UNIVERSITY OF DELAWARE

# Development of a mesoscopic simulation method for atmospheric convection


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10:50 – 11:10, December 1 (Thursday)

*The 4th International Workshop on Nonhydrostatic Models*

Nov. 30 (Wed) - Dec. 2 (Fri), 2016

The Prince Hakone Lake Ashinoko, Hakone, Japan

# Outline

- ❖ Background, motivation, and objectives
- ❖ The DUGKS method
- ❖ Some results
- ❖ Summary

## Background & Motivation

- ✧ Mesoscopic methods based on the Boltzmann equation to solve complex turbulent flows have been rapidly developed over the last 30 years
- ✧ But very limited applications to geophysical flows

## Overall objectives

- ✧ Simulate high-Rayleigh number convection flows using DUGKS

- ✧ How to treat unresolved local gradients?

  Controlled local numerical diffusion (TVD, monotone, ….)

  Explicit SGS model

- ✧ Compare DUGKS and Navier-Stokes based solvers

  in terms of accuracy, numerical stability, and efficiency

# Thermal convection flows

Macroscopic world

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\bar{\rho}} \frac{\partial \tilde{p}}{\partial x_i} + \boxed{\beta g\left(\theta - \theta_0\right)\delta_{i3}} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

$$\frac{\partial \theta}{\partial t} + \frac{\partial}{\partial x_j}\left(u_j \theta\right) = \frac{\partial}{\partial x_i}\left(\kappa \frac{\partial \theta}{\partial x_i}\right)$$

$$\theta = T - \bar{T}$$

$$u_0 = \sqrt{g\beta\Delta T H}$$

$$\mathrm{Ra} = \frac{g\beta\Delta T H^3}{\nu\kappa}$$

$$Pr = \frac{\nu}{\kappa} = 0.71$$

Mesoscopic world

$$\partial_t f + \xi \cdot \nabla f = \tilde{\Omega} \equiv -\frac{f - f^{eq}}{\tau_v} + \Phi, \quad \Phi_i \approx \boxed{\frac{\beta \vec{g}\theta \cdot \left(\vec{e}_i - \vec{u}\right)}{RT} f_i^{(eq)}}$$

$$\partial_t h + \xi \cdot \nabla h = \Psi \equiv -\frac{h - h^{eq}}{\tau_c}, \quad \theta = \sum_i h_i$$

$$\rho = \sum_i h_i, \quad \rho\vec{u} = \sum_i f_i \xi_i + \boxed{\frac{\delta t}{2}\rho\beta\vec{g}\theta,} \quad p = \rho R\theta$$

$$f^{eq} = \rho\, w_i \left[1 + \frac{\vec{e}_i \cdot \vec{u}}{c_s^2} + \frac{\left(\vec{e}_i \cdot \vec{u}\right)^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2}\right], \quad h^{eq} = \theta\, w_i \left[1 + \boxed{\frac{\vec{e}_i \cdot \vec{u}}{c_s^2} + \frac{\left(\vec{e}_i \cdot \vec{u}\right)^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2}}\right]$$

## DUGKS: Discrete Unified Gas Kinetic Scheme

- ✧ Based directly on the Boltzmann equation with BGK collision model
- ✧ Gas Kinetic Scheme combined with certain good features of LBM (simplicity and low numerical dissipation)
- ✧ The kinetic advection is treated as fluxes through cell interfaces
- ✧ Fluxes are computed using distributions at the half time step, with streaming and collision coupled together (low numerical dissipation)
- ✧ A much more general approach than LBM
  - Key advantages: all flow types, all Kn and Ma
  - Non-uniform grid

K Xu and J-C Huang, J. Comp. Phys. 229, 7747 (201)
ZL Guo, K Xu, RJ Wang, PRE 88, 033305 (2013); PRE 91, 033313 (2015)
P Wang, S Tao, ZL Guo, Computers & Fluids, 120 70-81 (2015).

# DUGKS: finite-volume discretization for hydrodynamic velocity

$$\partial_t f + \xi \cdot \nabla f = \tilde{\Omega} \equiv -\frac{f - f^{eq}}{\tau_v} + \Phi$$

$$\xi \to \boldsymbol{e}_i, \quad \Phi_i \approx \frac{\beta \vec{g}\left(T - \bar{T}\right) \cdot \left(\vec{e}_i - \vec{u}\right)}{RT} f_i^{(eq)}$$

**For nearly incompressible flow, D3Q19**

Updating rule for cell-center distribution functions

$$f_i^{n+1}\left(\boldsymbol{x}\right) - f_i^{n}\left(\boldsymbol{x}\right) + \underbrace{\frac{dt}{\left|V_j\right|} \sum_{dS} f_i^{n+0.5}\left(\boldsymbol{x}_s\right) \boldsymbol{e}_i \cdot d\boldsymbol{S}}_{\text{Mid-point}} = \underbrace{\frac{dt}{2}\left[\tilde{\Omega}_i^{n+1} + \tilde{\Omega}_i^{n}\right]}_{\text{Trapezoidal}}$$

Constructing $f_i^{n+0.5}\left(\boldsymbol{x}_s\right)$: Integrate from $t_n$ to $t_n + 0.5dt$ along the characteristic path

$$f_i^{n+0.5}\left(\boldsymbol{x}_s\right) - f_i^{n}\left(\boldsymbol{x}_s - 0.5dt\ \boldsymbol{e}_i\right) = \frac{dt}{4}\left[\tilde{\Omega}_i^{n+0.5}\left(\boldsymbol{x}_s\right) + \tilde{\Omega}_i^{n}\left(\boldsymbol{x}_s - 0.5dt\ \boldsymbol{e}_i\right)\right]$$

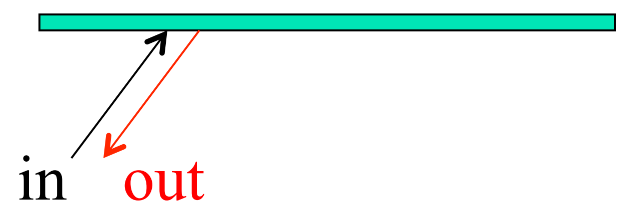
$\boldsymbol{x}$ = cell center, $\boldsymbol{x}_s$ = cell boundary

Similar transformations as in LBM are used to make all explicit

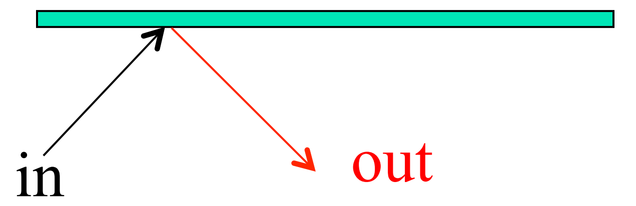
K Xu and J-C Huang, J. Comp. Phys. 229, 7747 (201)
ZL Guo, K Xu, RJ Wang, PRE 88, 033305 (2013); PRE 91, 033313 (2015)

# DUGKS: Boundary conditions
# – all done to distributions at cell interfaces

No-slip wall: bounce-back




Free-slip wall: mirror reflection




Fixed temperature

$$h_{\bar{\alpha}}^{n+0.5}\left(\boldsymbol{x}_s\right) = -h_{\alpha}^{n+0.5}\left(\boldsymbol{x}_s\right) + 2W_{\alpha}T_{wall}$$

Zero heat flux

$$h_{\bar{\alpha}}^{n+0.5}\left(\boldsymbol{x}_s\right) = h_{\alpha}^{n+0.5}\left(\boldsymbol{x}_s\right)$$

# DNS of turbulent flows using DUGKS

Homogeneous isotropic turbulence in a periodic box

Wang P, Wang L-P, Guo ZL, 2016, Comparison of the LBE and DUGKS methods for DNS of decaying turbulent flows. Phys. Rev. E., 94, 043304

Turbulent channel flow [non-uniform mesh with large grid aspect ratios]

Bo YT, Wang P, Guo ZL, Wang L-P, 2016, Parallel implementation and validation of DUGKS for three-dimensional Taylor-Green vortex flow and turbulent channel flow, *Computers & Fluids, submitted.*

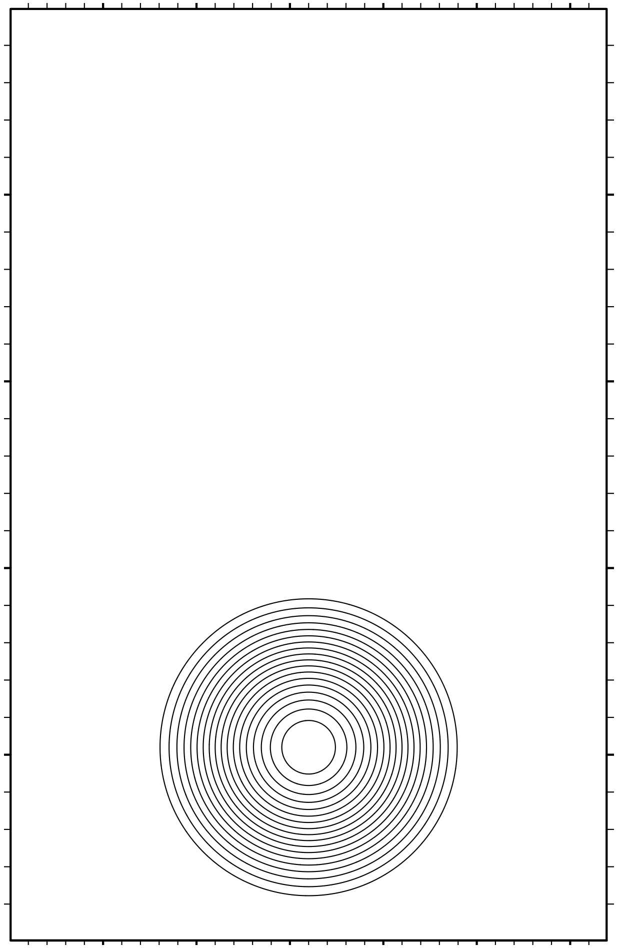
DNS of thermal convection in an enclosure

Wang L-P, Wen X, Geneva N, Wang P, Guo ZL, 2016, Simulations of high-Rayleigh-number convection flows using mesoscopic methods, Discrete Simulation of Fluid Dynamics 2016.

Ra ~ $10^{11}$ in 3D

MPI, non-uniform mesh, external forcing, boundary conditions

# The physical problem: Rising and evolution of a warm dry bubble



Background

$$\rho_0 = 1.0, \quad \theta_0 = 300K, \quad \Delta T = 2 \text{ K}$$

$$\theta = \theta_0 + \begin{cases} \Delta T \left[ \cos\left( \frac{\pi r}{2000} \right) \right]^2 & r < 1000\ m \\ 0, & \text{otherwise} \end{cases}$$

Centered at 1040 m height

Domain: 3200 m H, 5000m V

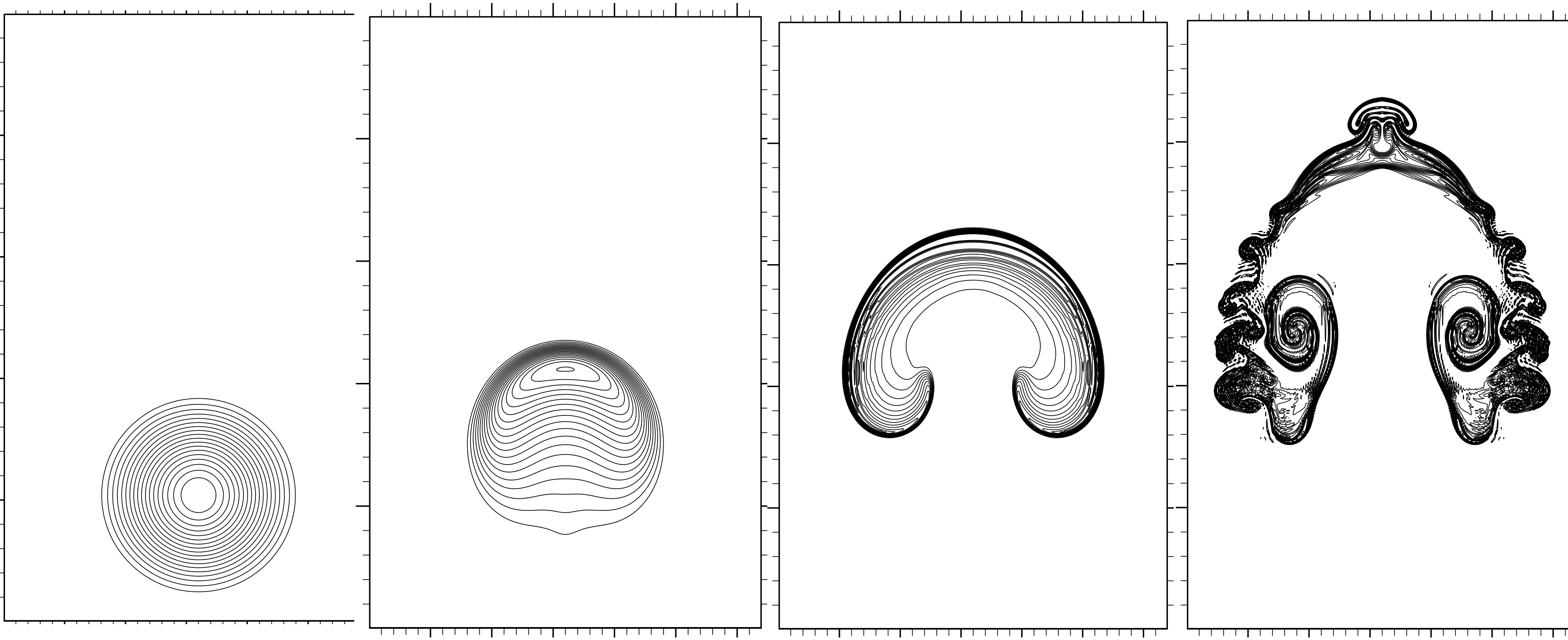
$$H = 1000\ m, \quad \Pr = 0.71, \quad \nu = 1.57 \times 10^{-5}$$

$$Ra = \frac{Pr\, G \Delta T H^3}{\nu^2} = 1.89 \times 10^{17}$$

Periodic BC in horozontal

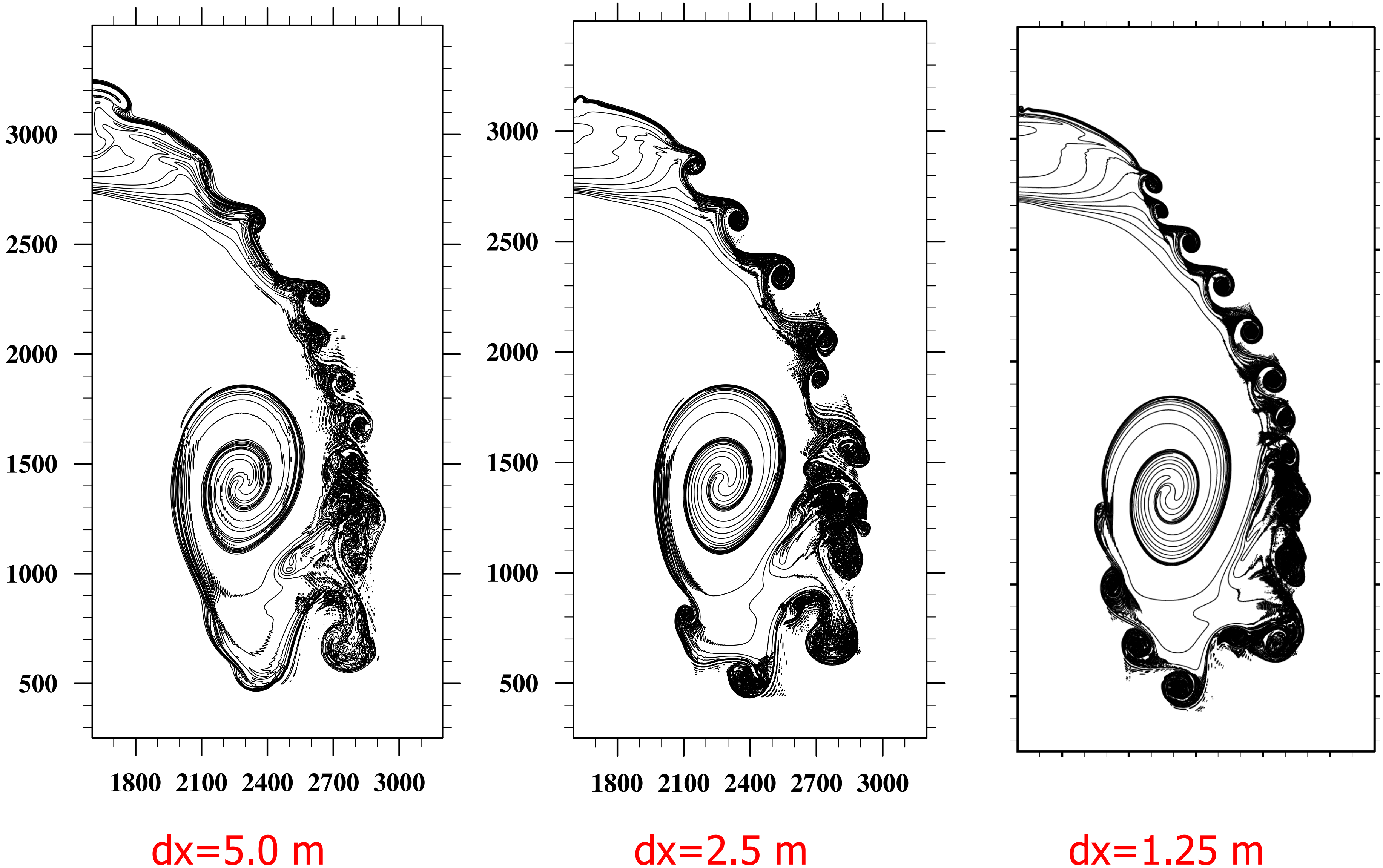
Vertical boundaries: zero heat flux & stress free

**Evolution at a given grid resolution of dx = 10 m**
**No numerical limiter applied**

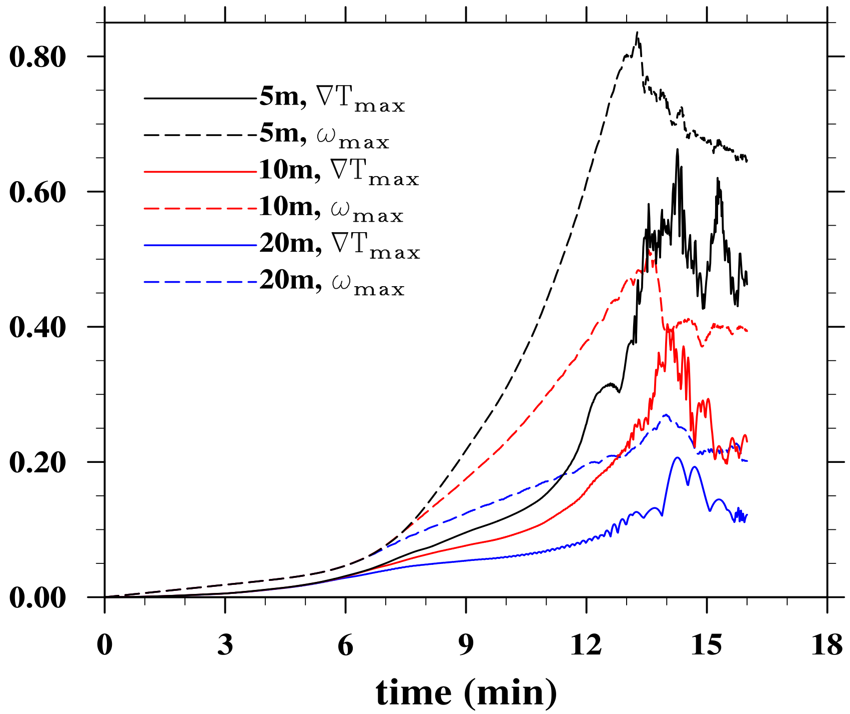


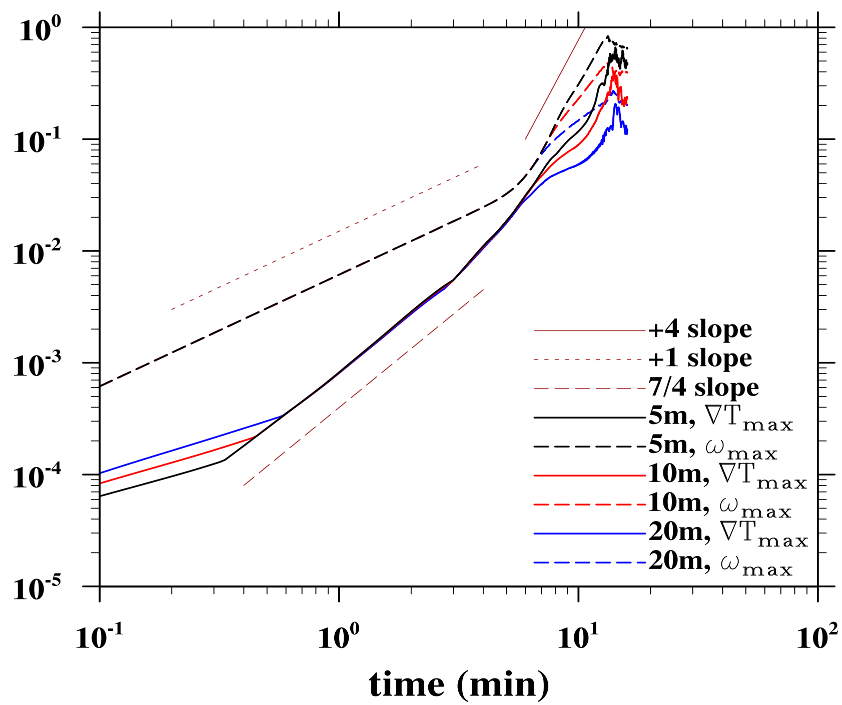
0 min | 5 min | 10 min | 15 min

# How about increasing the grid resolution?
# No numerical limiter applied



# Maximum local temperature gradient and maximum local vorticity
# → Rapid evolution of the smallest spatial scale




- The higher the resolution, the more rapid the smallest scale is formed

# The van-Leer slope limiter (the monotonized central limiter)

## Slope in a cell for field reconstruction

$$\sigma_j^n = minmod\left(2\frac{U_{j+1}^n - U_j^n}{\Delta x}, \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}, 2\frac{U_j^n - U_{j-1}^n}{\Delta x}\right)$$

(Form 1)

where

$$minmod(a_1, a_2, a_3) = \begin{cases} sign(a_1)\, min(|a_1|,|a_2|,|a_3|), & \text{if } sgn(a_1) = sgn(a_2) = sgn(a_3) \\ 0, & \text{otherwise} \end{cases}$$

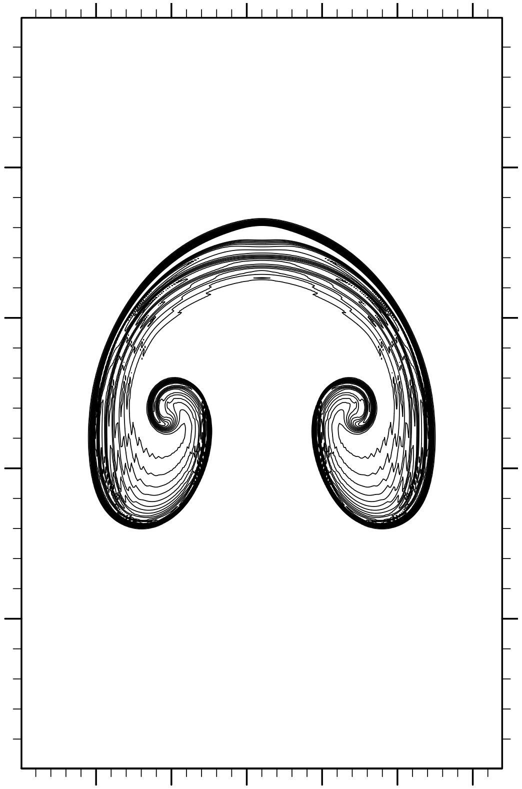
(Form 2)

Variation

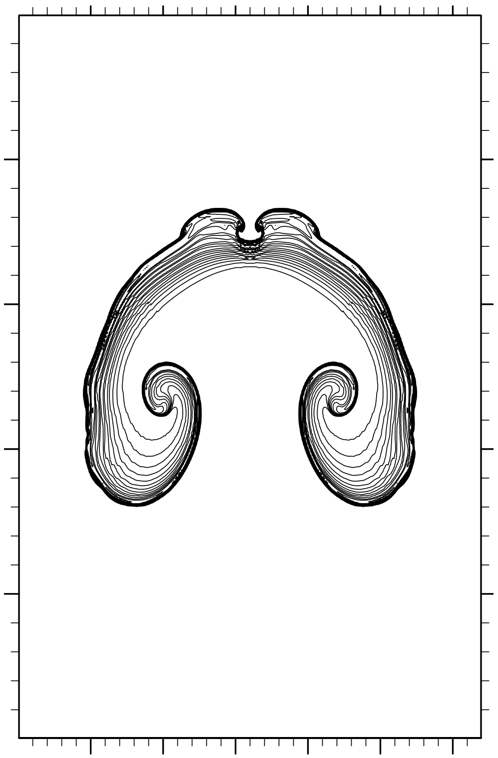
$$\sigma_j^n = \left[sgn(s_1) + sgn(s_2)\right]\frac{|s_1||s_2|}{|s_1| + |s_2|}, \quad \text{where } s_1 = \frac{U_{j+1}^n - U_j^n}{\Delta x}, \; s_2 = \frac{U_j^n - U_{j-1}^n}{\Delta x}$$

B. van Leer, J. Comput. Phys. 23, 276 (1977).

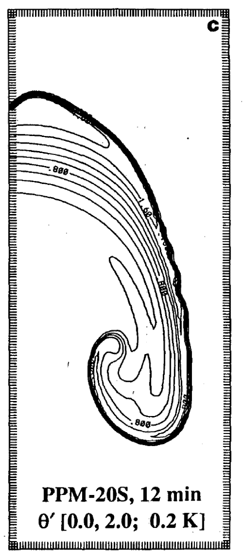
# Time =12.0 min, dx = 10 m, comparison of T field



No limiter



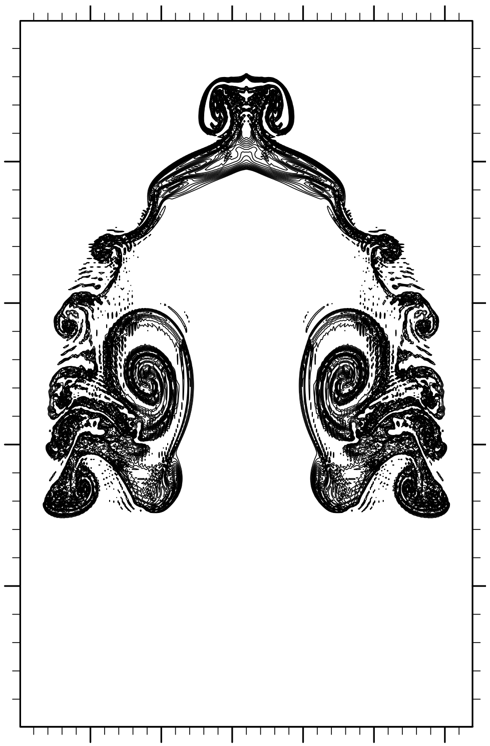
van Leer limiter



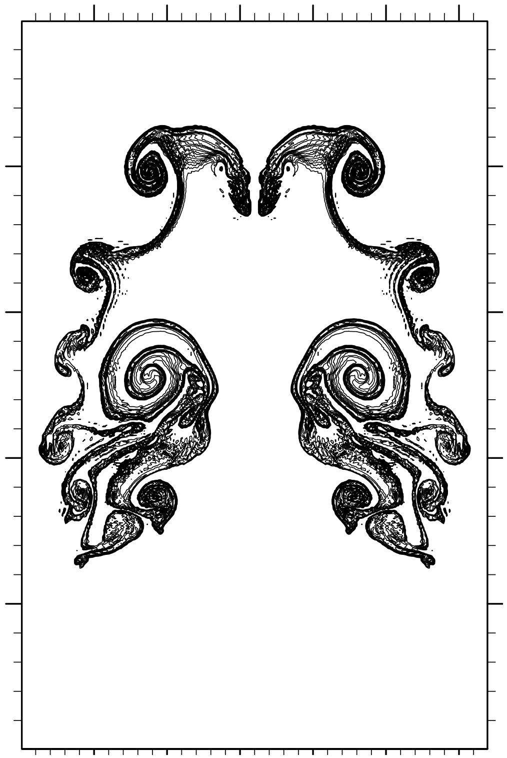

Piecewise parabolic method
Carpenter et al (1990)

Carpenter et al., 1990, Monthly Weather Rev. 118: 586 – 612.

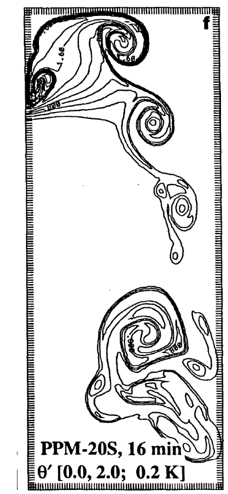
Time =16.0 min, dx = 10 m, comparison of T field



No limiter



van Leer limiter




Piecewise parabolic method
Carpenter et al (1990)

# Codes to be compared

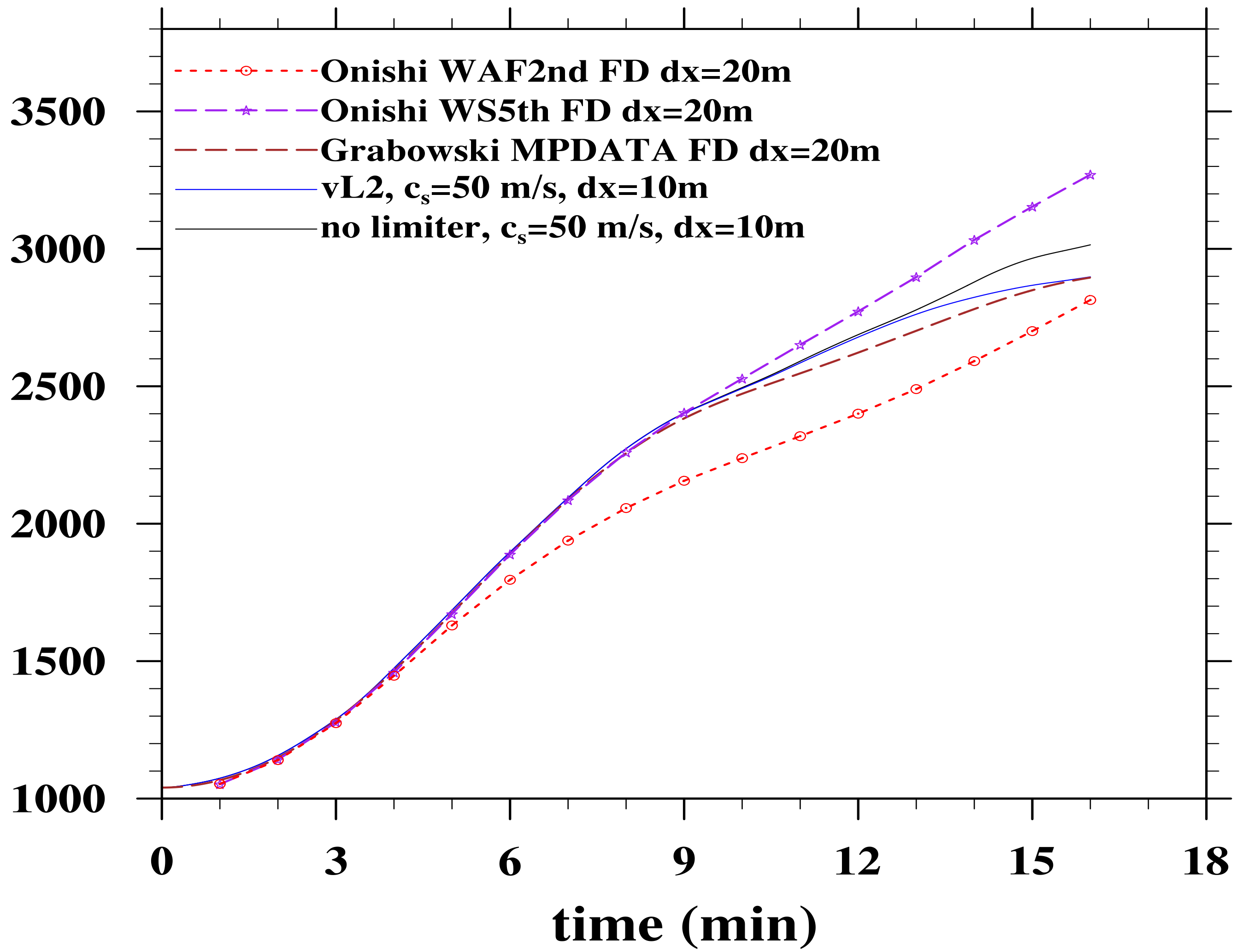
NCAR Grabowski: 2$^{nd}$-order finite difference code with MPDATA (the multidimensional positive definite advection transport), set to constant background density

JAMSTec Onishi: atmospheric background density
WAF2nd: 2$^{nd}$-order Weighted-Averaged Flux method with SUPER-BEE flux limiter

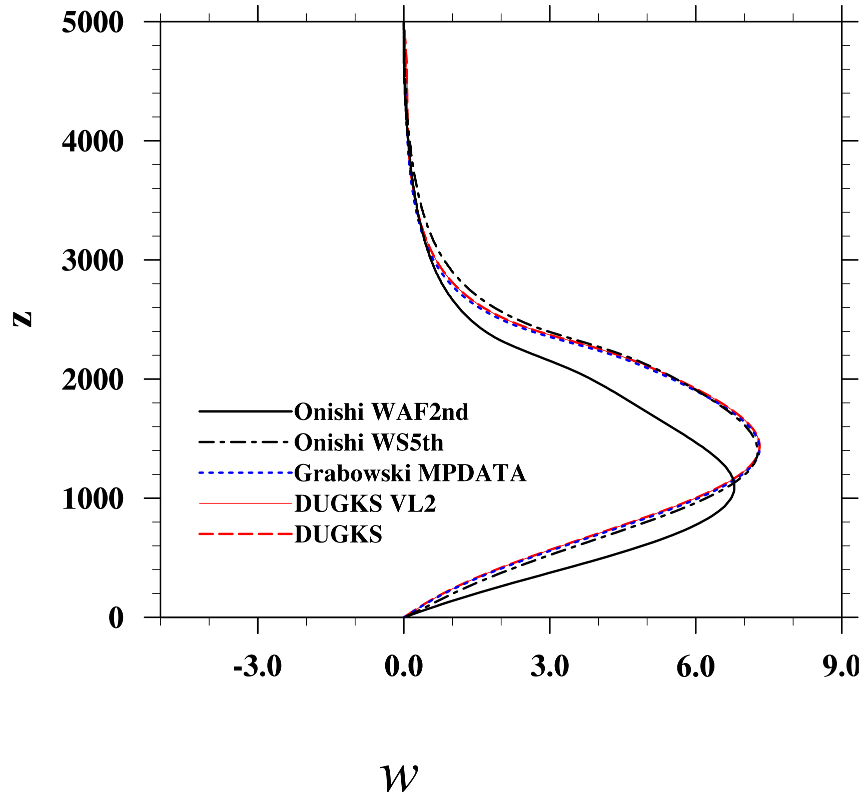
WS5th:  Wicker-Skamarock 5$^{th}$-order upwind scheme

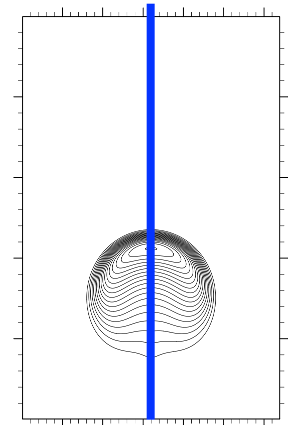
# The center of the thermal

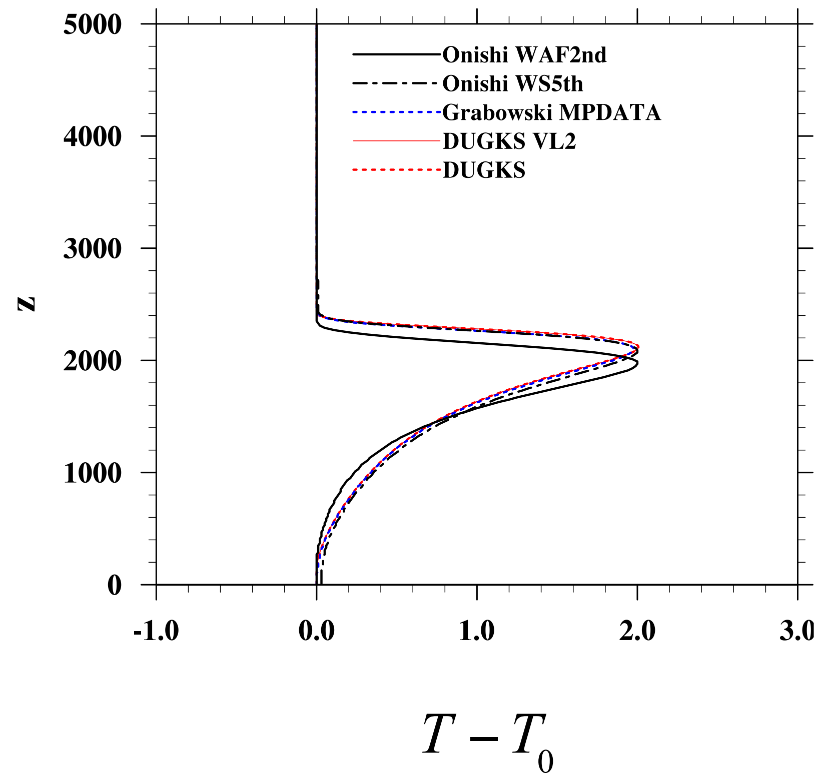
$$Z_c = \frac{\int \left(\theta - \theta_0\right) z\, dV}{\int \left(\theta - \theta_0\right) dV}$$



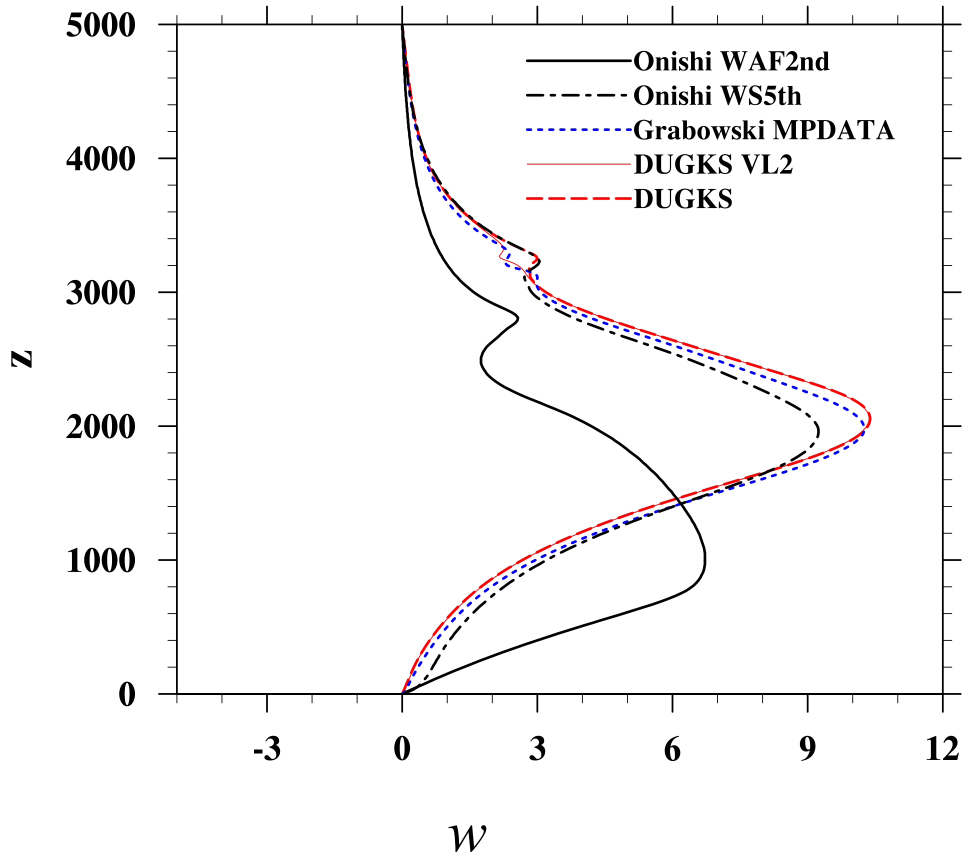
# Vertical profiles at 5 min

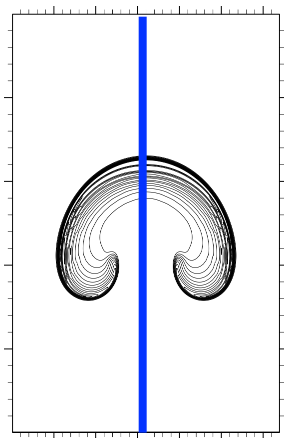


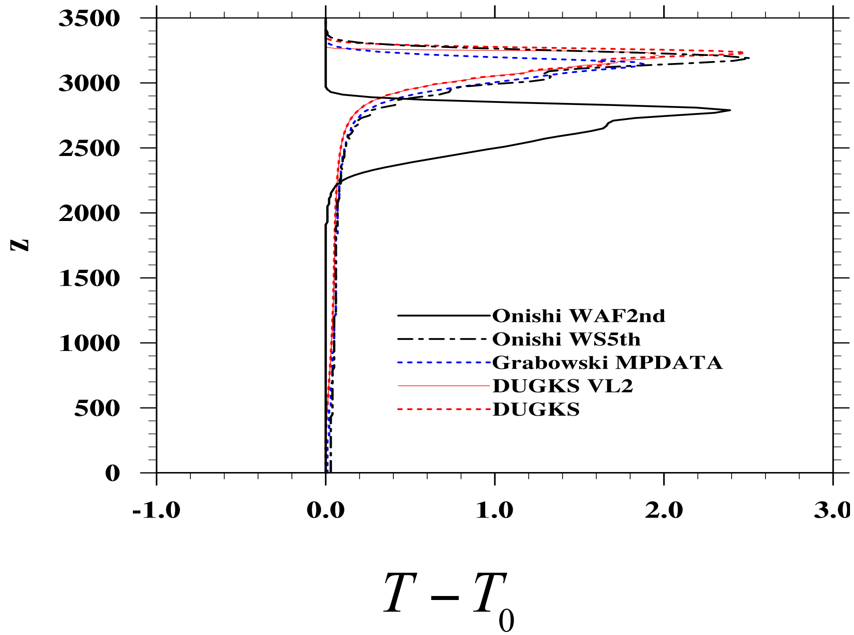





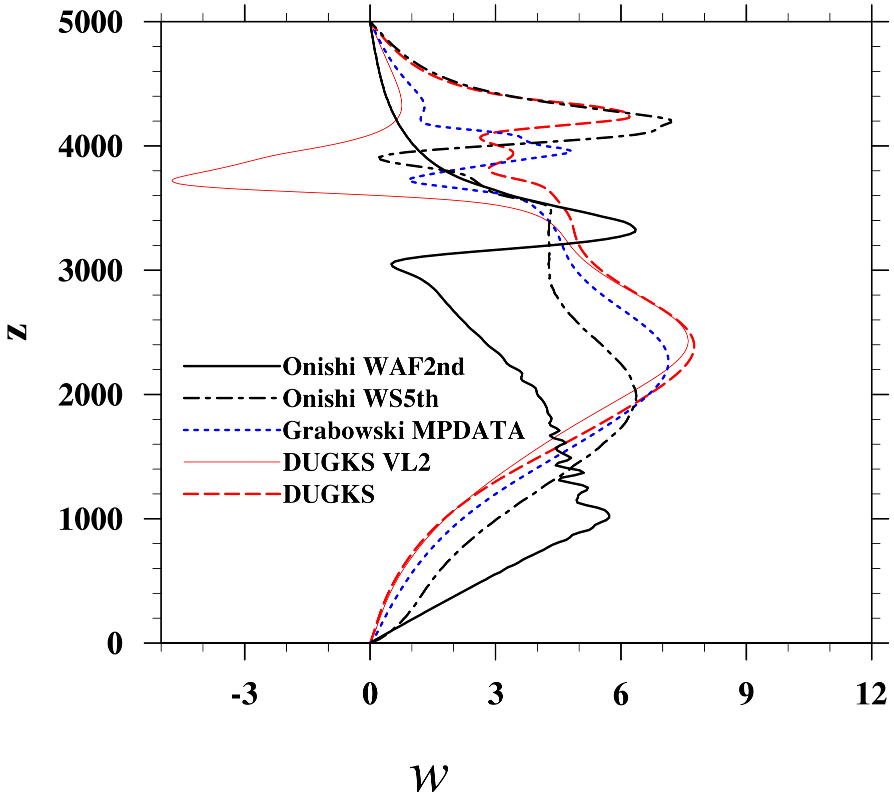
# Vertical profiles at 10 min

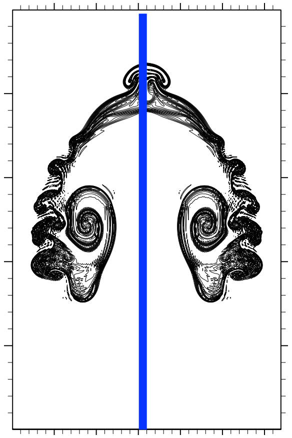


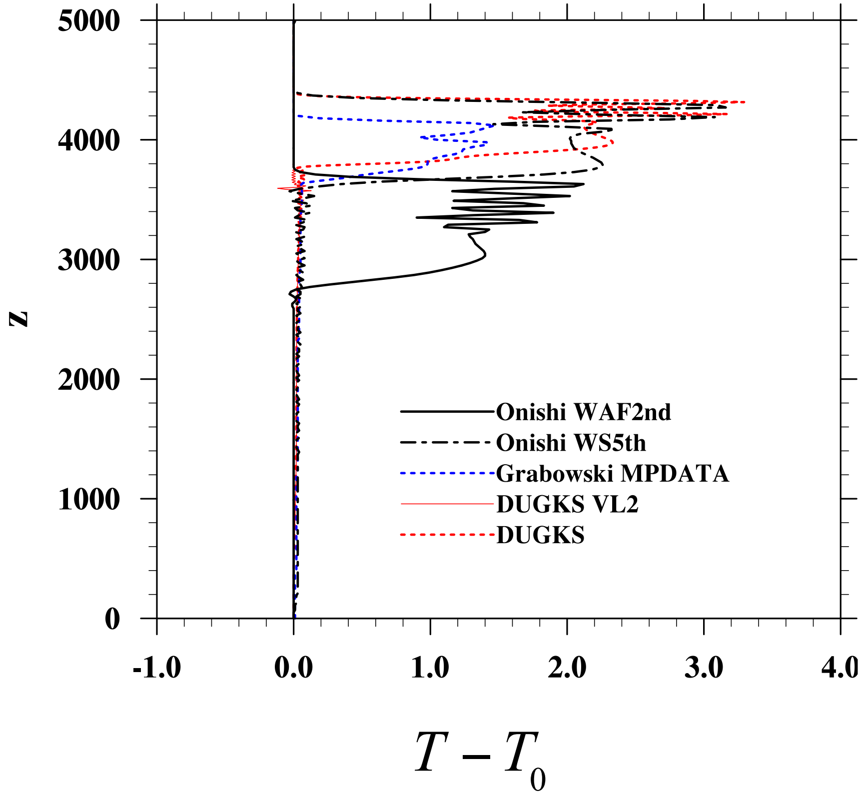





# Vertical profiles at 15 min





# Summary

Demonstrated the feasibility of using DUGKS for high Ra convection flows

- DUGKS has low numerical diffusivity and provides accurate solution for convection flow
- DUGKS code is stable even when the flow is not resolved
- When the flow is unresolved, local oscillations occur
- Numerical limiter help suppress oscillations

At later times, the solution could depend sensitively on the treatment of the advection term, details of the numerical limiter, grid resolution *etc*., or even how grids are set up relative to the center of the bubble

- How do we develop benchmark solutions at later times?

Potential benefits: fast scalable computation, low numerical dissipation, ….

Next steps

- Directional splitting may be tested
- Better slope / flux limiter scheme: MPDATA, WENO
- Atmospheric background density / temperature