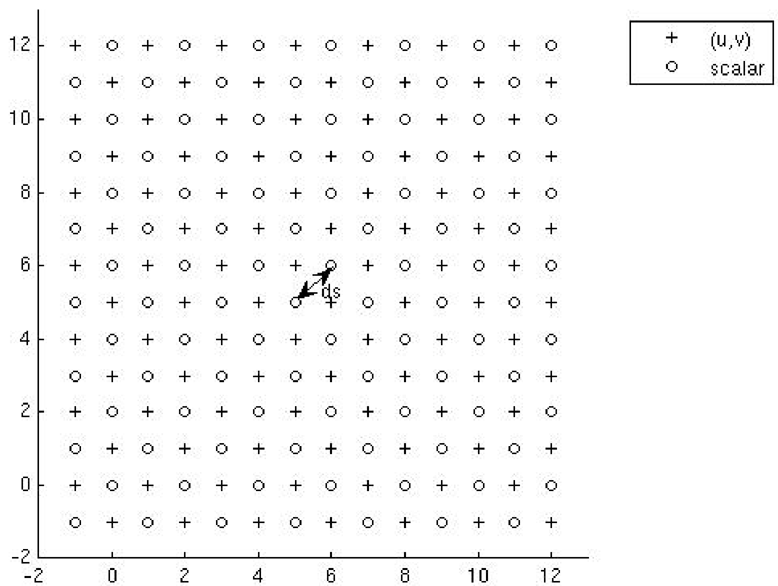
Dimension for Grid Point

	Dot-Point	Cross-Point	Flux-Point
For MM5 (MCIP)	(NCOL+1 , NROW+1)	(NCOL , NROW)	X-dir (NCOL+1 , NROW) Y-dir (NCOL , NROW+1)
For WRF/EM (WCIP)	(NCOL+1 , NROW+1)	(NCOL , NROW)	X-dir (NCOL+1 , NROW) Y-dir (NCOL , NROW+1)
For WRF/NMM	(NCOL , NROW)	(NCOL , NROW)	(NCOL , NROW)

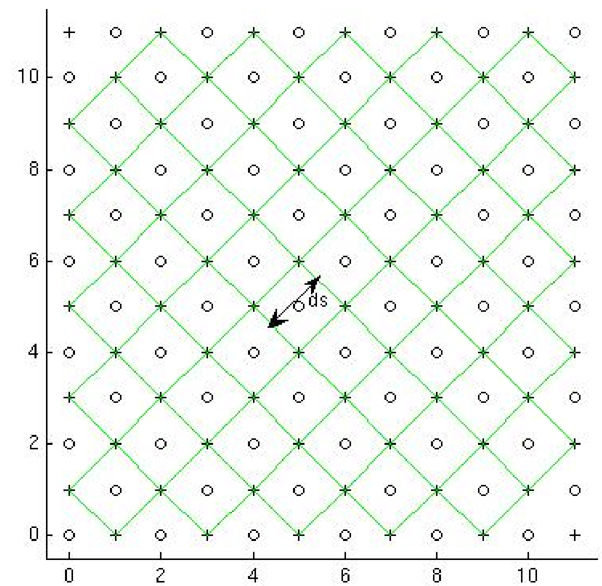
How to Utilize Arakawa-E for CMAQ?

- Develop a horizontal advection algorithm in CMAQ for Arakawa E-grids
- Split 2-D horizontal advection operator into 1-D operators and use CMAQ-proven 1-D schemes, such as PPM, with alternation between appropriate X and Y directions
- Work directly with meteorological variables on the E-grid - avoid spatial interpolation

Option 1: Rotated square cells (rotated B-grid then on C-grid



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



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

Advantages

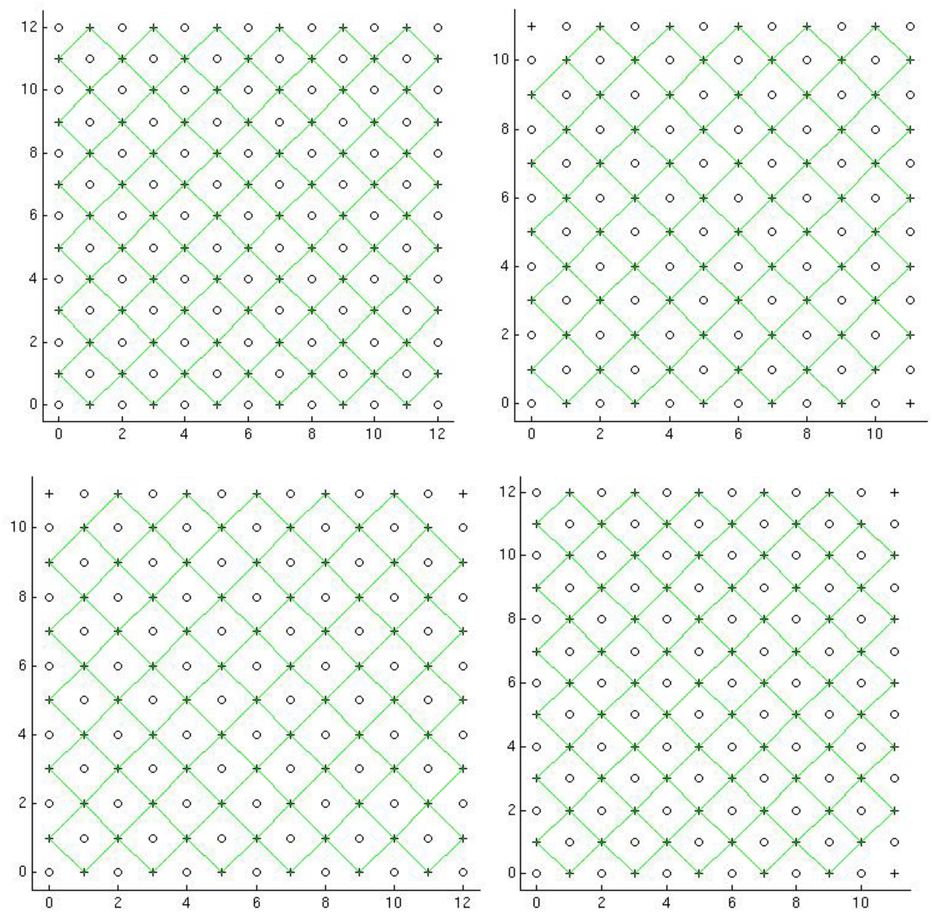
- Makes the E-Grid look like a B-grid whose “rows” and “columns” are along diagonal SW→NE and SE→NW lines
- Can use 1-D algorithm, e.g. PPM, along these lines
- CMAQ (and preprocessors) are familiar with turning B-grid data into C-grid flux point data

Disadvantages

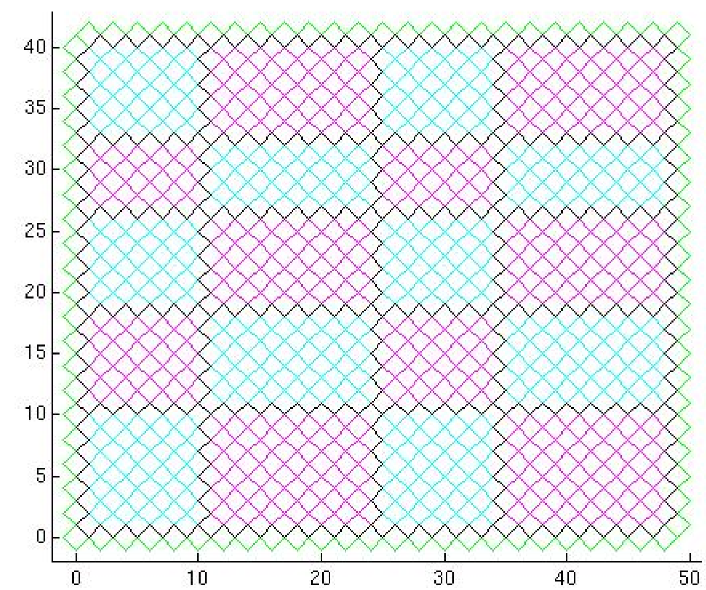
- Diagonal lines of cells have variable lengths, which requires non-trivial extra book-keeping (in EGRID_MODULE.F)
- Requires interpolation of wind velocities to get flux point values
- Jagged boundary effect
- Parallelization is more difficult

Bookkeeping issues

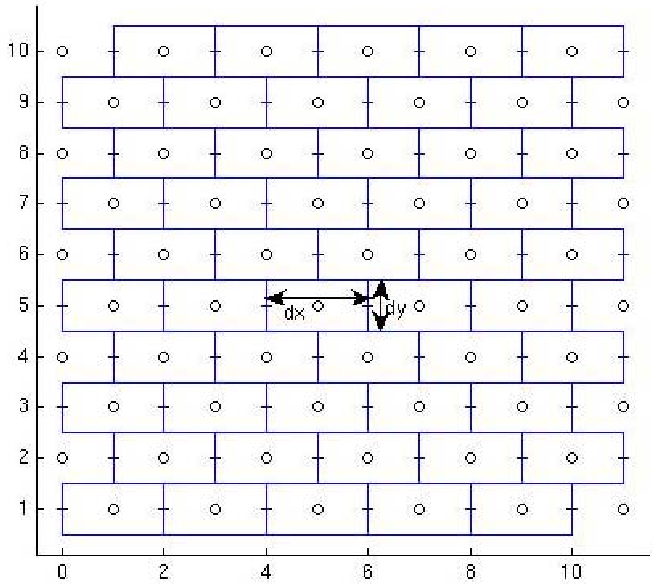
Grid geometry changes depending on whether the number of columns or rows is even or odd

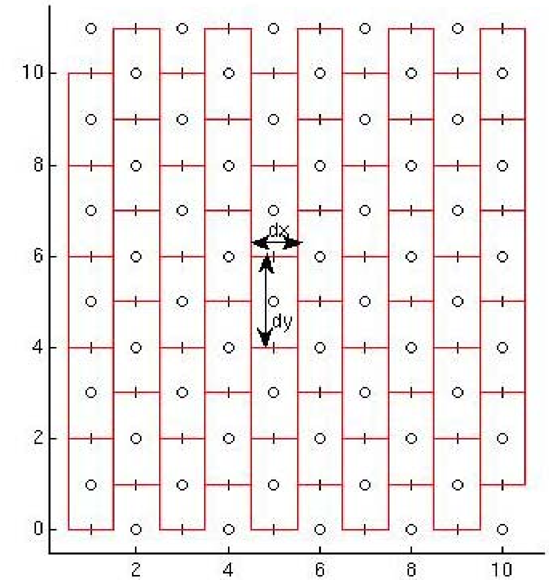


Partitioning for parallelization



Option 2: Rotated square cells (XY-Elongated cell)





Cells have the same area as the rotated cells

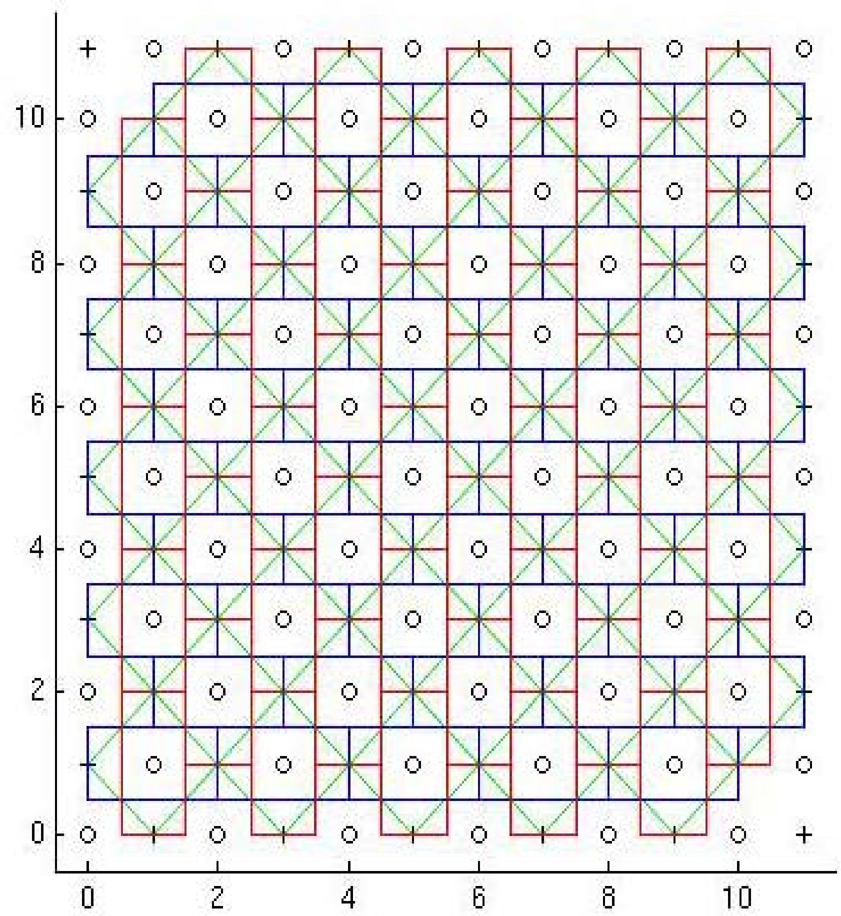
Advantages

- 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

Disadvantages

- Grid separation effect – **DEAL KILLER**
  (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

Option 3: mixed grid

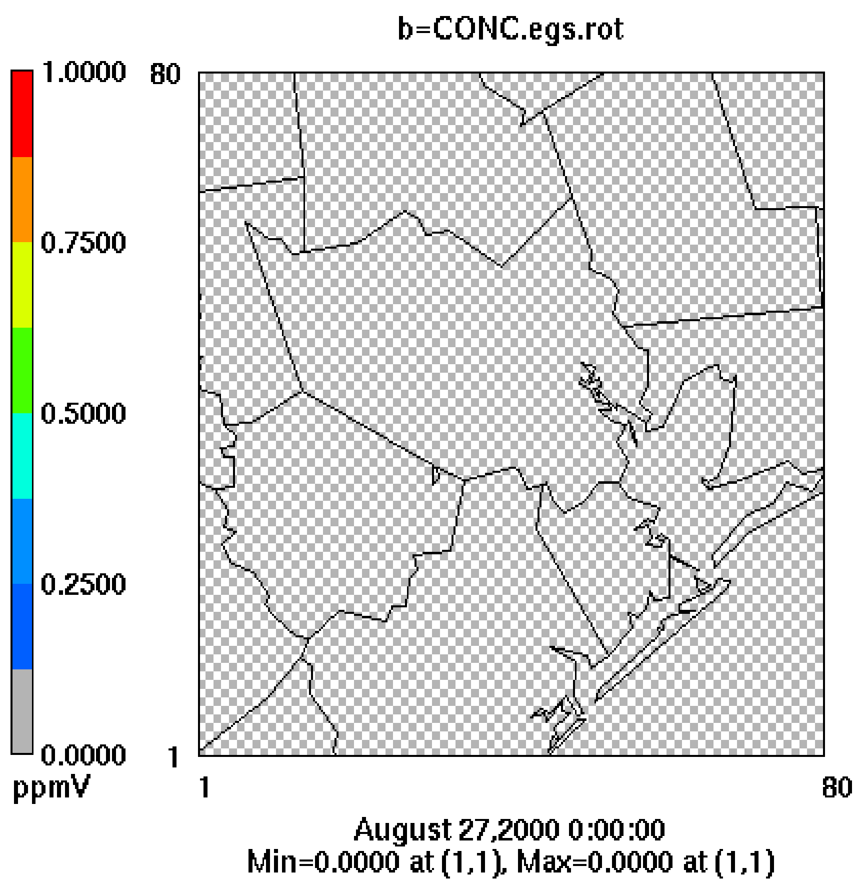


Alternate between rotated cell advection and XY cell advection – mitigates the drawbacks of each method alone

Jagged Boundary Effect

Option 1: rotated B-grid then on C-grid

Horizontal Wind; IC0_BC1; Rotated Cell E-grid

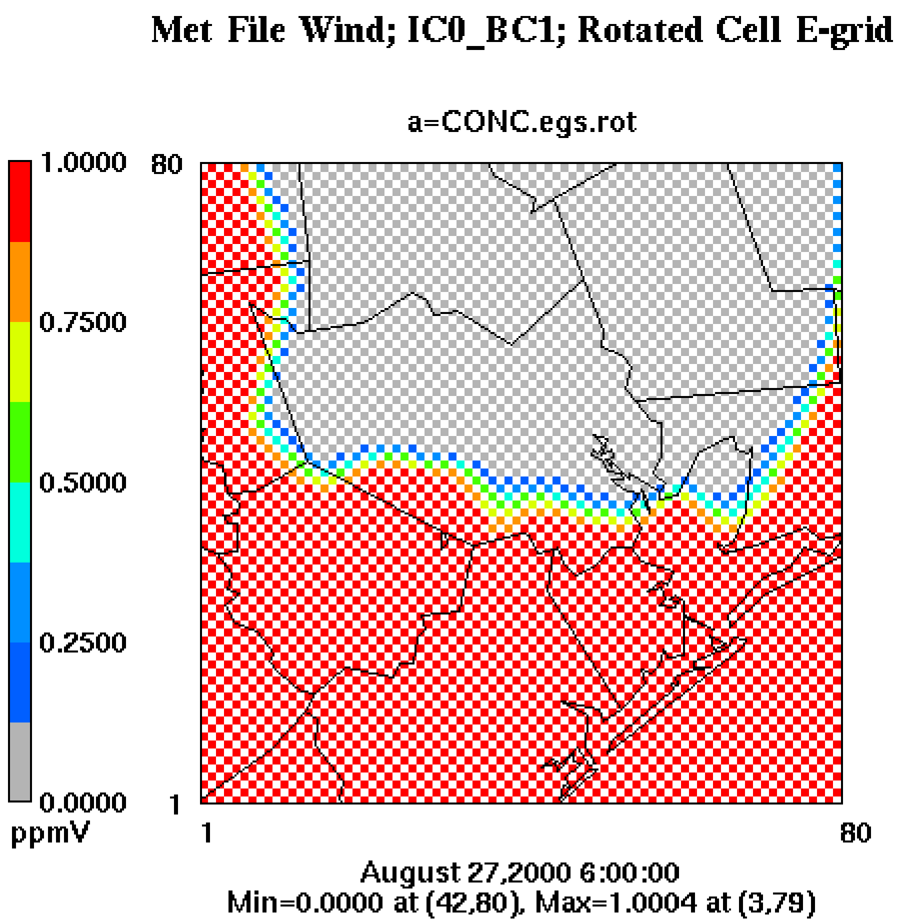


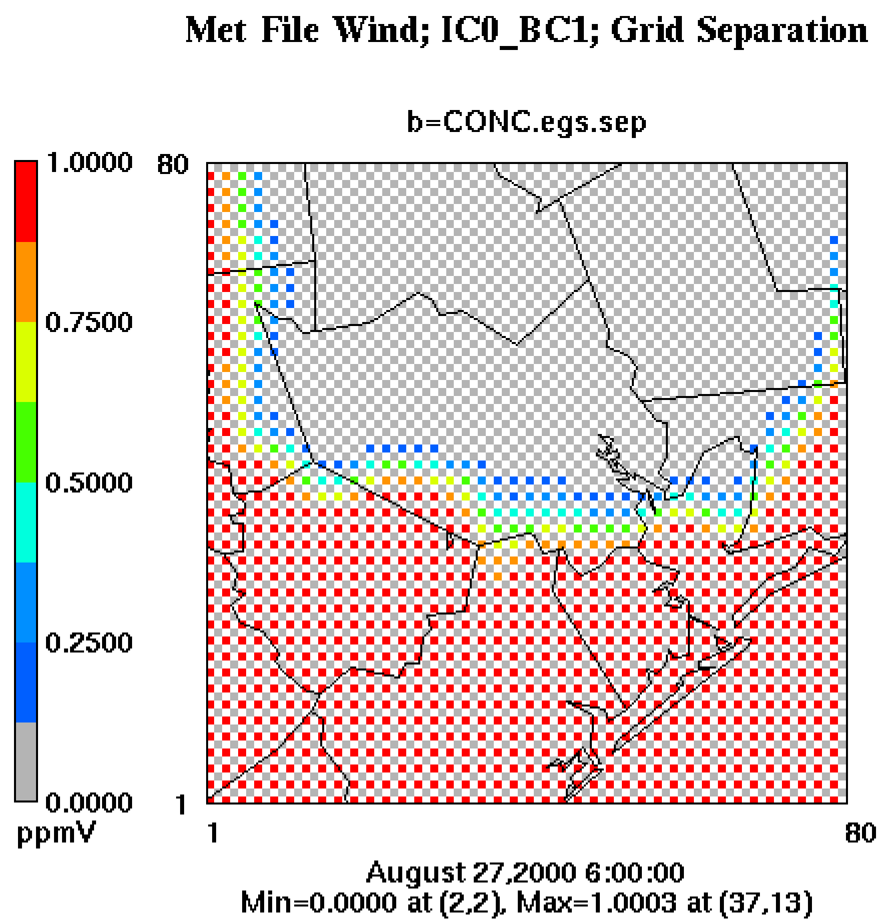
Boundary values propagate into the domain because boundaries are angled 45 degree

Grid Separation Effect: signals moving x- and y-direction each do not interact

Option 1: rotated B-grid then on C-grid

Option 2: XY-Elongated cell

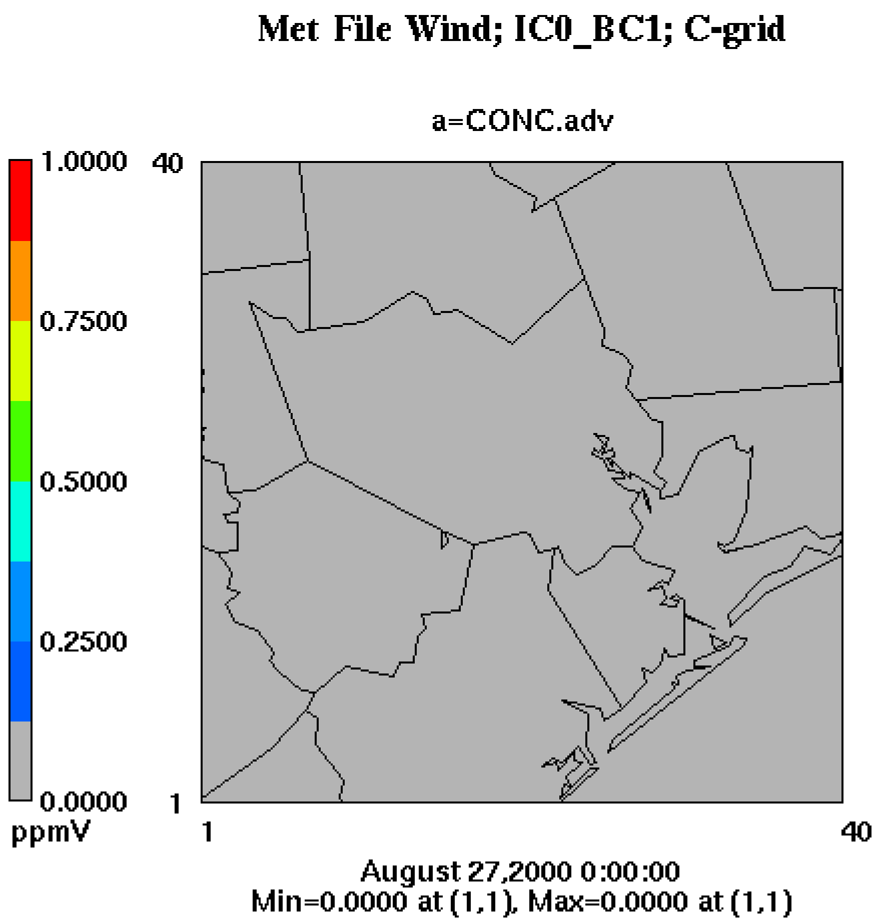


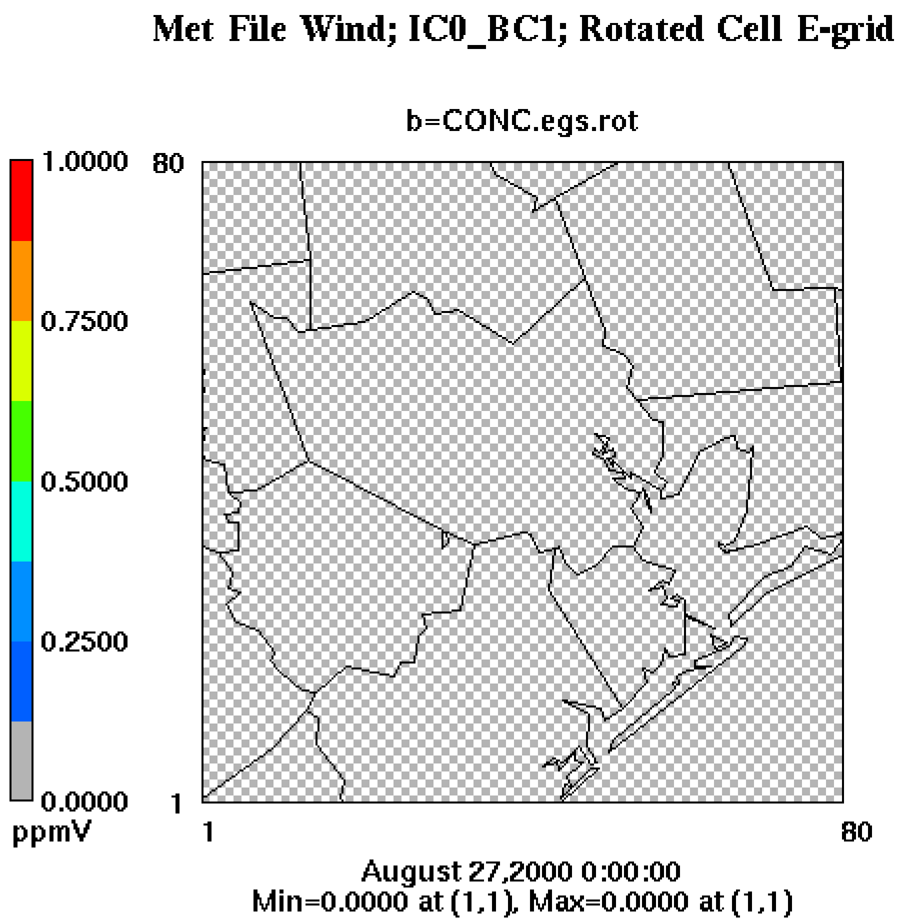


Comparison between regular CMAQ and Option 1

CMAQ C-grid

Option 1: rotated B-grid then on C-grid



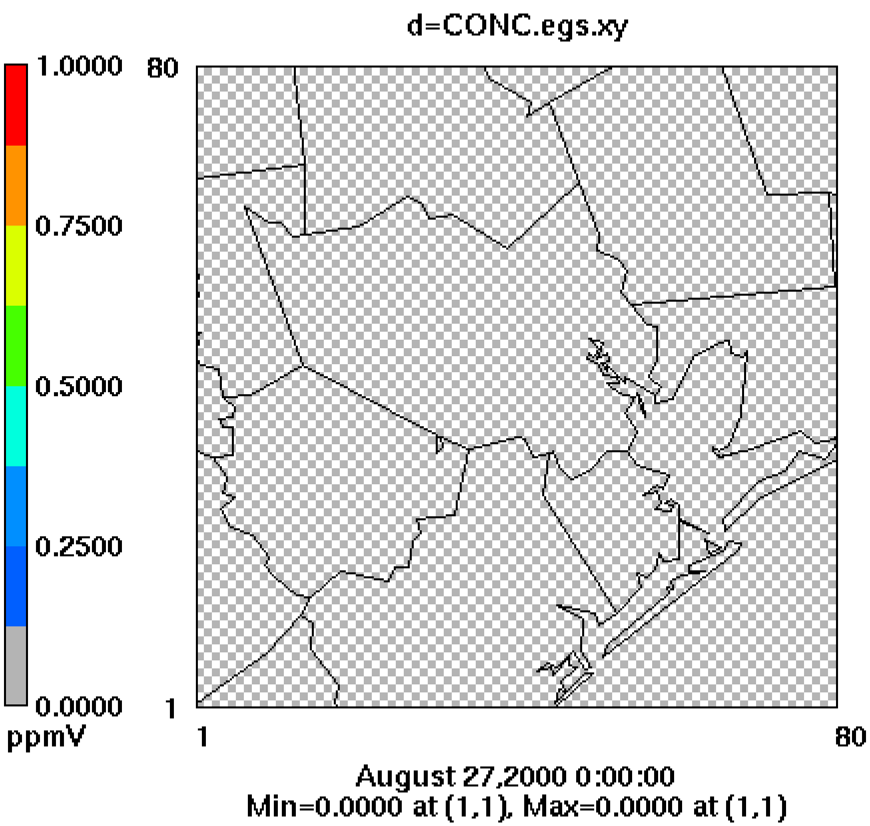


Comparison between Option 2 & 3

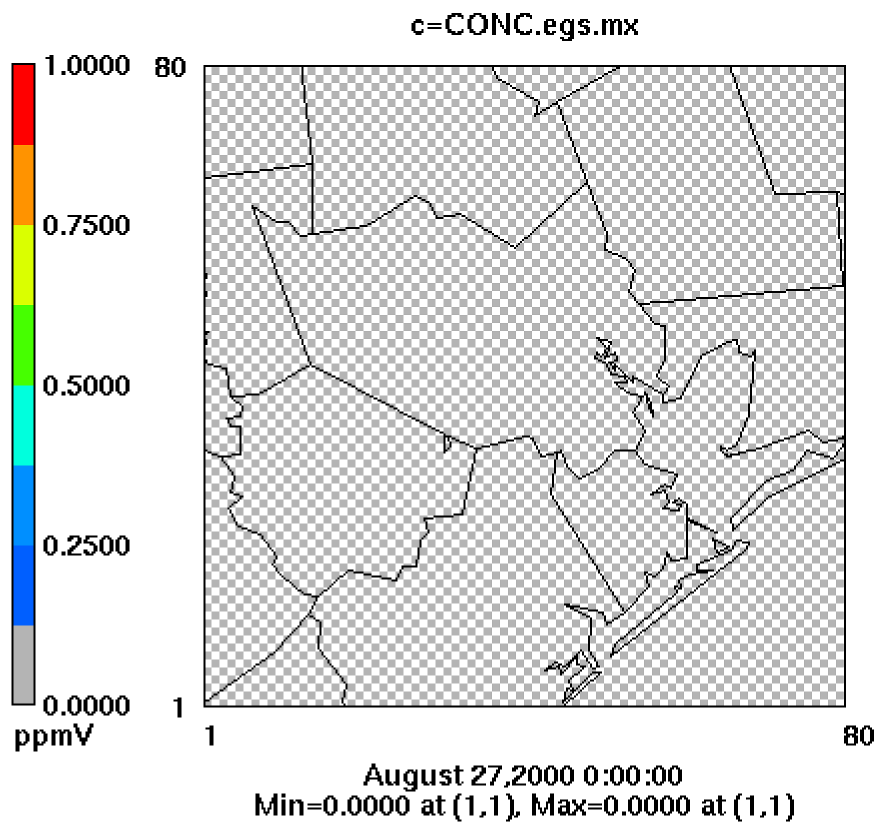
Option 2: XY-Elongated cell

Option 3: mixed grid

Met File Wind; IC0_BC1; XY Cell E-grid



Met File Wind; IC0_BC1; Mixed Cell E-grid



Development of the interface code for WRF/NMM and CMAQ

We will prototype the WCIP for WRF/NMM. A sample NMM data set will be used to test the code implementation. The following is current plan for the WCIP code development.

(1) We have to compare two choices to use the WRF/NMM coordinate itself for CMAQ modeling

(a) To use non-constant grid resolutions

(Δx = variant, Δy = constant, and map scale factor = 1 (constant))

A simplified CMAQ-SAFE code or a variant of it can be used.

(b) To use 'fake' grid resolutions

(Assume 'fake' $\Delta x = \Delta y$ = constant, and define 'fake' map scale factor for x-direction as $m_x = m_x(i, j)$)

(2) In order to utilize WCIP for WRF/NMM, we will generate Arakawa-C grid structure with the Lambert Conic Conformal projection and perform an interpolation from variables on E-grid with rotated Lat./Lon. Coordinate.

(3) We expect that some of physical/dynamical variables of WRF/NMM should be adjusted for such changes and recalculated into those of CMAQ by using the WRF/NMM registry information.

Variables required for linking WCIP and WRF-EM

! Dynamics
:: u_m(:,:,:) ! U wind (m/s)
:: v_m(:,:,:) ! V wind (m/s)
:: w_m(:,:,:) ! W wind (m/s)
:: ww_mm(:,:,:)! Eta-dot (Pa s-1)

! Geopotential
:: ph_m(:,:,:) ! perturbation geopotential
:: phb_m(:,:,:) ! base-state geopotential

! Temperature
:: t_m(:,:,:) ! Temperature - 300 (K)

! Pressure
:: p_m(:,:,:) ! perturbation pressure [Pa]
:: pb_m(:,:,:) ! base-state pressure [Pa]
:: psfc_m(:,:) ! surface pressure [Pa]

! TKE
:: tke_m(:,:,:) ! turbulent kinetic energy
:: tke_myj_m(:,:,:) ! TKE in the MYJ scheme

! Water mixing ratio
:: qvapor_m(:,:,:) ! water vapoar [kg/kg]
:: qcloud_m(:,:,:) ! cloud water [kg/kg]
:: qrain_m(:,:,:) ! rain water [kg/kg]
:: qice_m(:,:,:) ! ice [kg/kg]
:: qsnow_m(:,:,:) ! snow [kg/kg]

! Density
:: alt_m(:,:,:) ! inverse density [m3 kg-1]

! 2D (J,I,ITIME)

:: mu_m(:,:) ! perturbation dry air mass in column [Pa]
:: mub_m(:,:) ! base-state dry air mass in column [Pa]
:: q2_m(:,:) ! QV at 2m [kg/kg]
:: t2_m(:,:) ! Temp at 2m [K]
:: th2_m(:,:) ! Pot. Temp. at 2m [K]
:: u10_m(:,:) ! U at 10 m [m/s]
:: v10_m(:,:) ! V at 10 m [m/s]
:: mapfac_m_m(:,:) ! map scale factor at cross
:: mapfac_u_m(:,:) ! map scale factor at square
:: mapfac_v_m(:,:) ! map scale factor at Triangle
:: hgt_m(:,:) ! Terrain height [m]
:: tsk_m(:,:) ! surface skin temperature [K]
:: sst_m(:,:) ! sea surface temp [K]
:: rainc_m(:,:) ! accumulated total CU precipitation [mm]
:: rainnc_m(:,:)! accumulated total Grid scale precip. [mm]
:: swdown_m(:,:) !sfc downward shortwave flux [W m-2]
:: gsw_m(:,:) ! sfc downdward shortwave flux [W m-2]
:: glw_m(:,:) ! sfc downdward longwave flux [W m-2]
:: xlat_m(:,:) ! latitude at cross [deg]
:: xlong_m(:,:) ! longitude at cross [deg]
:: lu_index_m(:,:) ! land use
:: hfx_m(:,:) ! sfc upward heat flux [W m-2]
:: qfx_m(:,:) ! sfc upward moisture flux [kg m-2 s-1]
:: snowc_m(:,:) ! snow cover (1=snow)

! add
:: mavail_m(:,:) ! surface moisture availability
:: hol_m(:,:) ! PBL height over M-O length [m/m]
:: ust_m(:,:) ! u* [m s-1]
:: zpbl_m(:,:) ! PBL height [m]
:: ivgtyp_m(:,:) ! dominant vegetation category
:: isltyp_m(:,:) ! dominant soil category
:: vegfra_m(:,:) ! vegetation fraction
:: canwat_m(:,:) ! canopy water [kg m-2]
:: albedo_m(:,:) ! albedo
:: emiss_m(:,:) ! surface emissivity
:: znt_m(:,:) ! surface roughness length [m]

! 1D (K,ITIME)
:: znu_m(:)
:: znw_m(:)

! ...
! 1D (E,ITIME) ---> E: ext_scalar
:: p_top
:: itimestep
:: mp_physics

Variables saved in WRF-NMM output

**** Need to know the name and characteristics (i.e., unit) for the variables typed in bold and blue font**

int LMH(:,:) ;
int LMV(:,:) ;
float HBM2(:,:) ;
float HBM3(:,:) ;
float VBM2(:,:) ;
float VBM3(:,:) ;
float SM(:,:) ;
float SICE(:,:) ;
float HTM(:,:,:) ;
float VTM(:,:,:) ;
float PD(:,:) ;
float FIS(:,:) ;
float RES(:,:) ;
float T(:,:,:) ;
float Q(:,:,:) ;
float U(:,:,:) ;
float V(:,:,:) ;
float DX_NMM(:,:) ;
float WPDAR(:,:) ;
float CPGFU(:,:) ;
float CURV(:,:) ;
float FCP(:,:) ;
float FDIV(:,:) ;
float F(:,:) ;
float FAD(:,:) ;
float DDMPU(:,:) ;
float DDMPV(:,:) ;

float PDTOP(:) ;
float PT(:) ;
float PSDT(:,:) ;
float THS(:,:) ;
float APREC(:,:) ;
float ACPREC(:,:) ;
float CUPREC(:,:) ;
float PSHLTR(:,:) ;
float TSHLTR(:,:) ;
float QSHLTR(:,:) ;
float ALBASE(:,:) ;
float CZEN(:,:) ;
float EPSR(:,:) ;
float GFFC(:,:) ;
float GLAT(:,:) ;
float GLON(:,:) ;
float HDAC(:,:) ;
float HDACV(:,:) ;
float MXSNAL(:,:) ;
float SOILTB(:,:) ;
float CWM(:,:,:) ;
float ISLOPE(:,:) ;
float VEGFRC(:,:) ;
float SH2O(:,:,:) ;
float SMC(:,:,:) ;
float STC(:,:,:) ;
float PINT(:,:,:) ;

float W(:,:,:) ;
float QVAPOR(:,:,:) ;
float QCLOUD(:,:,:) ;
float SMOIS(:,:,:) ;
float TH2(:,:) ;
float U10(:,:) ;
float V10(:,:) ;
float SMSTAV(:,:) ;
float SFROFF(:,:) ;
float UDROFF(:,:) ;
int IVGTYP(:,:) ;
int ISLTYP(:,:) ;
float ACSNOW(:,:) ;
float ACSNOM(:,:) ;
float SNOW(:,:) ;
float CANWAT(:,:) ;
float SST(:,:) ;
float WEASD(:,:) ;
float TKE_MYJ(:,:,:) ;
float THZ0(:,:) ;
float QZ0(:,:) ;
float UZ0(:,:) ;
float VZ0(:,:) ;
float QSFC(:,:) ;
float AKHS(:,:) ;
float AKMS(:,:) ;
int ITIMESTEP(:) ;

Summary

Issues related with linking WRF models with CMAQ discussed

- Studied differences in the governing equations and coordinates, their interactions with transport algorithms in WRF and the CMAQ chemistry-transport model

- Presented several methods to cast the WRF meteorological data on CMAQ grid and coordinate structures to represent transportation of pollutants.

- Contrasted the differences in dynamics descriptions between the WRF/NMM and WRF/EM and their implication on the development of the linking strategy.