# A Scale-Aware Treatment of Subgrid Mixing in the WRF Model

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Reference:

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# What is Subgrid Mixing?

Transport equation for the grid resolved part of a generic physical property $\psi$

$$d\overline{\psi} / dt = -\partial \overline{u_i' \psi'} / \partial x_i + \ldots$$

Split the subgrid scale (SGS) flux divergence

$$\partial \overline{u_i' \psi'} / \partial x_i = (\partial \overline{u_i' \psi'} / \partial x_i)_{convection} + (\partial \overline{u_i' \psi'} / \partial x_i)_{turbulence}$$

Convection (quasi-organized)

mass-flux closure

Turbulence (quasi-random)

ensemble-mean closure

# What does "scale-aware" mean in subgrid mixing parameterization?

The total flux of $\psi$ is approximately unchanged regardless of resolution, but the contributions from the resolved and parameterized components may vary greatly (with the latter decreasing with an increase in resolution).

# Outline

1. Review of theoretical foundation
2. Development in WRF-ARW: Minimal complexity for CBL simulations
3. Examples of numerical results
4. Summary and future work

# Toward Numerical Modeling in the "Terra Incognita"

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ABSTRACT

In mesoscale modeling the scale $l$ of the energy- and flux-containing turbulence is much smaller than the scale $\Delta$ of the spatial filter used on the equations of motion, and in large-eddy simulation (LES) it is much larger. Since their models of the subfilter-scale (SFS) turbulence were not designed to be used when $l$ and $\Delta$ are of the same order, this numerical region can be called the "terra incognita."

The most common SFS model, a scalar eddy diffusivity acting on the filtered fields, emerges from the conservation equations for SFS fluxes when several terms, including all but one of the production terms, are neglected. Analysis of data from the recent Horizontal Array Turbulence Study (HATS) shows that the neglected production terms can be significant. Including them in the modeled SFS flux equations yields a more general SFS model, one with a tensor rather than a scalar eddy diffusivity. This more general SFS model is probably not necessary in fine-resolution LES or in coarse-resolution mesoscale modeling, but it could improve model performance in the terra incognita.

- **The exact but unclosed governing equations for subgrid turbulent mixing are mathematically identical for any grid scale.**
- **There exists a general mathematical framework for properly parameterizing subgrid turbulent mixing of any grid scale from mesoscale to LES.**

# Governing Equations of Subgrid Turbulent Mixing (Mellor-Yamada Level 3 Model)

Reynolds stress equation

$$\overline{u_i'u_j'} = -\frac{3l_1}{\sqrt{e}}\left[(\overline{u_i'u_k'} - C_1 e\delta_{ki})\frac{\partial \bar{u}_j}{\partial x_k} + (\overline{u_k'u_j'} - C_1 e\delta_{kj})\frac{\partial \bar{u}_i}{\partial x_k} - \frac{g}{\overline{\theta_v}}\left(\delta_{j3}\overline{u_i'\theta'} + \delta_{i3}\overline{u_j'\theta'}\right)\right]$$

(where $i \neq j$)

Thermal flux equation

$$\overline{u_i'\theta'} = -\frac{3l_2}{\sqrt{e}}\left[(\overline{u_i'u_j'})\frac{\partial \bar{\theta}}{\partial x_j} + (\overline{\theta'u_j'})\frac{\partial \bar{u}_i}{\partial x_j} - \delta_{i3}\left(\frac{\overline{\theta'^2}}{\overline{\theta}}\right)g\right]$$

TKE equation

$$\frac{\partial e}{\partial t} + \bar{u}_j\frac{\partial e}{\partial x_j} - \frac{\partial}{\partial x_j}\left[l\sqrt{e}S_q\frac{\partial e}{\partial x_j}\right] = -\overline{u_i'u_j'}\frac{\partial \bar{u}_i}{\partial x_j} + \delta_{i3}\frac{g}{\overline{\theta}}\overline{u_i'\theta'} - \frac{C_e e^{3/2}}{l}$$

Thermal variance equation

$$\frac{\partial \overline{\theta'^2}}{\partial t} + \bar{u}_j\frac{\partial \overline{\theta'^2}}{\partial x_j} - \frac{\partial}{\partial x_j}\left[l\sqrt{e}S_\theta\frac{\partial \overline{\theta'^2}}{\partial x_j}\right] = -2\overline{\theta'u_j'}\frac{\partial \bar{\theta}}{\partial x_j} - C_\theta\frac{\sqrt{e}}{l}\overline{\theta'^2}$$

# LES Limit: 3-D TKE Closure

Deardorff's three-dimensional TKE-based closure scheme (Deardorff 1980) is the most widely used subgrid-scale model in LES.

$$\frac{\partial e}{\partial t}+\bar{u}_j\frac{\partial e}{\partial x_j}+\frac{\partial}{\partial x_j}\left[\frac{\partial \overline{u_i'(e+p'/\bar{\rho})}}{\partial x_i}\right]=-\overline{u_i'u_j'}\frac{\partial \bar{u}_i}{\partial x_j}+\delta_{i3}\frac{g}{\bar{\theta}}\overline{u_i'\theta'}-\varepsilon$$

$$\lim_{\Delta x_i \to LES}(\overline{u_i'u_j'})=-K_M\left(\partial\bar{u}_i/\partial x_j+\partial\bar{u}_j/\partial x_i\right)+\frac{2}{3}\delta_{ij}e$$

$$\lim_{\Delta x_i \to LES}(\overline{u_i'\theta'})=-K_H\,\partial\bar{\theta}/\partial x_i$$

$$\overline{u_i'(e+p'/\bar{\rho})}=-2K_M\frac{\partial e}{\partial x_i}$$

$$K_M=c_K l e^{1/2} \qquad K_H=\left(1+\frac{2l}{\Delta s}\right)K_M \qquad \varepsilon=\frac{C_e e^{3/2}}{l}$$

$$l=\begin{cases}\min\left[0.76e^{1/2}\left|\frac{g}{\theta}\frac{\partial\theta}{\partial z}\right|^{-1/2},\Delta s\right] & \text{for } N^2>0\\ \Delta s & \text{for } N^2\le 0\end{cases} \qquad \Delta s=\left(\Delta x\Delta y\Delta z\right)^{1/3}$$

# Mesoscale Limit

$$\lim_{\Delta x_i \to mesoscale} (\overline{u_i'u_j'}) = \lim_{\Delta x_i \to mesoscale} \left( -\frac{3l_1}{\sqrt{e}} \left[ (\overline{u_i'u_k'} - C_1 e\delta_{ki}) \frac{\partial \overline{u}_j}{\partial x_k} + (\overline{u_k'u_j'} - C_1 e\delta_{kj}) \frac{\partial \overline{u}_i}{\partial x_k} - \frac{g}{\overline{\overline{\theta}}} \left( \delta_{j3} \overline{u_i'\theta_v'} + \delta_{i3} \overline{u_j'\theta'} \right) \right] \right)$$

$$= -K_{ij}^{M} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) + \delta_{j3} \overline{u_i'u_j'}^{NL} \qquad (i \neq j)$$

$$\lim_{\Delta x_i \to mesoscale} (\overline{u_i'\theta'}) = \lim_{\Delta x_i \to mesoscale} \left( -\frac{3l_2}{\sqrt{e}} \left[ (\overline{u_i'u_j'}) \frac{\partial \overline{\theta}}{\partial x_j} + (\overline{\theta'u_j'}) \frac{\partial \overline{u}_i}{\partial x_j} - \delta_{i3} \left( \frac{\overline{\theta'^2}}{\overline{\overline{\theta}}} \right) g \right] \right)$$

$$= -K_{ij}^{H} \frac{\partial \overline{\theta}}{\partial x_j} + \delta_{i3} \overline{u_i'\theta'}^{NL}$$

- **The first two terms on the right can be regarded as the local component of turbulent fluxes given in the PBL scheme.**
- **The third term on the right is conventionally regarded as the nonlocal component of the turbulent flux due to buoyancy.**

# Mesoscale limit (cont'd)

$$\frac{\partial \overline{u}}{\partial t} = -\overline{u}\frac{\partial \overline{u}}{\partial x} - \overline{v}\frac{\partial \overline{u}}{\partial y} - \overline{w}\frac{\partial \overline{u}}{\partial z} - \frac{1}{\rho}\frac{\partial p}{\partial x} - f\overline{v} + \mu\nabla^2\overline{u}$$

$$-\frac{\partial \overline{u'u'}}{\partial x} - \frac{\partial \overline{u'v'}}{\partial y} - \frac{\partial \overline{u'w'}}{\partial z}$$

$2^{nd}$ order

horizontal subgrid mixing

Vertical subgrid mixing

$$\frac{\partial \overline{v}}{\partial t} = -\overline{u}\frac{\partial \overline{v}}{\partial x} - \overline{v}\frac{\partial \overline{v}}{\partial y} - \overline{w}\frac{\partial \overline{v}}{\partial z} - \frac{1}{\rho}\frac{\partial p}{\partial y} + f\overline{v} + \mu\nabla^2\overline{v}$$

$$-\frac{\partial \overline{v'u'}}{\partial x} - \frac{\partial \overline{v'v'}}{\partial y} - \frac{\partial \overline{v'w'}}{\partial z}$$

$2^{nd}$ order

**<u>Horizontal subgrid mixing</u>: resolved strain rate dependent, mostly numerical (Smagorinsky first-order closure based on horizontal deformation in WRF)**

**<u>Vertical subgrid mixing</u>: stability dependent, PBL scheme**

# Key Points:

1. Based on the assumption of scale separation, the conventional subgrid turbulent mixing in mesoscale NWP and LES models utilize different closure formulations.

2. The exact but unclosed governing equations for subgrid turbulent mixing in mesoscale NWP and LES models are mathematically identical.

3. A generalized closure to unify the governing equations for subgrid mixing across mesoscale and LES scale is desirable and possible.

# Starting Point of Our Development in WRF: the Mellor-Yamada Level 2.5 Formulation

$$\frac{\partial e}{\partial t} = \bar{u}_j \frac{\partial e}{\partial x_j} - \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{g}{\bar{\bar{\theta}}} \overline{w'\theta'} - \frac{\partial}{\partial x_i}\left[ K_{ij}^{M} \frac{\partial e}{\partial x_j} \right] - \frac{C_e e^{3/2}}{l}$$

$$\overline{u_i' u_j'} = -\frac{3 l_1}{\sqrt{e}} \left[ (\overline{u_i' u_k'} - C_1 e \delta_{ki}) \frac{\partial \bar{u}_j}{\partial x_k} + (\overline{u_k' u_j'} - C_1 e \delta_{kj}) \frac{\partial \bar{u}_i}{\partial x_k} - \frac{g}{\bar{\bar{\theta}}} \left( \delta_{j3} \overline{u_i'\theta'} + \delta_{i3} \overline{u_j'\theta'} \right) \right] \quad (i \neq j)$$

$$\overline{u_i'\theta'} = -\frac{3 l_2}{\sqrt{e}} \left[ (\overline{u_i' u_j'}) \frac{\partial \bar{\theta}}{\partial x_j} + (\overline{\theta' u_j'}) \frac{\partial \bar{u}_i}{\partial x_j} - \delta_{i3} \left( \frac{\overline{\theta'^2}}{\bar{\bar{\theta}}} \right) g \right]$$

Minimal requirements for extending the 3D TKE subgrid-scale model in WRF to the mesoscale limit include the following two key specifications:

- The diffusivities (i.e., horizontal and vertical length scales) suitable for the mesoscale
- The nonlocal fluxes (i.e., terms other than the down-gradient terms)

# Simplest Closure

$$\overline{u_i' u_j'} = -K_{ij}^{M}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) + \overline{u_i' u_j'}^{NL} \qquad (i \neq j)$$

$$\overline{u_i' \theta'} = -K_{ij}^{H} \frac{\partial \overline{\theta}}{\partial x_j} + \delta_{i3}\, \overline{u_i' \theta'}^{NL}$$

$$K_{horizontal}^{M} = C_{horizontal}^{M} e^{1/2} l_{horizontal} \qquad K_{vertical}^{M} = C_{vertical}^{M} e^{1/2} l_{vertical}$$

$$K_{ij}^{H} = \left(1 + \frac{C_l\, l_{vertical}}{l_{horizontal}}\right) K_{ij}^{M}$$

# In the LES Limit

Deardorff's length scale is applied:

$$l_{horizontal} = l_{vertical} = l_{LES} = \begin{cases} \min\left[ 0.76e^{1/2} \left| \dfrac{g}{\theta} \dfrac{\partial \theta}{\partial z} \right|^{-1/2}, \Delta s \right] & \text{for } N^2 > 0 \\ \Delta s & \text{for } N^2 \leq 0 \end{cases}$$

$$\Delta s = \left( \Delta x \Delta y \Delta z \right)^{1/3}$$

# In the Mesoscale Limit

Following MYNN Level-3 scheme, the vertical length scale is given as:

$$\frac{1}{l_{vertical}} = \frac{1}{l_{MESO}} = \frac{1}{l_S} + \frac{1}{l_T} + \frac{1}{l_B}$$

where $$l_S = \alpha_1 kz \qquad l_T = \alpha_2 \frac{\int_0^\infty e^{1/2} z dz}{\int_0^\infty e^{1/2} dz}$$

$$l_B = \begin{cases} \left[\alpha_3 e^{1/2} + \alpha_4 e^{1/2} (q_c / l_T N)^{1/2}\right] / N, & \partial\overline{\theta}/\partial z > 0 \\ \infty, & \partial\overline{\theta}/\partial z \le 0 \end{cases}$$

$$l_{horizontal} = Func\left[\left(\Delta x \Delta y\right)^{1/2}\right]$$

$l_S$ is the length scale in the surface layer controlled by the characteristics of the surface and stability, $l_T$ is the length scale depending on the turbulent structure of the PBL and $l_B$ the length scale limited by the thermal stability.

# Numerical Consideration

- It was found that the 3DTKE scheme can be unstable when it is used in mesoscale simulations in which dx,dy>>dz (highly anisotropic grid).

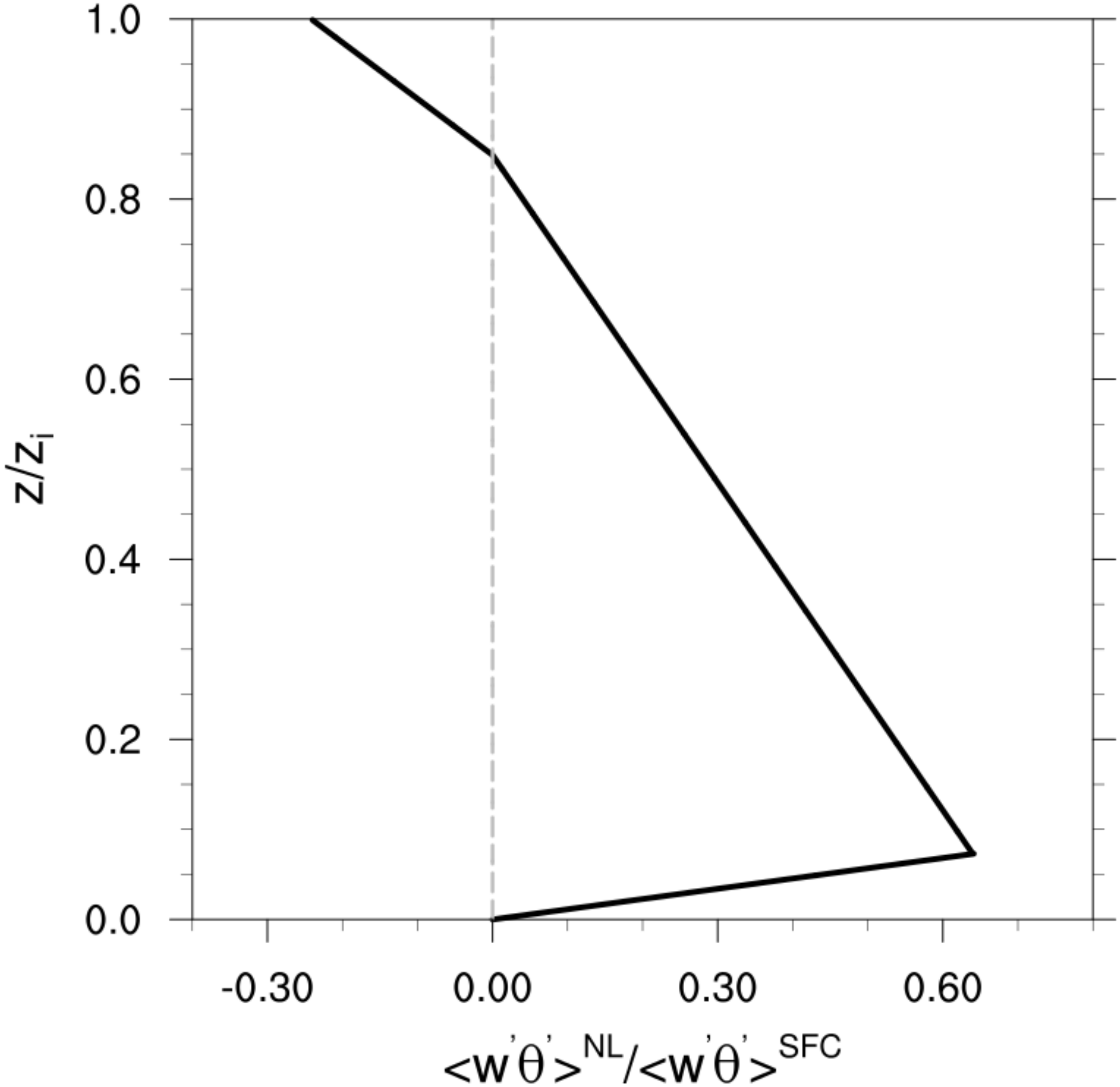
- To make the model stable, an implicit method instead of original explicit method to solve the TKE equation and model diffusion equations.

$$\frac{\partial e}{\partial t}+\overline{U}_j\frac{\partial e}{\partial x_j}=-(\overline{u_i'u_j'})\frac{\partial \overline{U_i}}{\partial x_j}+\delta_{i3}\frac{g}{\overline{\theta}_v}\overline{u_i'\theta_v'}-\frac{1}{\overline{\rho}}\frac{\partial(\overline{p'u_i'})}{\partial x_i}-\frac{\partial(\overline{u_j'e})}{\partial x_j}-\varepsilon$$

$$e_k^{n+1}-e_k^n=\Delta t\left(D_h-A_h+P\right)_k^n+\Delta t\left(D_v-A_v-\frac{c_e e^{1/2}}{l}e\right)_k^{n+1}$$

# In the Mesoscale Limit

$\overline{w'\theta'}^{NL}$ is the prescribed nonlocal heat flux from Shin and Hong (2013)



# In the Mesoscale Limit: Nonlocal Momentum Flux

Following the suggestion by Brown and Grant (1997) and Noh et al. (2003), the effect of nonlocal momentum flux is included in the momentum flux profile as

$$-\overline{u'w'} = K_M \left( \frac{\partial \overline{u}}{\partial z} + \frac{\partial \overline{w}}{\partial x} + \gamma_m \frac{u}{\sqrt{u^2 + v^2}} \right)$$

$$-\overline{v'w'} = K_M \left( \frac{\partial \overline{v}}{\partial z} + \frac{\partial \overline{w}}{\partial y} + \gamma_m \frac{v}{\sqrt{u^2 + v^2}} \right)$$

The counter-gradient term $\gamma_m$ of momentum flux is given as

$$\gamma_m = S_m \frac{u_*^2}{w_s z_i} \left( \frac{w_*}{w_s} \right)^3$$

$$w_s = \left( u_*^3 + 8k w_*^3 z / h \right)^{1/3} \qquad w_* = (g/\theta_0 \, Q_0 z_i)^{1/3}$$

# Scale-Adaptive Transition Between LES and Mesoscale Limit

$$\overline{w'\theta'}^{\Delta x} = \overline{w'\theta'}^{\Delta x, L} + \overline{w'\theta'}^{\Delta x, NL}$$

$$\overline{w'\theta'}^{\Delta x, L} = -K_{\Delta x}^{H} \frac{\partial \overline{\theta}^{\Delta x}}{\partial z} \qquad \overline{w'\theta'}^{\Delta x, NL} = \overline{w'\theta'}^{NL} P_{NL}(\Delta x / z_i)$$

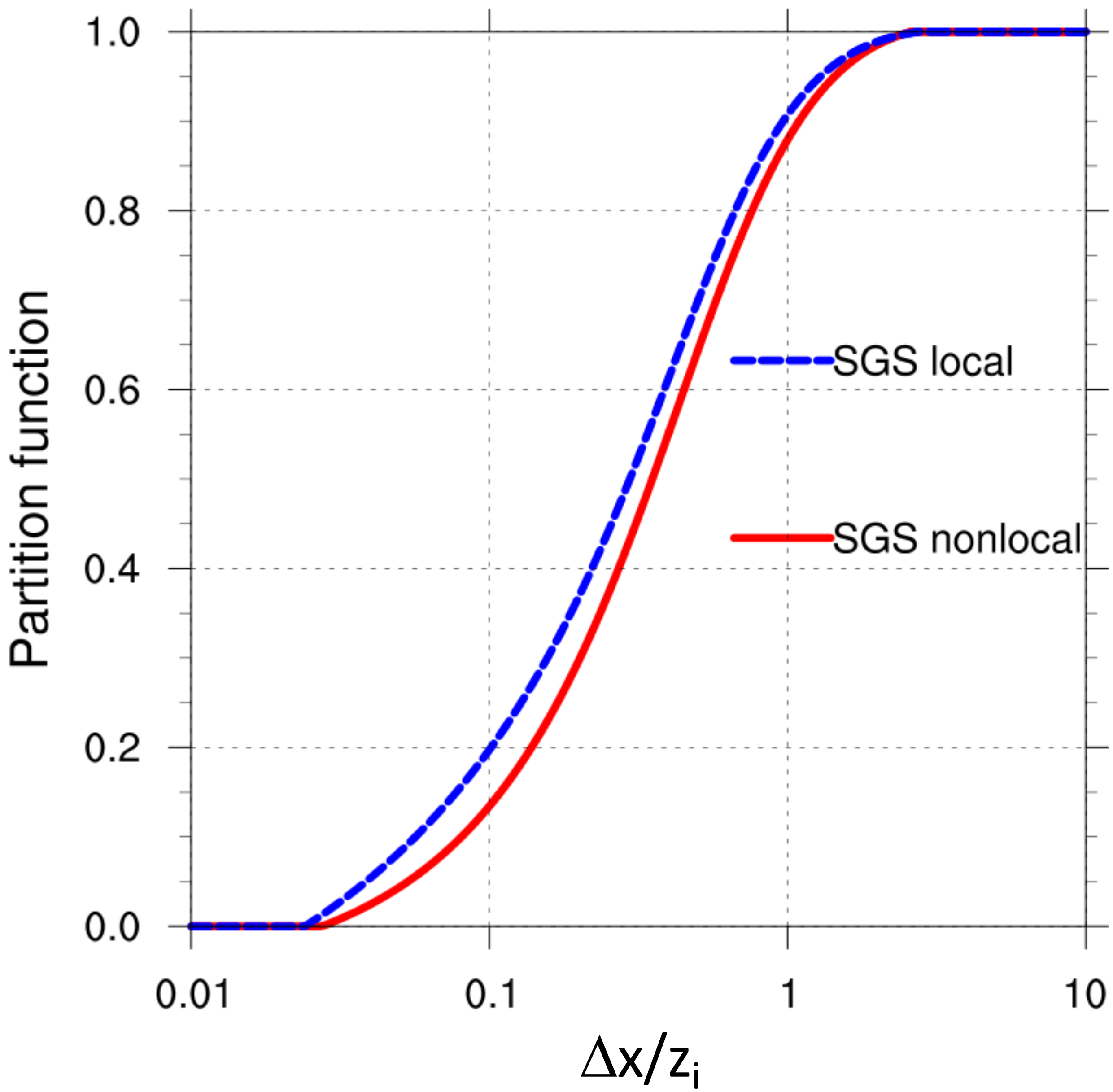
$$K_{\Delta x}^{H} = C_{vertical}\, l_{\Delta x} e^{1/2}$$

$$l_{\Delta x} = P_L(\Delta x / z_i)\, l_{MESO} + \left[1 - P_L(\Delta x / z_i)\right] l_{LES}$$

$$\Rightarrow \quad K_{\Delta x}^{H} = P_L(\Delta x / z_i) K_{MESO}^{H} + \left[1 - P_L(\Delta x / z_i)\right] K_{LES}^{H}$$

$P_L(\Delta x / z_i)$ and $P_{NL}(\Delta x / z_i)$ are scale-adaptive transition weighting functions.

# Weighting functions $P_{NL}(\Delta x/z_i)$ and $P_L(\Delta x/z_i)$ from Shin and Hong (2013)



# A Remark on the Numerical Diffusivity (a.k.a., the Background Diffusivity)

Practically, if the numerical diffusivity is needed, it should be combined with the turbulence-induced diffusivity in question. For example, the total horizontal diffusivity model has the following form:

$$
\begin{aligned}
K_{horizontal} &= K_{numerical} + K^{M}_{horizontal} \\
&= (C_{numerical}\Delta)^2 D + K^{M}_{horizontal}
\end{aligned}
$$

$$
D = (D_{ij}D_{ij})^{1/2} \qquad D_{ij} = \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}
$$

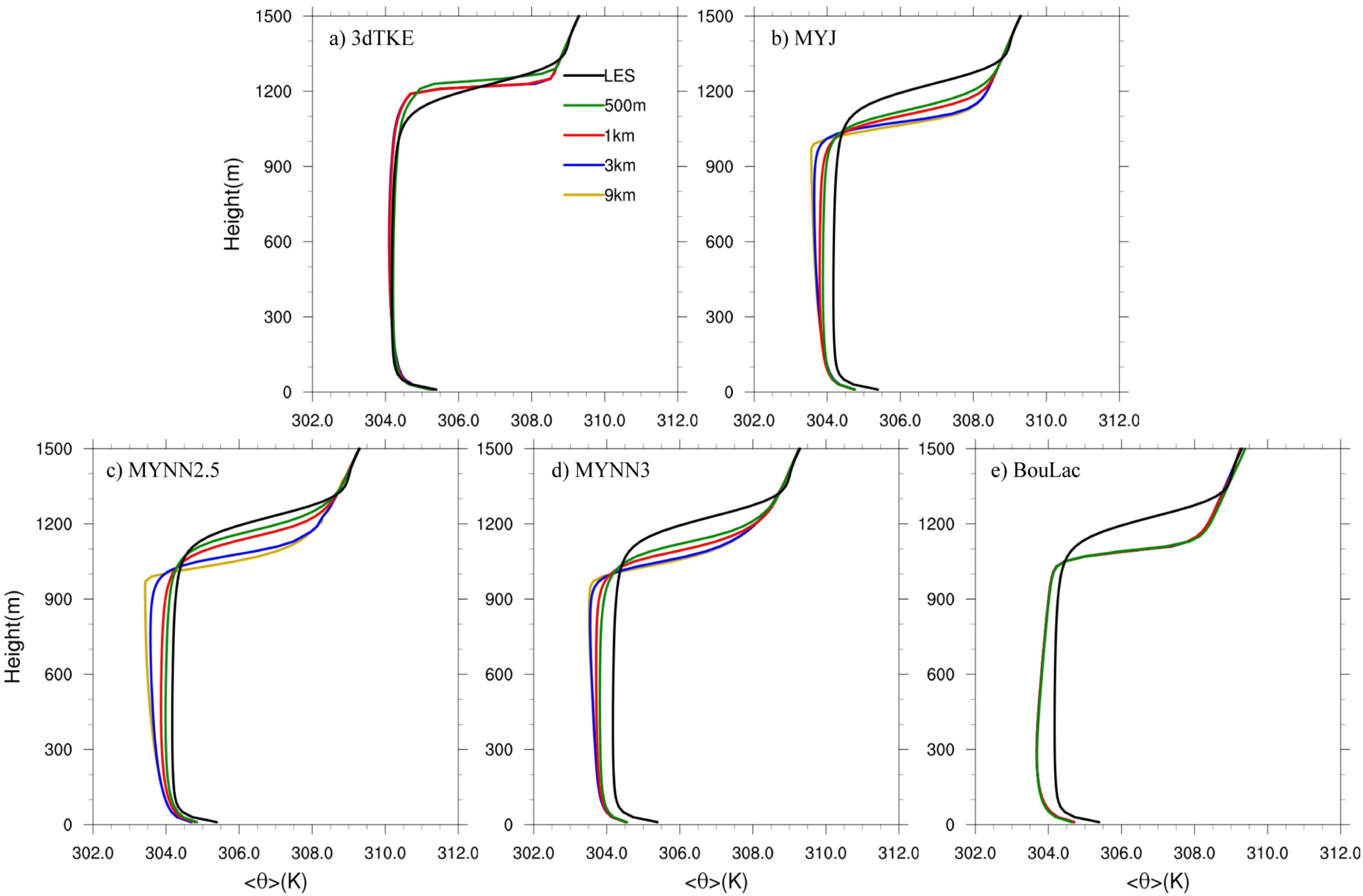
# Highlight of Numerical Results: Idealized Dry CBL Development

| Name of experiments | H-Diff. | V-Diff. | Vertical grid size | Horizontal grid size |
|---|---|---|---|---|
| Benchmark LES | 3dTKE | 3dTKE | 20 m | 50m |
| 3dTKE | 3dTKE | 3dTKE | 20 m | 9 km, 3km, 1 km, 500 m |
| MYJ | 2D Smag | MYJ | 20 m | 9 km, 3km, 1 km, 500 m |
| MYNN2.5/MYNN3 | 2D Smag | MYNN | 20 m | 9 km, 3km, 1 km, 500 m |
| BouLac | 2D Smag | BouLac | 20 m | 9 km, 3km, 1 km, 500 m |

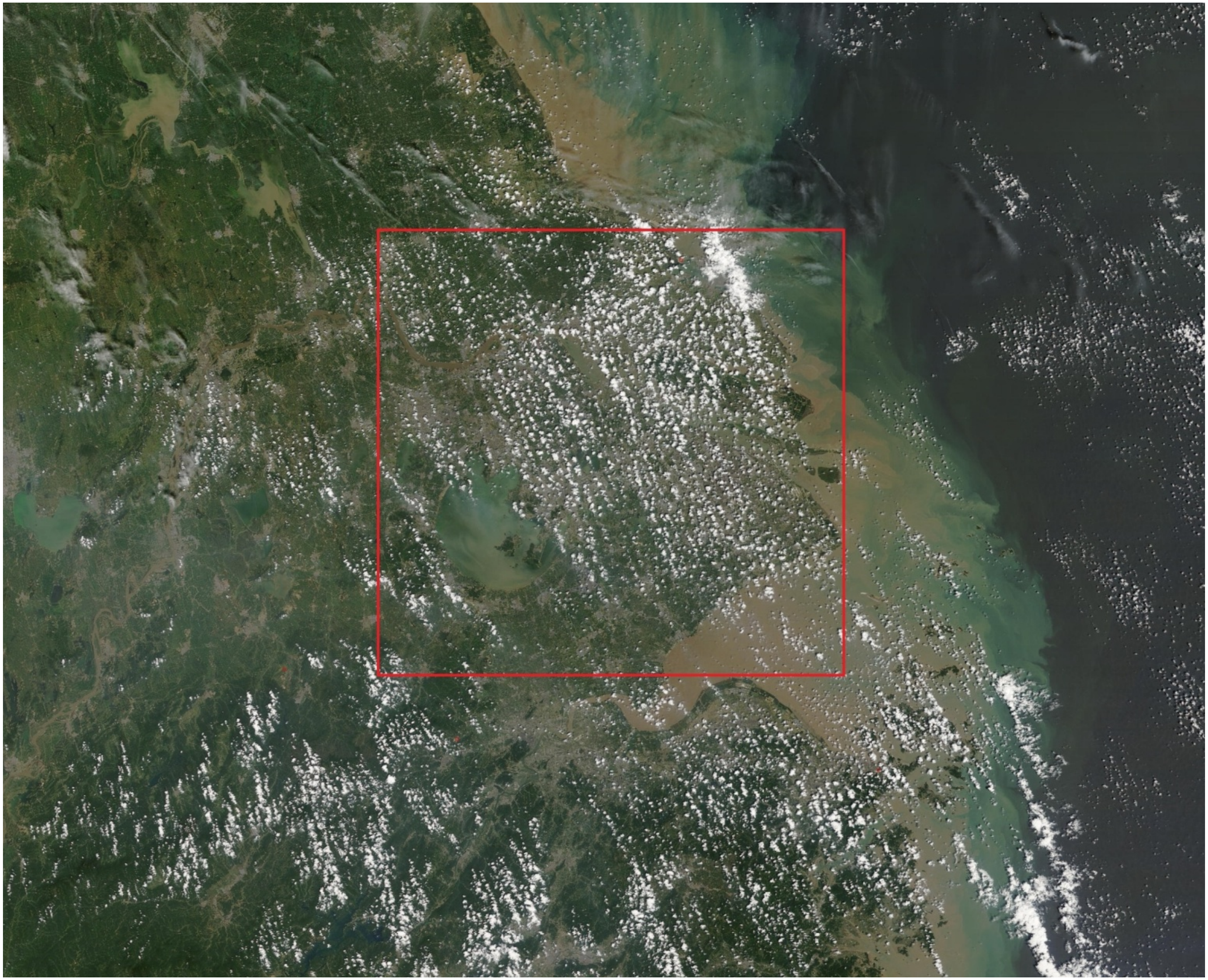
- The benchmark LES run was driven by constant kinematic heat flux ($Q_0$ = 0.24 K m s$^{-1}$) and geostrophic wind in the *x* direction ($U_g$ = 10 m s$^{-1}$).

- In the PBL experiments, the surface heat flux is prescribed with the same value as the LES (0.24 K m s$^{-1}$) .

# Mean Profiles of Potential Temperature



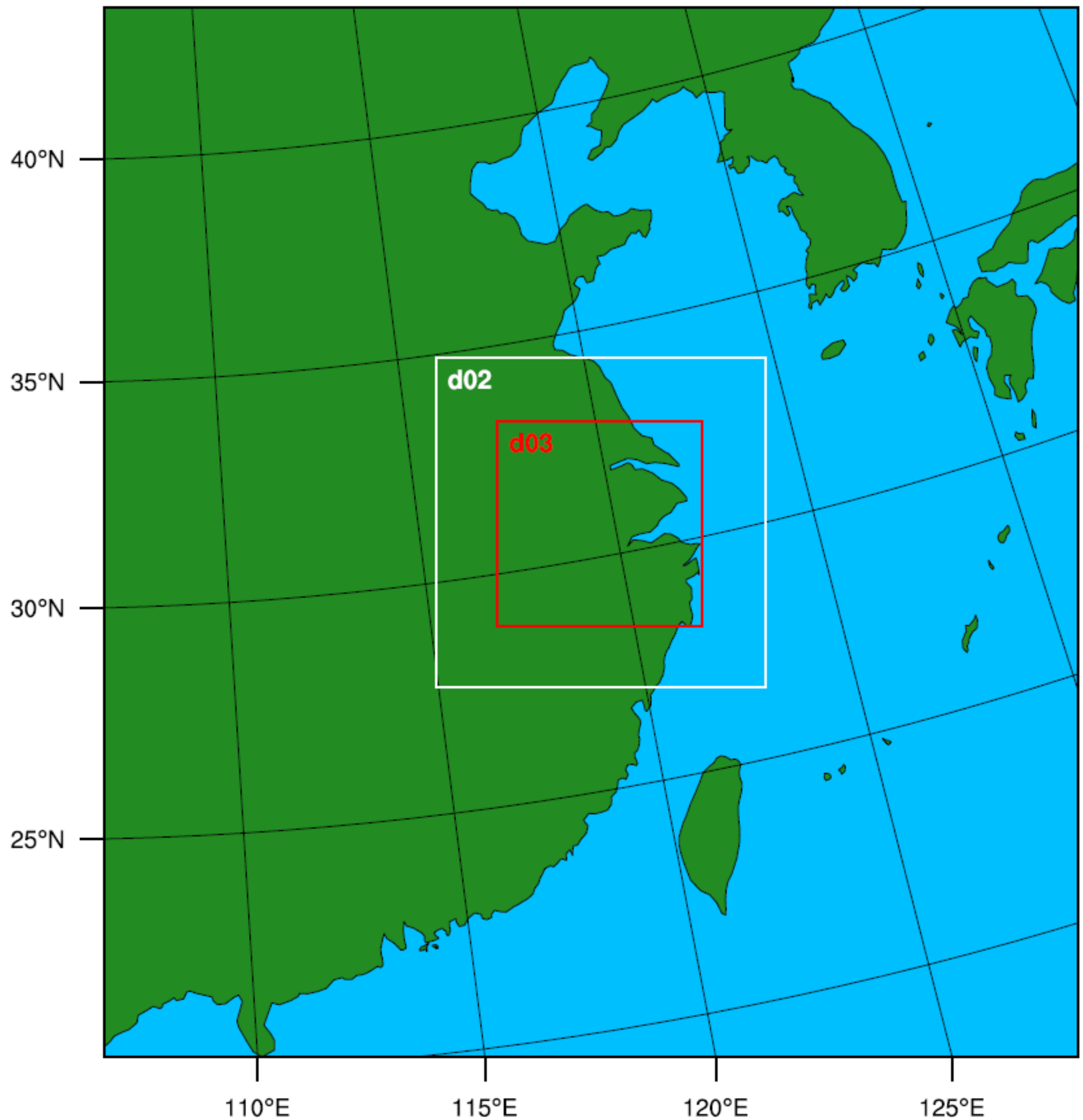
# 250-m resolution visible MODIS-*Terra* image at 02:40 UTC 29 Aug 2016

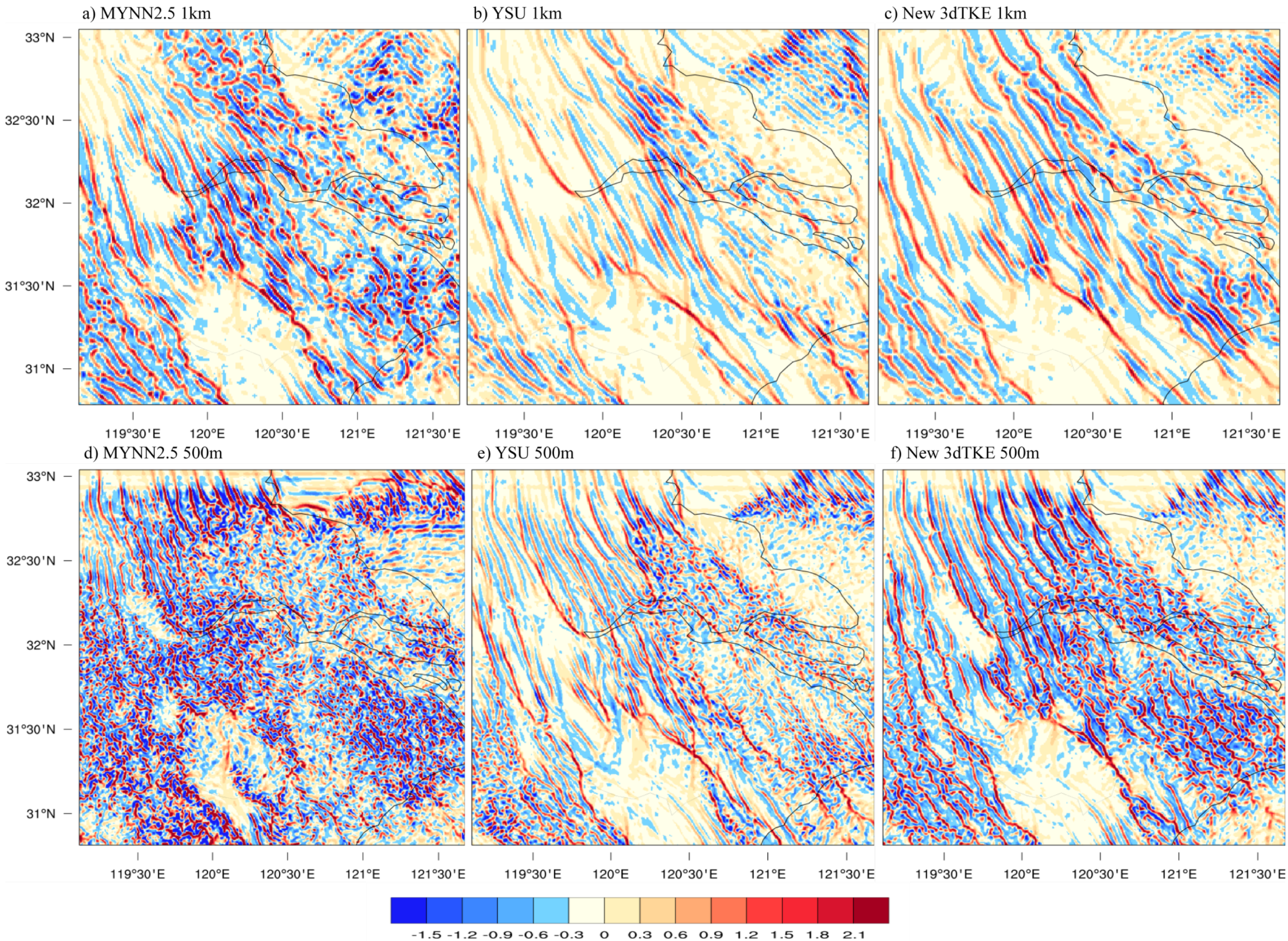


# D01:3km
# D02:1km
# D03:500m

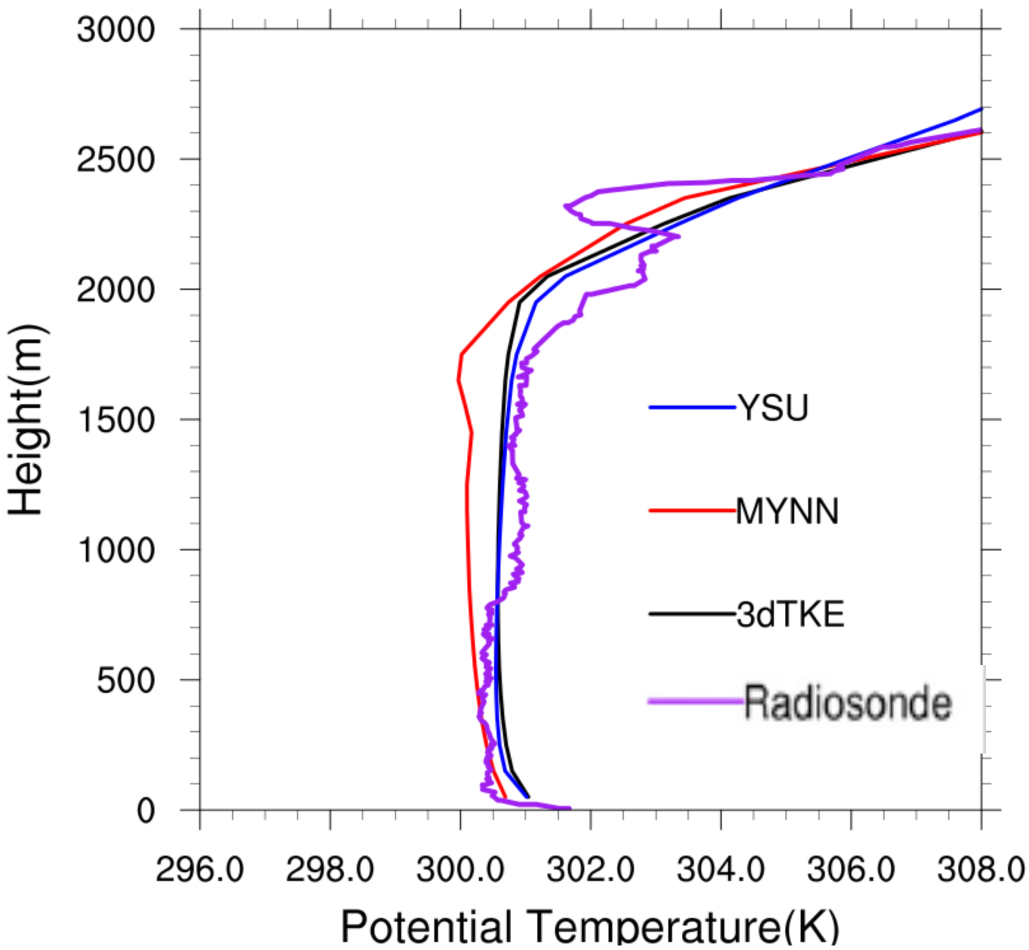
**From: 2016.08.29.08**
**To: 2016.08.30.08**

| Res | nx*ny | dt |
|---|---|---|
| 3km | 793*853 | 15s |
| 1km | 805*805 | 5s |
| 500m | 1001*1001 | 2s |

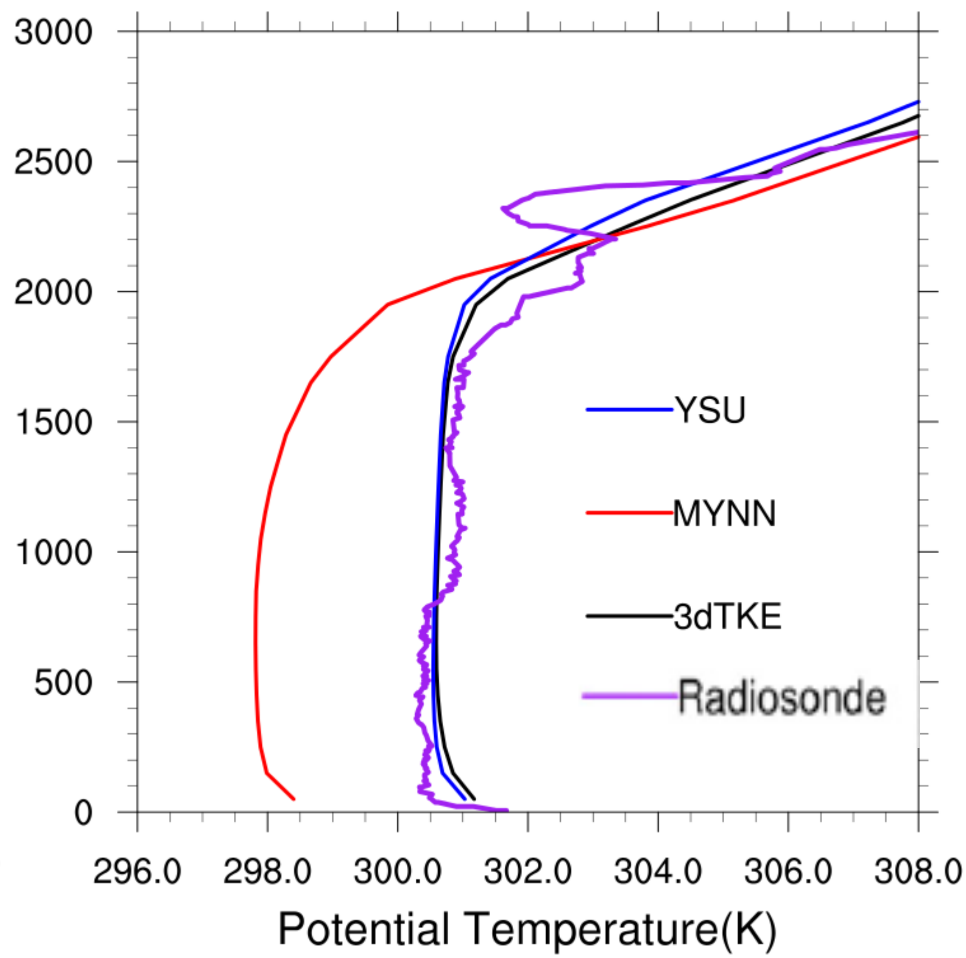



a) MYNN2.5 1km
b) YSU 1km
c) New 3dTKE 1km
d) MYNN2.5 500m
e) YSU 500m
f) New 3dTKE 500m
33°N
32°30'N
32°N
31°30'N
31°N
119°30'E
120°E
120°30'E
121°E
121°30'E
-1.5 -1.2 -0.9 -0.6 -0.3 0 0.3 0.6 0.9 1.2 1.5 1.8 2.1

# Vertical profiles of simulated potential temperature at 0500 UTC 29 Aug 2016 for the Station Baoshan (31.40$^{o}$N, 121.45 $^{o}$E)




1km




500m

# Summary and Future Work

- A scale-adaptive parameterization scheme based on the general form of the TKE equation has been developed in the WRF model to simulate 3-D subgrid turbulent mixing.

- The scheme shows promise in making the transition between the mesoscale and LES limits smooth, not only in the amount of subgrid mixing, but also in the parameterization formula (an appealing feature for nesting simulations).

- It is feasible to apply the new scheme in lieu of conventional planetary boundary layer parameterization schemes.

- Including the contribution to vertical momentum and heat fluxes due to nonlocal buoyancy flux is important for mesoscale simulations.

- Further evaluation and improvements using more realistic cases are underway.