Design and Configuration of MPAS for Deep-Atmosphere NWP and Geospace Applications

Joe Klemp and Bill Skamarock

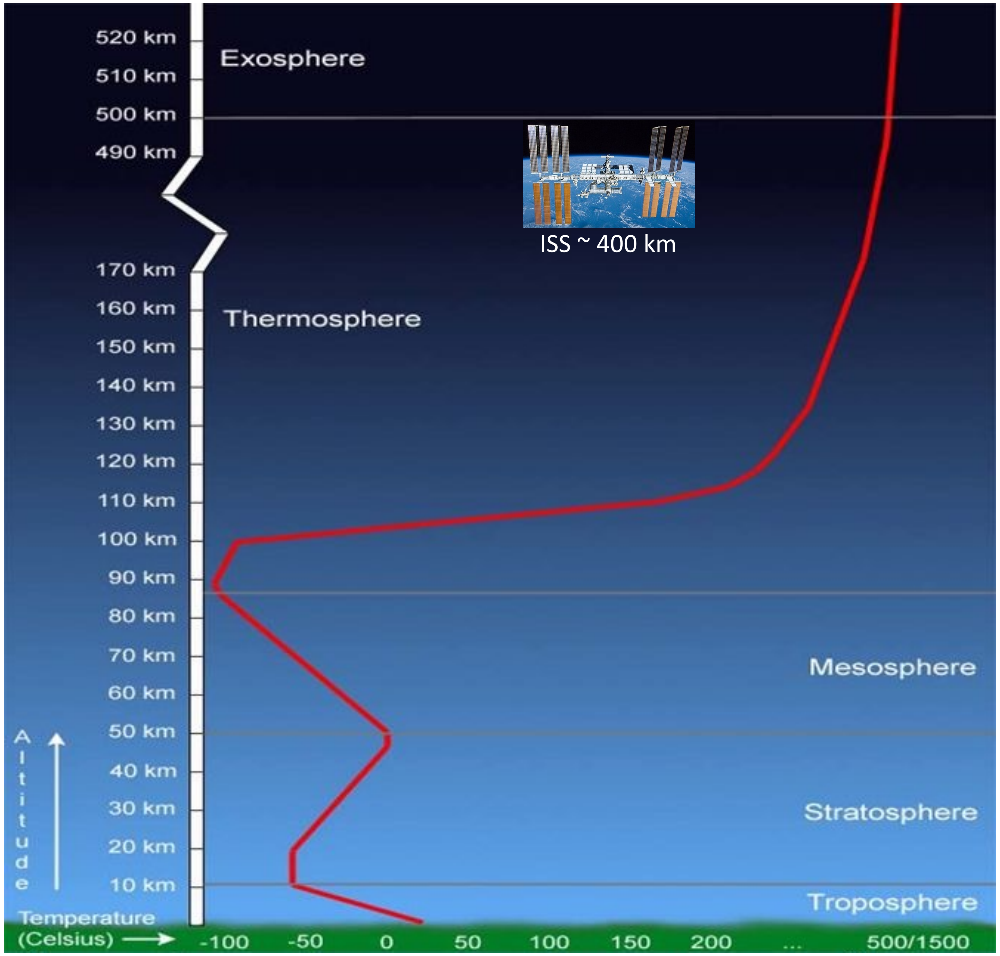
NCAR Mesoscale and Microscale Meteorology Laboratory

Boulder, Colorado, USA

Geospace Extensions for MPAS

Average Temperature Profile in the Earth's Atmosphere

p (hPa)	ρ (kg/m³)	θ (K)	ν (m²/s)
10^{-8}	10^{-12}		10^{7}
10^{-6}	10^{-9}	10^{7}	10^{4}
10^{-4}	10^{-6}	10^{5}	10^{2}
		10^{4}	10^{-1}
10^{0}	10^{-3}	10^{3}	
10^{3}	10^{0}	300	10^{-5}



MPAS Extensions Deep Atmosphere and Geospace Applications

Deep Atmosphere (Full 3-D MPAS model):

- Use actual geocentric distance r instead of the Earth radius r_e in the governing equations and the grid mesh configuration
- Allow gravity to vary with height, $g(z) = g_0 \frac{r_e^2}{(r_e+z)^2}$
- Include Coriolis force terms involving vertical velocity components

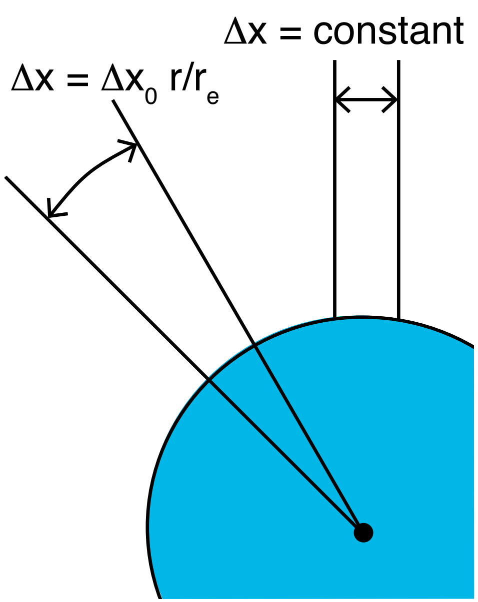
Geospace, above ~ 150 km (2-D MPAS slab model):

- Include variable atmospheric composition and its coupling to the dynamics
- Modify the thermodynamic equation to account for variable composition
- Include (large) kinematic viscosity and thermal diffusivity terms
- Add appropriate physics and chemistry for the upper atmosphere (solar and Joule heating, ion drag, oxygen disassociation, etc.)

MPAS

Model for Prediction Across Scales

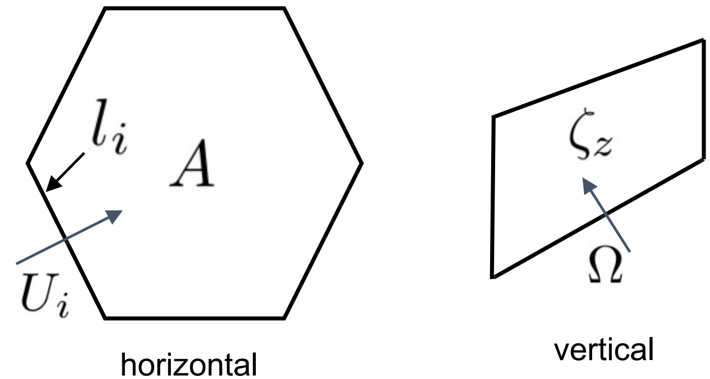
Deep Atmosphere Extensions for MPAS: Geometry



$$\frac{\partial \tilde{\rho}}{\partial t} = \nabla_\zeta \cdot \mathbf{V_H} + \frac{\partial \Omega}{\partial \zeta}$$

$$\tilde{\rho} = \frac{\rho}{\zeta_z}, \quad \mathbf{V_H} = (U, V) = (\tilde{\rho} u, \tilde{\rho} v), \quad \Omega = \tilde{\rho}\dot{\eta}$$ (shallow atmosphere)

Hexagonal grid cell:



$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{A_0} \sum_{i=1}^{n} U_i l_{0_i} + \frac{\Delta \Omega}{\Delta \zeta}$$

$A_0, l_{0_i} =$ Cell area and edge lengths at surface

Deep Atmosphere: $\tilde{\rho} = \frac{A}{A_0}\frac{\rho}{\zeta_z}, \quad U_i = \frac{A_0}{A}\frac{l_i}{l_{0_i}}\tilde{\rho} u_i, \quad \Omega = \tilde{\rho}\dot{\eta}$

Shallow Atmosphere: $\tilde{\rho} = \frac{\rho}{\zeta_z}, \quad U_i = \tilde{\rho} u_i, \quad \Omega = \tilde{\rho}\dot{\eta} \quad (A = A_0, \quad l_i = l_{0_i})$

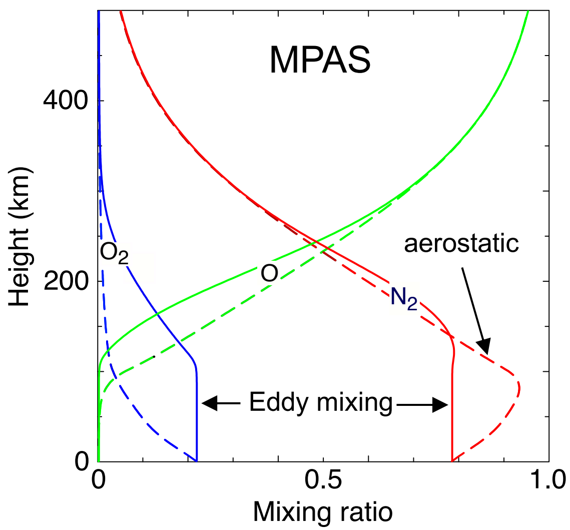
Geospace Extensions for MPAS: Composition

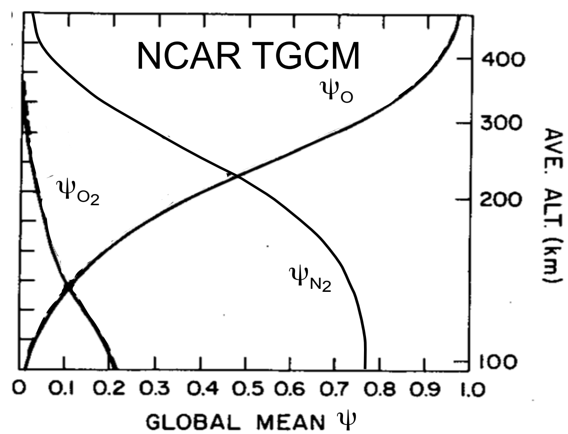
Model for Prediction Across Scales

Primary atmospheric constituents: $n = 3$ (N_2, O_2, O)

Aerostatic balance: constituents distributed according to their molecular weights:

$$\frac{\partial \ln p_i}{\partial z} = -\frac{g M_i}{k_b T}$$



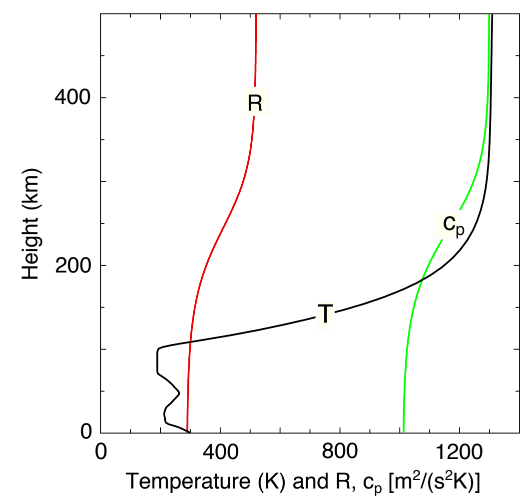


Dickinson et al. JAS, 1984

Thermodynamic Coefficients

$$\bar{R} = \frac{k_b}{\bar{M}} = k_b \sum_{i=1}^{n} \frac{\psi_i}{M_i}$$

$$\bar{c}_p = \sum_{i=1}^{n} c_{p_i} \psi_i$$



Composite thermodynamic properties vary only with the mixing ratios of the atmospheric constituents:

Geospace Extensions for MPAS: Thermodynamic Equation

Internal energy equation: $$c_p \frac{dT}{dt} - RT\frac{d\ln p}{dt} = Q$$

From definition of potential temperature, $\theta = Tp^{-\kappa}$ $\qquad \kappa = \frac{R}{c_p}$

$$\frac{d\ln\theta}{dt} = \frac{d\ln T}{dt} - \kappa\frac{d\ln p}{dt} - \ln p\frac{d\kappa}{dt}$$

$$\frac{d\ln\theta}{dt} = \frac{Q}{c_p T} - \ln p\frac{d\kappa}{dt} \qquad (\neq 0 \text{ for } Q = 0)$$

Flux form thermodynamic equation:

$$\frac{\partial\Theta}{\partial t} + \nabla\cdot\mathbf{V}\theta = \frac{\rho Q}{c_p\pi} - \Theta\ln p\frac{d\kappa}{dt} \qquad \Theta = \rho\theta, \quad \mathbf{V} = \rho\mathbf{v}$$

Small but potentially significant correction !

MPAS
Model for Prediction Across Scales

Geospace Extensions for MPAS: Equations and Constituents

$$\partial_t \mathbf{V}_H = -\mathbf{v}_H \nabla_\zeta \cdot \mathbf{V}_H - \partial_\zeta(\Omega \mathbf{v}_H) - \tilde{\rho}_d \nabla_\zeta K - p\left[\frac{\rho_d}{\rho_m} z_\zeta \nabla_\zeta \phi + z_H \frac{g z_\zeta}{R_d T_m}\right]$$

$$- \eta \mathbf{k} \times \mathbf{V}_H - \frac{\mathbf{v}_H W}{r} - eW\cos\alpha_r + (\nabla \tilde{\rho}_d \nu \cdot \nabla)\mathbf{v}_H + F_{\mathbf{V}_H}$$

$$\partial_t W = -(\nabla \cdot \mathbf{v} W)_\zeta - p\left[\frac{\rho_d}{\rho_m}\partial_\zeta \phi + \frac{g z_\zeta}{R_d T_m}\right]$$

$$+ \frac{uU + vV}{r} + e(U\cos\alpha_r - V\sin\alpha_r) + \nabla \tilde{\rho}_d \nu \cdot \nabla w + F_W$$

$$\partial_t \Theta_m = -(\nabla \cdot \mathbf{V}\theta_m)_\zeta - \theta_m \phi\left[\frac{\partial \tilde{\rho}_d \kappa}{\partial t} + (\nabla \cdot \tilde{\rho}_d \kappa \mathbf{v})_\zeta\right] + \frac{1}{c_p \pi}\nabla \cdot (k_c \nabla T) + F_{\Theta_m}$$

$$\partial_t \tilde{\rho}_d = -(\nabla \cdot \mathbf{V})_\zeta$$

$$\partial_t Q_j = -(\nabla \cdot \mathbf{V} q_j)_\zeta + F_{Q_j},$$

$$\frac{\partial \Psi_i}{\partial t} = -\nabla \cdot \mathbf{V}\psi_i - \frac{\partial}{\partial \zeta}\left[\alpha^{-1}\mathbf{L}\psi\right] + \frac{\partial}{\partial \zeta}\left[\tilde{\rho}_d K_e(\zeta)\frac{\partial \psi_i}{\partial \zeta}\right] + \mathbf{S} - \mathbf{R}$$

$$\Theta_m = \tilde{\rho}_d \theta\left[1 + \frac{M_d}{M_v} q_v\right]$$

$$\kappa = \frac{R_d}{c_p}$$

$$p = p_0\left(\frac{R_d \Theta_m}{p_0 z_\zeta}\right)^{\frac{1}{1-\kappa}}$$

$$\phi = \ln\frac{p}{p_o}$$

$$\eta = \mathbf{k} \cdot \nabla \times \mathbf{v}_H + f$$

$$e = 2\Omega_e \cos\psi$$

$$f = 2\Omega_e \sin\psi$$

Geospace Extensions for MPAS: Equations and Constituents

MPAS
Model for Prediction Across Scales

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$$+ \frac{uU + vV}{r} + e(U \cos\alpha_r - V \sin\alpha_r) + \nabla \tilde{\rho}_d \nu \cdot \nabla w + F_W$$

Coriolis terms involving *w*

$$\partial_t \Theta_m = -(\nabla \cdot \mathbf{V} \theta_m)_\zeta - \theta_m \phi \left[\frac{\partial \tilde{\rho}_d \kappa}{\partial t} + (\nabla \cdot \tilde{\rho}_d \kappa \mathbf{v})_\zeta\right] + \frac{1}{c_p \pi} \nabla \cdot (k_c \nabla T) + F_{\Theta_m}$$

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$$\partial_t Q_j = -(\nabla \cdot \mathbf{V} q_j)_\zeta + F_{Q_j},$$

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$$\Theta_m = \tilde{\rho}_d \theta\left[1 + \frac{M_d}{M_v} q_v\right]$$

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Pressure gradients are calculated using ln *p* instead of *p*

MPAS
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Geospace Extensions for MPAS: Equations and Constituents

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Molecular diffusivity terms

Thermal Conductivity term

$$\partial_t \tilde{\rho}_d = -(\nabla \cdot \mathbf{V})_\zeta$$

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Multiple equations are integrated for the atmospheric constituents, which determine R and c_p

Geospace Extensions for MPAS: Equations and Constituents

MPAS
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$$p = p_0 \left(\frac{R_d \Theta_m}{p_0 z_\zeta}\right)^{\frac{1}{1-\kappa}}$$

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$$\eta = \mathbf{k} \cdot \nabla \times \mathbf{v}_H + f$$
$$e = 2\Omega_e \cos\psi$$
$$f = 2\Omega_e \sin\psi$$

Only equations where variations in atmospheric composition feed back into the dynamics

Dynamical equations are solved using the same split-explicit time integration as in MPAS for the shallow atmosphere

Geospace Extensions for MPAS: Mountain-wave test cases

MPAS Model for Prediction Across Scales

2-D slab model

z_t = 500 km Δz = 2 km $\bar{U}$ = 50 m/s

$$h(x) = \frac{a^2 h_m}{(x - x_c)^2 + a^2}$$

$a = 5\Delta x$

Δx = 5, 20, 100 km h_m = 100 m

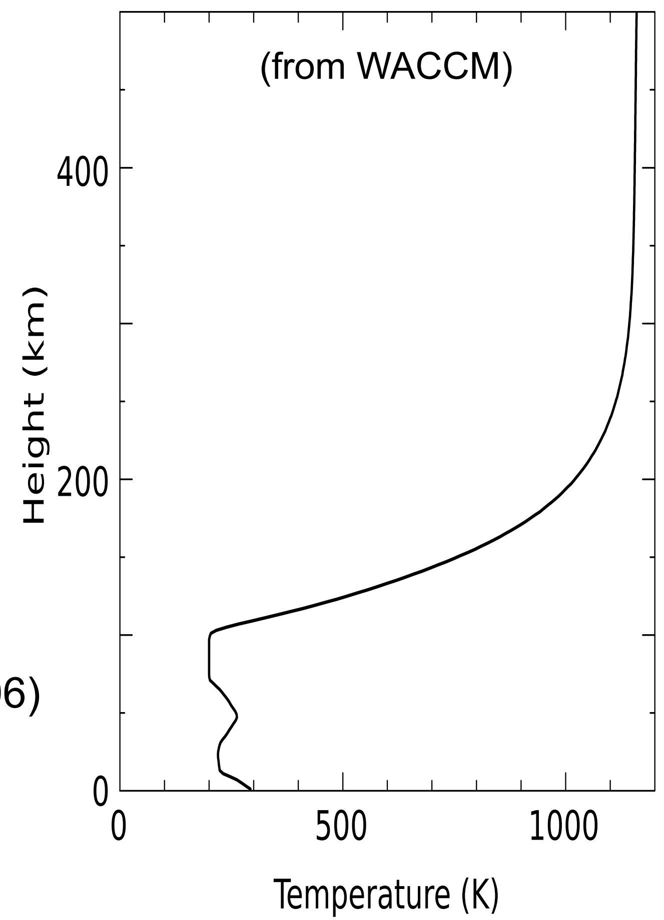
$\Delta t = 4\,\Delta x$ $\Delta\tau = \Delta t/6$

$$K_m = K_b + \ell^2 f(Ri)\frac{\partial u}{\partial z}$$

(Hong et al. *MWR* 2006)

$$Ri = \frac{g}{\theta}\left[\frac{\partial\theta/\partial z}{(\partial u/\partial z)^2}\right]$$

Temperature Sounding



Impulsive startup produces large amplitude acoustic modes in the upper domain. This startup noise is controlled by imposing Rayleigh damping on deviations from the initial state at early times.

MPAS
Model for Prediction Across Scales

Mountain-wave test case
hydrostatic scales

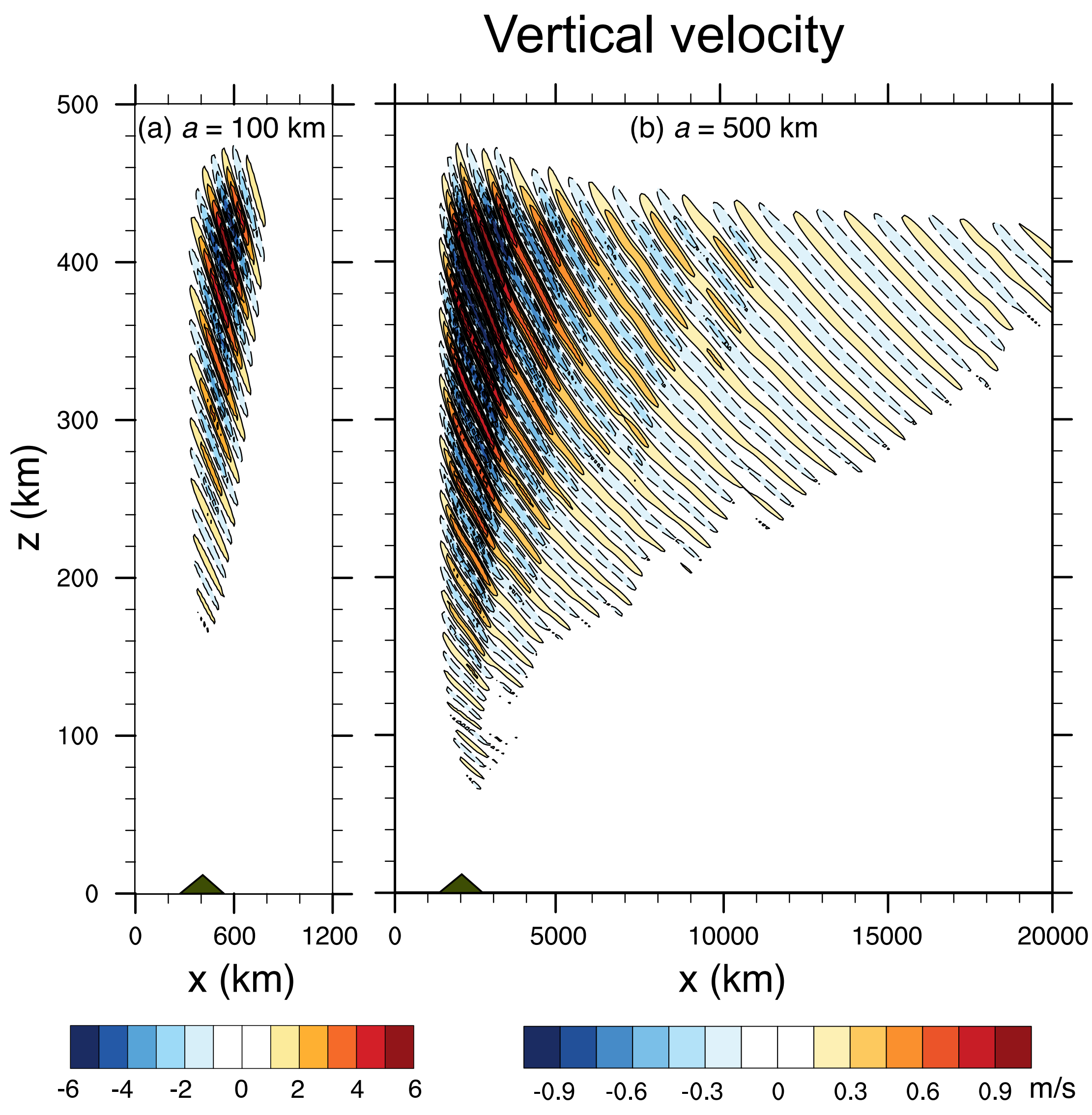
$h_m = 100$ m

$\Delta x =$ (a) 20 km,
(b) 100 km

$K_b \Delta t / \Delta z^2 =$ (a) .03,
(b) .005

No molecular viscosity
or thermal conductivity

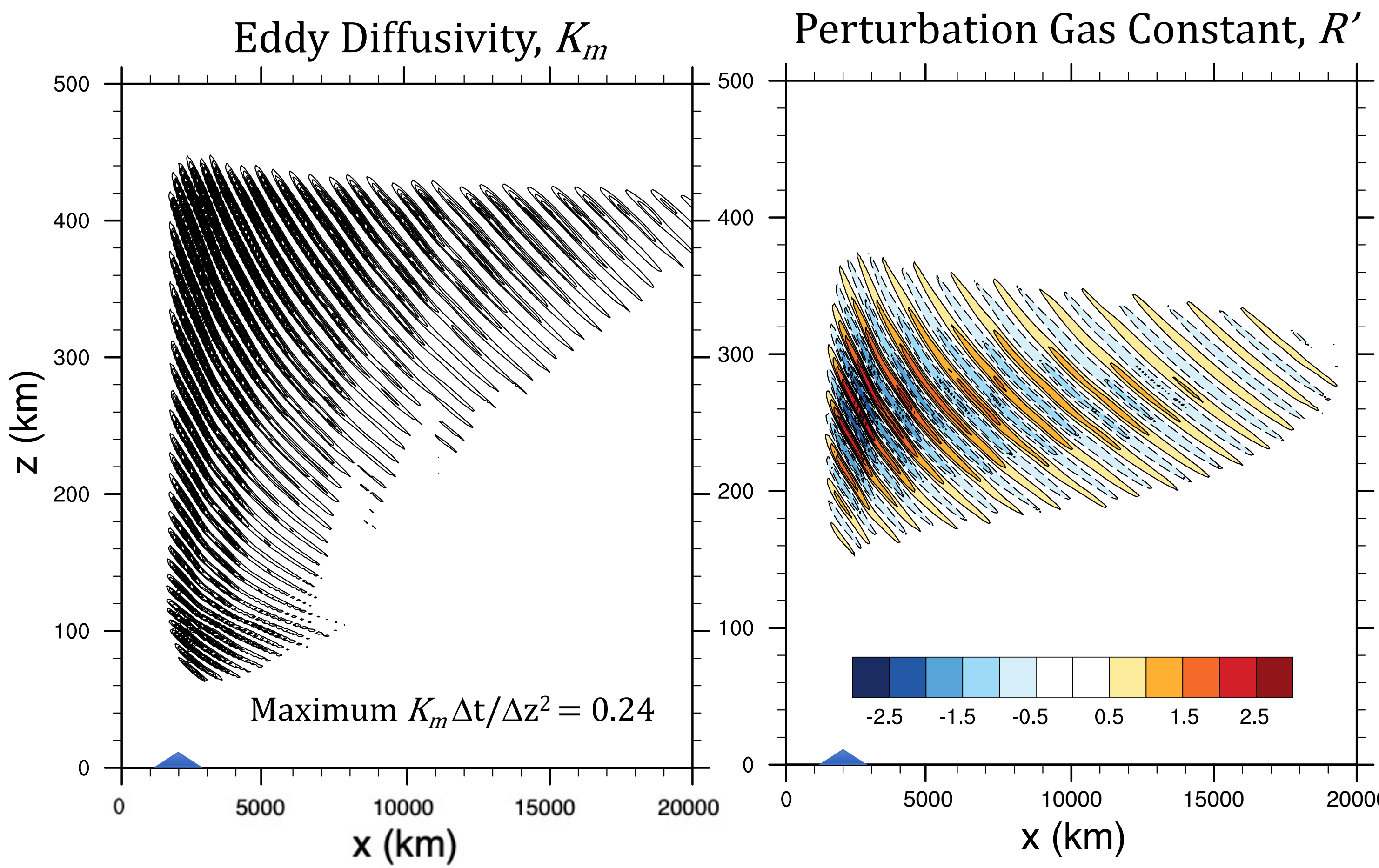
$$\ell^2 = k^2 \frac{N^2 - k^2 U^2}{k^2 U^2 - f^2}$$



MPAS
Model for Prediction Across Scales

Mountain-wave test case
hydrostatic scales

$h_m = 100$ m $\quad a = 500$ km $\quad K_b \Delta t / \Delta z^2 = 0.005$



No molecular viscosity or thermal conductivity

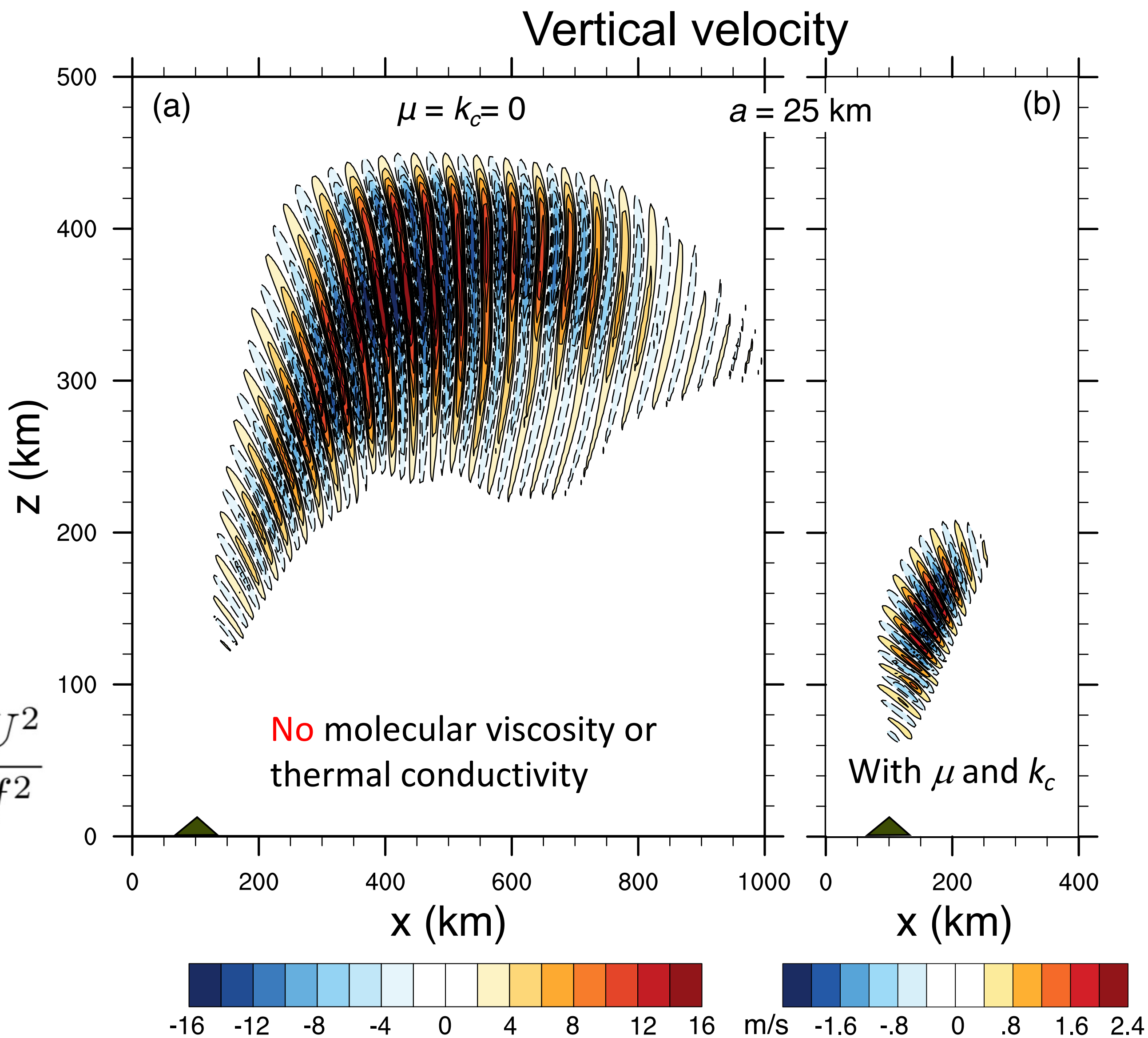
Mountain-wave test case
nonhydrostatic scales

$h_m = 100$ m

$\Delta x = 5$ km

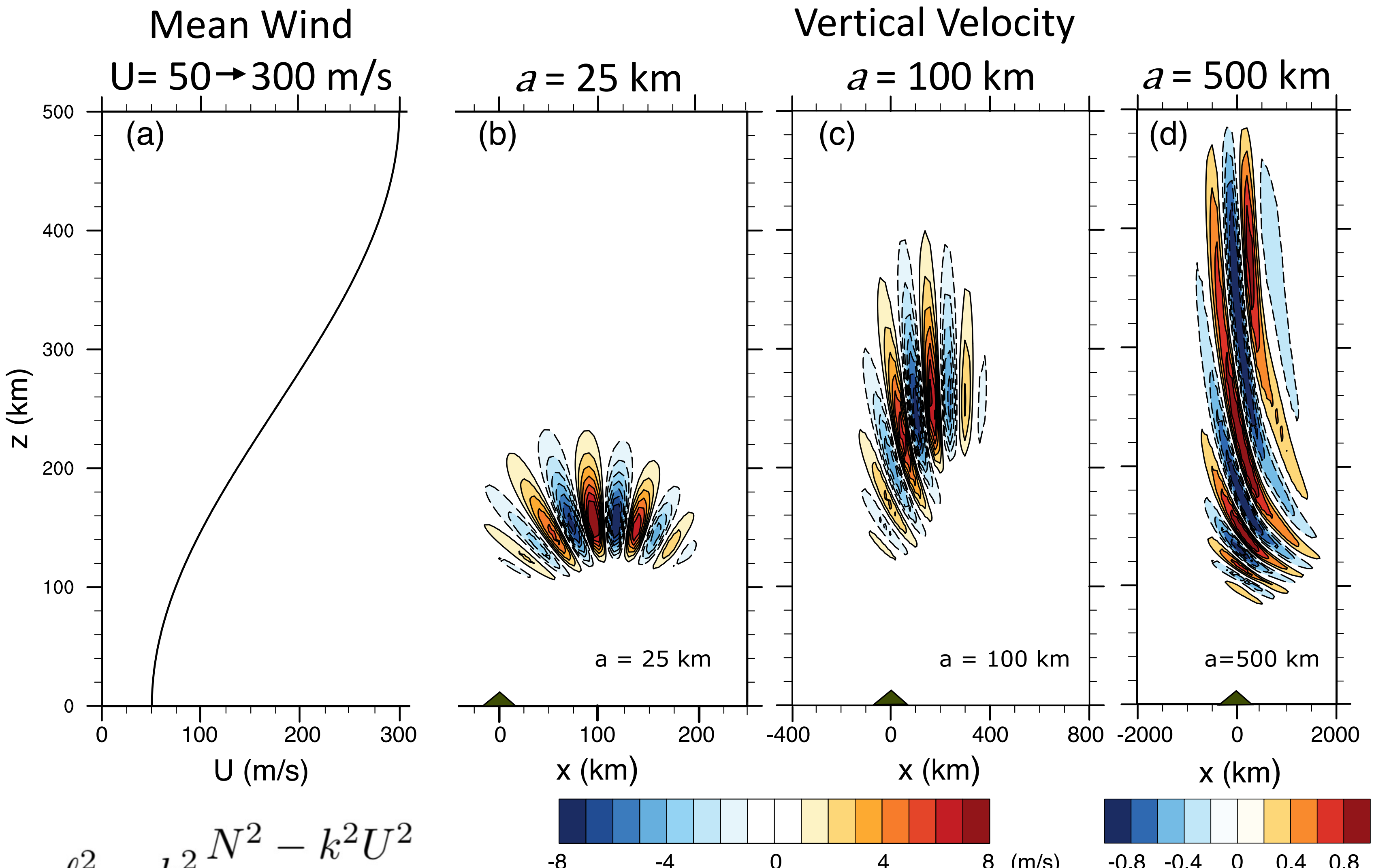
$K_b = .027 \Delta z^2 / \Delta t$

$$\ell^2 = k^2 \frac{N^2 - k^2U^2}{k^2U^2 - f^2}$$



Mountain-wave test case

Stronger mean wind



$$\ell^2 = k^2 \frac{N^2 - k^2 U^2}{k^2 U^2 - f^2}$$

With molecular viscosity and thermal conductivity

MPAS
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Geospace extensions for MPAS: Summary

- Height-based hybrid terrain-following coordinate seems well suited for deep atmosphere domains.
- Split-explicit finite-volume numerics for solving the nonhydrostatic dynamical equations appear to remain viable for the deep atmosphere.
- Equations are solved in double precision using full thermodynamic variables (not as perturbations from a reference state).
- Large molecular diffusivity and conductivity terms require special implicit treatment (currently using ADI).
- Large acoustic noise due to impulsive startup may require special filtering.
- Next steps: Implement in 3-D MPAS code, evaluate more realistic test cases, begin adding thermospheric physics.