MicroHH – An Overview

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Outline of the Talk

- Introduction to MicroHH
- Dynamical Core: Governing Equations
- Dynamical Core: Numerical Implementation
- Case Studies

An Overview of MicroHH

What is MicroHH ?

A CFD Setup for Simulation of Turbulent flows in periodic domains with focus on atmosphere

Stevens et al., MWR., 113, 2005
Heus et al., GMD, 3,2010)
Maronga et al., GMD,8, 2015)
(Van Heerwaarden et al, GMD, 10., 2017)

An Overview of MicroHH

Why MicroHH ?

- To come up with solver that is ready for massively parallel simulations
  - Performance, Scaling & Design
  - Fixing these problems often requires a substantial structural change to entire code
  - May require a new version implementation algorithm

- To take advantage modern trends of computing on Graphic Processing Units

- To support both DNS & LES on a common MPI-OMP-CUDA enabled platform with more than 10000 cores

- To cater to a wide range of applications ranging from Neutral Channel flows to Cloudy Atmospheric Boundary Layers in Large Domains

An Overview of MicroHH

How is MicroHH Designed?

View Dynamical Core

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

- **Dynamical core of MicroHH solves the conservation of Mass, Momentum and energy under the *Anelastic Approximation*.**

- ***1st Anelastic approximations:***

  The Buoyancy Force is a major component of vertical momentum equation.

  - **Motivated by geophysical flows for which the effects of stratification are important**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

- ***2nd Anelastic approximations:***

The characteristic vertical displacement, D, of an air parcel is comparable to the density scale height i.e. $D \sim H_\rho$

- **This removes the limitation of the Boussinesq approximation, which is valid only for flows whose vertical displacements are small compared to the density scale height**

- **Anelastic approximation subsumes the physics of Boussinesq approximation.**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

- ***3rd Anelastic approximations:***

The horizontal variations of the thermodynamic state variables at any height are small compared to the static value at that height, for example:

$$\theta'(x, y, z, t) \ll \theta_s(z),$$

$$\frac{\theta'(x, y, z, t)}{\theta_s(z)} = O(\epsilon) \ll 1.$$

- **This suggests that linearization of thermo-dynamics relations is valid in the anelastic approximation.**
- **Lipps & Hemler (1982) argue that**
- **Is it a constraint on the structure of the base-state atmosphere?**
- **Is it valid ONLYfor adiabatic flow?**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Conservation of Mass:

$$\frac{\partial \rho_0 u_i}{\partial x_i} = \rho_0 \frac{\partial u_i}{\partial x_i} + \rho_0 w H_\rho^{-1} = 0. \qquad (1)$$

Where the scale height for density H_ρ

$$H_\rho \equiv \left(\frac{1}{\rho_0} \frac{\mathrm{d}\rho_0}{\mathrm{d}z} \right)^{-1} \qquad (2)$$

$H_\rho \rightarrow \infty$ **then** (1) → $\frac{\partial u_i}{\partial x_i} = 0.$ (3)

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Thermodynamic Relations & Conservation of Momentum:

Some notations:

θ_v' **Perturbation of virtual potential temperature**

θ_{v0} **Reference virtual potential temperature**

p' **Perturbation Pressure**

ρ' **Perturbation density**

ρ_0 **Reference density**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

More notations & Relations :

θ **Dry Potential temperature**

θ_l **Liquid Water potential temperature**

$$\theta_l \approx \theta - \frac{L_v}{c_p\ \Pi} q_l$$

q_t **Total Specific Humidity**

q_v **Water Vapor Specific Humidity**

q_l **The Cloud Liquid Water Specific Humidity**

$$q_l = \max(0,\ q_t - q_s)$$

L_v **Latent Heat of Vaporization**

c_p **Specific Heat of dry air at constant pressure**

Π **Exner Function**

$$\Pi = \left(\frac{p}{p_{00}}\right)^{R_d/c_p}$$

q_s **Saturation specific humidity**

$$q_s = \frac{\epsilon\ e_s}{p - (1-\epsilon)\ e_s}$$

ϵ **Dry air and water vapour gas const. ratio** R_d/R_v

e_s **Saturation vapour pressure**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

More notations & Relations :

θ_{v} **Virtual Potential temperature**

$$\theta_{\mathrm{v}} \equiv \theta \left(1 - \left[1 - \frac{R_{\mathrm{v}}}{R_{\mathrm{d}}} \right] q_{\mathrm{t}} - \frac{R_{\mathrm{v}}}{R_{\mathrm{d}}} q_{\mathrm{l}} \right)$$

$\mathrm{d}p_0$ **Base Static Pressure**

$$\mathrm{d}p_0 = -\rho_0 g \, \mathrm{d}z$$

ρ_0 **Base Density**

$$\rho_0 = p_0 / (R_{\mathrm{d}} \, \Pi \, \theta_{\mathrm{v}0})$$

Integration with height results in

$$p_{0;k+1} = p_{0;k} \exp\left(\frac{-g(z_{k+1} - z_k)}{R_{\mathrm{d}} \, \Pi \, \theta_{\mathrm{v}0}} \right)$$

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Thermodynamic Relations & Conservation of Momentum:

$$\frac{\theta_v'}{\theta_{v0}} = \frac{p'}{\rho_0 g H_\rho} - \frac{\rho'}{\rho_0} \tag{4}$$

$$\frac{\partial u_i}{\partial t} = -\frac{1}{\rho_0}\frac{\partial \rho_0 u_i u_j}{\partial x_j} - \frac{\partial}{\partial x_i}\left(\frac{p'}{\rho_0}\right) + \delta_{i3} g \frac{\theta_v'}{\theta_{v0}} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + F_i, \tag{5}$$

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Thermodynamic Relations & Conservation of Momentum:

Under Boussinesq approximation (4-5) reduce to:

$$\frac{\theta_v'}{\theta_{v0}} = -\frac{\rho'}{\rho_0}, \tag{6}$$

$$\frac{\partial u_i}{\partial t} = -\frac{\partial u_i u_j}{\partial x_j} - \frac{1}{\rho_0}\frac{\partial p'}{\partial x_i} + \delta_{i3} g \frac{\theta_v'}{\theta_{v0}} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + F_i \tag{7}$$

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Pressure Equation

$$\frac{\partial}{\partial x_i}\left[\rho_0 \frac{\partial}{\partial x_i}\left(\frac{p'}{\rho_0}\right)\right] = \frac{\partial \rho_0 f(u_i)}{\partial x_i} \qquad (8)$$

Under Boussinesq approximation (8) reduce to:

$$\frac{\partial^2}{\partial x_i^2}\left(\frac{p'}{\rho_0}\right) = \frac{\partial f(u_i)}{\partial x_i} \qquad (9)$$

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Conservation of an Scalar

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\rho_0}\frac{\partial \rho_0 u_j \phi}{\partial x_j} + \kappa_\phi \frac{\partial^2 \phi}{\partial x_j^2} + S_\phi \qquad (10)$$

κ_ϕ **The Diffusivity**

S_ϕ **Source/Sink**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Conservation of Energy:

MicroHH supports different Energy Conservation Equations

For Dry Dynamics

$$\frac{\partial \theta}{\partial t} = -\frac{1}{\rho_0}\frac{\partial \rho_0 u_j \theta}{\partial x_j} + \kappa_\theta \frac{\partial^2 \theta}{\partial x_j^2} + \frac{\theta_0}{\rho_0 c_p T_0} Q \qquad (11)$$

For Wet Dynamics replace θ by θ_l **Liquid water potential temperature**

Dynamical Core: Governing Equations

Bannon, P.R, JASci., 53, 1996

Simplified Conservation of Momentum & Energy:

Using Buoyancy

$$b \equiv (g/\theta_{v0})\,\theta_v' \qquad (13)$$

Eqns. (6-7), (11) become

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p'}{\partial x_i} + \delta_{i3} b + \nu \frac{\partial^2 u_i}{\partial x_j^2} \qquad (14)$$

$$\frac{\partial b}{\partial t} + \frac{\partial b u_j}{\partial x_j} = \kappa_b \frac{\partial^2 b}{\partial x_j^2} + Q_b \qquad (15)$$

Dynamical Core: Governing Equations

For Slope Flows in periodic Domians with linear thermal stratification:

Fedorovich & Shapiro, 2009

$$\frac{\partial u}{\partial t} + \frac{\partial u_j u}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p'}{\partial x} + \sin(\alpha) b + \nu \frac{\partial^2 u}{\partial x_j^2} \qquad (16)$$

$$\frac{\partial w}{\partial t} + \frac{\partial u_j w}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p'}{\partial z} + \cos(\alpha) b + \nu \frac{\partial^2 w}{\partial x_j^2} \qquad (17)$$

$$\frac{\partial b}{\partial t} + \frac{\partial b u_j}{\partial x_j} = \kappa_b \frac{\partial^2 b}{\partial x_j^2} - (u \sin(\alpha) + w \cos(\alpha)) N^2 + Q_b \qquad (18)$$

Background stratificaton in units of buoyancy $N^2 \equiv (g/\theta_{v0})(d\theta_v/dz)_0$

Dynamical Core: Numerical Implementation

Few Relevant Comments on Grids:

- **Galilean Transformation is possible**
  - **One can apply a uniform translation velocity to the grid and thus let it move with flow.**
- **Governing Equations are invariant under the translation**
- **Has potential for larger time steps and can also increase accuracy**
- **Has a default equal order representation of advection, diffusion etc. but allows overriding as desired.**
- **Grids can be stretched in vertical dimension**
- **Grid Hieghts are w.r.t cell centers**

Time Integration

- **Prognostic Equations are solved using Runge-Kutta time integration schemes**
  - **Option One: A Three Stage Third Order RK scheme (Williamson, 1980)**
  - **OptionTwo: A Five Stage Fourth Order RK Scheme (Carpenter & Kennedy, 1994)**
    - **Generic Form:**

$$(\delta\phi)_n = f(\phi_n) + a_n(\delta\phi)_{n-1} \tag{16}$$

$$\phi_{n+1} = \phi_n + b_n \Delta t (\delta\phi)_n \tag{17}$$

Time Integration

- **For Three Stage Third Order RK scheme**

$$a_n = \left\{0, -\frac{5}{9}, -\frac{153}{128}\right\}$$
$$b_n = \left\{\frac{1}{3}, \frac{15}{16}, \frac{8}{15}\right\}. \qquad (19)$$

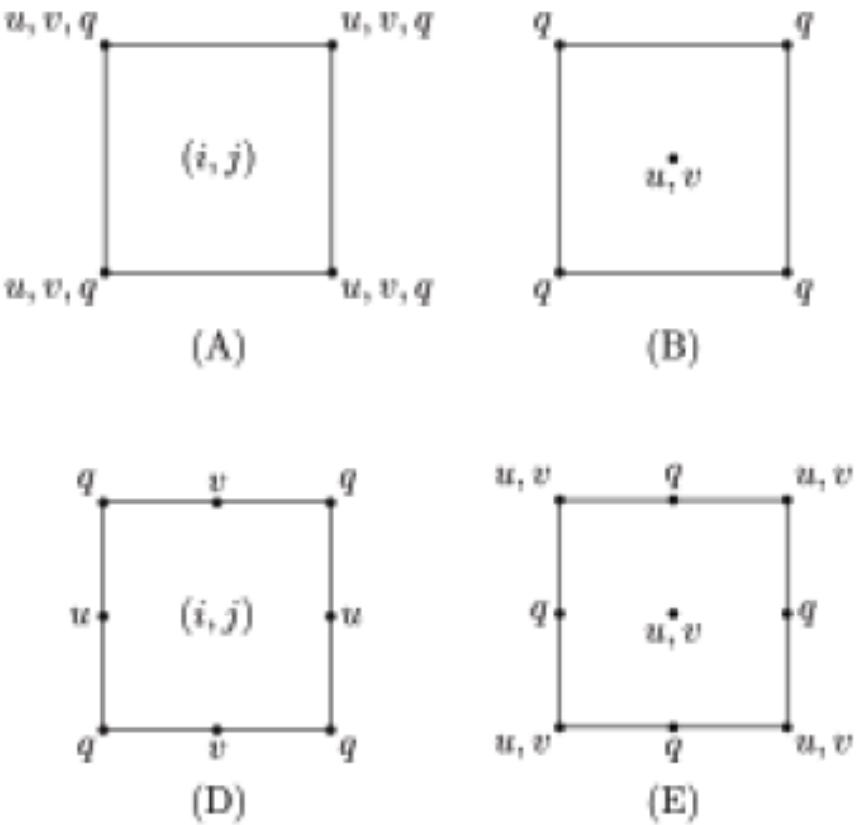
- **A Five Stage Fourth Order RK Scheme**

$$a_n = \left\{0, -\frac{567301805773}{1357537059087}, -\frac{2404267990393}{2016746695238}, -\frac{3550918686646}{2091501179385}, -\frac{1275806237668}{842570457699}\right\}$$

$$b_n = \left\{\frac{1432997174477}{9575080441755}, \frac{5161836677717}{13612068292357}, \frac{1720146321549}{2090206949498}, \frac{3134564353537}{4481467310338}, \frac{2277821191437}{14882151754819}\right\} \qquad (20)$$

Dynamical Core: Numerical Implementation

MicroHH is discretized on Staggered Arakawa C-grid



Arakawa A-grid

Arakawa B-grid

Arakawa C-grid

Arakawa D-grid

Arakawa E-grid

Building Blocks for Spatial Discretization Based on Finite Difference Method

(Morishini et al (1998), Vasilyev (2000)

2nd Order Interpolation Operators:

$$\phi_{i,j,k} \approx \overline{\phi}^{2x}_{i,j,k} \equiv \frac{\phi_{i-\frac{1}{2},j,k} + \phi_{i+\frac{1}{2},j,k}}{2}$$
$$\phi_{i,j,k} \approx \overline{\phi}^{2xL}_{i,j,k} \equiv \frac{\phi_{i-\frac{3}{2},j,k} + \phi_{i+\frac{3}{2},j,k}}{2} \qquad (21)$$

- **The Superscript indicates**
  - ✓ **The spatial order (2)**
  - ✓ **The Direction (x)**
  - ✓ **The extra qualifier (L) is taken when using wider stencil**

Building Blocks for Spatial Discretization Based on Finite Difference Method

The 2nd order scheme for Gradient Operators:

$$\left.\frac{\partial \phi}{\partial x}\right|_{i,j,k} \approx \delta^{2x}(\phi)_{i,j,k} \equiv \frac{\phi_{i+\frac{1}{2},j,k} - \phi_{i-\frac{1}{2},j,k}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}$$

$$\left.\frac{\partial \phi}{\partial x}\right|_{i,j,k} \approx \delta^{2xL}(\phi)_{i,j,k} \equiv \frac{\phi_{i+\frac{3}{2},j,k} - \phi_{i-\frac{3}{2},j,k}}{x_{i+\frac{3}{2}} - x_{i-\frac{3}{2}}} \qquad (22)$$

The 4th order scheme for Gradient Operators:

$$\phi_{i,j,k} \approx \overline{\phi}^{4x}_{i,j,k}$$

$$\equiv \frac{-\phi_{i-\frac{3}{2},j,k} + 9\phi_{i-\frac{1}{2},j,k} + 9\phi_{i+\frac{1}{2},j,k} - \phi_{i+\frac{3}{2},j,k}}{16} \qquad (23)$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

The Biased 4th order version for points near bottom boundary:

$$\phi_{i,j,k} \approx \overline{\phi}^{4zb}_{i,j,k} \equiv \frac{5\phi_{i,j,k-\frac{1}{2}} + 15\phi_{i,j,k+\frac{1}{2}} - 5\phi_{i,j,k+\frac{3}{2}} + \phi_{i,j,k+\frac{5}{2}}}{16} \tag{24}$$

The centered and Baised 4th order scheme for Gradient Operators:

$$\left.\frac{\partial \phi}{\partial x}\right|_{i,j,k} \approx \delta^{4x}(\phi)_{i,j,k} \equiv \frac{\phi_{i-\frac{3}{2},j,k} - 27\phi_{i-\frac{1}{2},j,k} + 27\phi_{i+\frac{1}{2},j,k} - \phi_{i+\frac{3}{2},j,k}}{x_{i-\frac{3}{2}} - 27x_{i-\frac{1}{2}} + 27x_{i+\frac{1}{2}} - x_{i+\frac{3}{2}}}, \tag{25}$$

and

$$\left.\frac{\partial \phi}{\partial z}\right|_{i,j,k} \approx \delta^{4zb}(\phi)_{i,j,k} \equiv \frac{-23\phi_{i,j,k-\frac{1}{2}} + 21\phi_{i,j,k+\frac{1}{2}} + 3\phi_{i,j,k+\frac{3}{2}} - \phi_{i,j,k+\frac{5}{2}}}{-23z_{k-\frac{1}{2}} + 21z_{k+\frac{1}{2}} + 3z_{k+\frac{3}{2}} - z_{k+\frac{5}{2}}} \tag{26}$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

2nd Order Advection& Velocity Interpolation:

$$\left.\frac{\partial u\phi}{\partial x}\right|_{i,j,k} + \left.\frac{\partial v\phi}{\partial y}\right|_{i,j,k} \approx \delta^{2x}\left(u\overline{\phi}^{2x}\right)_{i,j,k} + \delta^{2y}\left(v\overline{\phi}^{2y}\right)_{i,j,k}$$

$$= \frac{u_{i+\frac{1}{2},j,k}\overline{\phi}^{2x}_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}\overline{\phi}^{2x}_{i-\frac{1}{2},j,k}}{} + \frac{v_{i,j+\frac{1}{2},k}\overline{\phi}^{2y}_{i,j+\frac{1}{2},k} - v_{i,j-\frac{1}{2},k}\overline{\phi}^{2y}_{i,j-\frac{1}{2},k}}{y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}} \tag{27}$$

$$\left.\frac{\partial vu}{\partial x}\right|_{i,j,k} = \delta^{2x}\left(\overline{v}^{2y}\overline{u}^{2x}\right)_{i,j,k}$$

$$= \frac{\overline{v}^{2y}_{i+\frac{1}{2},j,k}\overline{u}^{2x}_{i+\frac{1}{2},j,k} - \overline{v}^{2y}_{i-\frac{1}{2},j,k}\overline{u}^{2x}_{i-\frac{1}{2},j,k}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}. \tag{28}$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

4th Order Advection & Velocity Interpolation :

$$\left.\frac{\partial u\phi}{\partial x}\right|_{i,j,k} \approx \delta^{4x}\left(u\overline{\phi}^{4x}\right)_{i,j,k}$$
$$= \left(u_{i-\frac{3}{2},j,k}\overline{\phi}^{4x}_{i-\frac{3}{2},j,k} - 27u_{i-\frac{1}{2},j,k}\overline{\phi}^{4x}_{i-\frac{1}{2},j,k}\right.$$
$$\left.+27u_{i+\frac{1}{2},j,k}\overline{\phi}^{4x}_{i+\frac{1}{2},j,k} - u_{i+\frac{3}{2},j,k}\overline{\phi}^{4x}_{i+\frac{3}{2},j,k}\right) \Big/$$
$$\left(x_{i-\frac{3}{2}} - 27x_{i-\frac{1}{2}} + 27x_{i+\frac{1}{2}} - x_{i+\frac{3}{2}}\right). \tag{29}$$

$$\left.\frac{\partial vu}{\partial x}\right|_{i,j,k} \approx \frac{9}{8}\delta^{2x}\left(\overline{v}^{4y}\overline{u}^{2x}\right)_{i,j,k}$$
$$- \frac{1}{8}\delta^{2xL}\left(\overline{v}^{4y}\overline{u}^{2xL}\right)_{i,j,k} \tag{30}$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

2nd & 4th Order Scheme for Diffusion Operator in x-direction

$$\kappa_\phi \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j,k} \approx \kappa_\phi \delta^{2x}\left(\delta^{2x}(\phi)\right)_{i,j,k}$$
$$\kappa_\phi \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j,k} \approx \kappa_\phi \delta^{4x}\left(\delta^{4x}(\phi)\right)_{i,j,k} \qquad (31)$$

2nd & 4th Order Scheme for Diffusion Operator on equidistant grid

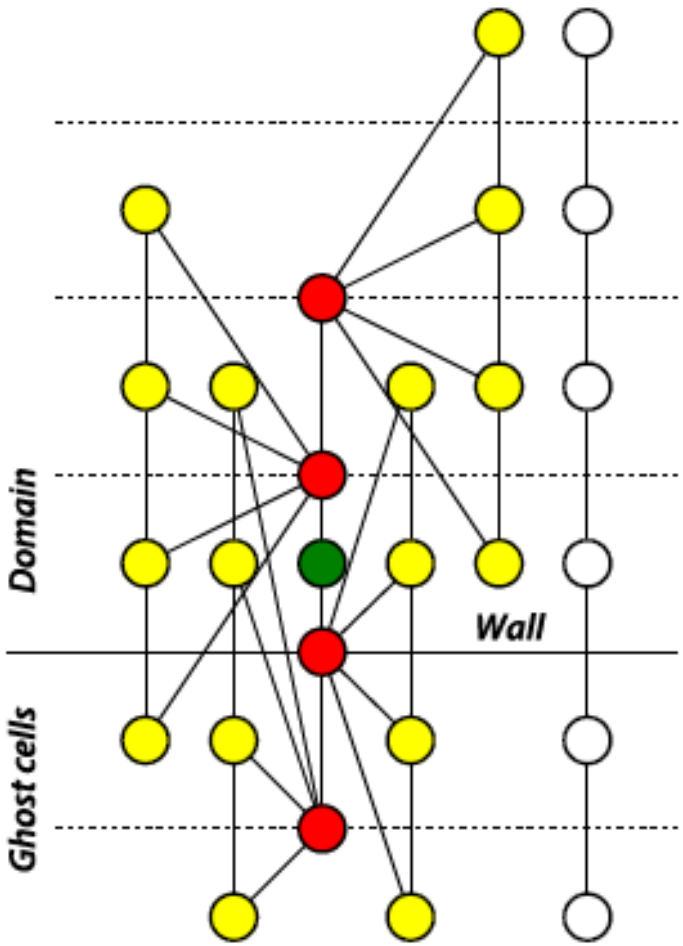
$$\kappa_\phi \delta^{2x}\left(\delta^{2x}(\phi)\right)_{i,j,k} = \kappa_\phi \frac{\phi_{i-1,j,k} - 2\phi_{i,j,k} + \phi_{i+1,j,k}}{(\Delta x)^2} \qquad (32)$$

$$\kappa_\phi \delta^{4x}\left(\delta^{4x}(\phi)\right)_{i,j,k}$$
$$= \frac{\kappa_\phi}{576(\Delta x)^2}\left(\phi_{i-3,j,k} - 54\phi_{i-2,j,k} + 783\phi_{i-1,j,k}\right. \qquad (33)$$
$$\left. -1460\phi_{i,j,k} + 783\phi_{i+1,j,k} - 54\phi_{i+2,j,k} + \phi_{i+3,j,k}\right)$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

Spl. Care near boundary for 4th Order Scheme for Diffusion using Seven-Point Stencil

Figure: Schematic of the diffusion discretization near the wall. The *GREEN* node is the evaluation point at the center of the first cell above the wall, the *RED* nodes are the stencil of the divergence operator, and *YELLOW* nodes show the stencils of the four gradient operators over which the divergence is evaluated. *WHITE* nodes indicate the extent of the stencil.



Building Blocks for Spatial Discretization Based on Finite Difference Method

Solution Methodology : Fractional Step Method of Chorin et al 1995

Step1) Calculation of Intermediate Velocity

$$u_i^* \Big|_{i,j,k}^{t+1} = u_i \Big|_{i,j,k}^{t} + \Delta t \; f_i \Big|_{i,j,k}^{t} \qquad (34)$$

Step2.1) Velocity Correction *(requires pressures)*

$$u_i \Big|_{i,j,k}^{t+1} = u_i^* \Big|_{i,j,k}^{t+1} - \Delta t \, \delta^{nx_i} \left(\frac{p}{\rho_0} \right) \Bigg|_{i,j,k}^{t} . \qquad (35)$$

Step2.2) Solve *Pressure Poisson Equation derived from (35)*

$$\frac{\delta^{nx_i} \left(\rho_0 u_i^* \right) \Big|_{i,j,k}^{t+1}}{\Delta t} = \delta^{nx_i} \left[\rho_0 \delta^{nx_i} \left(\frac{p}{\rho_0} \right) \right] \Bigg|_{i,j,k}^{t} . \qquad (36)$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

Solution Methodology : Fractional Step Method of Chorin et al 1995

Step2.3) Taking Advantage of Periodicity of fields in x, y direction use Fourier Transforms on (36) to get:

$$\widehat{\psi}_{l,m,k} = -k_{*n}^2 \widehat{\pi}_{l,m,k} - l_{*n}^2 \widehat{\pi}_{l,m,k} + \delta^{nz}\left[\rho_0 \delta^{nz}\left(\widehat{\pi}\right)\right]_{l,m,k}, \tag{37}$$

Where the l.h.s of (36) is denoted by: ψ (38)
and p/ρ_0 **by:** π

Further the modified wavenumbers are denoted by:

$$-k_{*2}^2 \equiv 2\frac{\cos(k\Delta x)}{(\Delta x)^2} - \frac{2}{(\Delta x)^2} \qquad -k_{*4}^2 \equiv 2\frac{\cos(3k\Delta x) - 54\cos(2k\Delta x) + 783\cos(k\Delta x)}{576(\Delta x)^2} - \frac{1460}{576(\Delta x)^2}, \tag{39}$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

Comments on Boundary Conditions:

- **Lateral Boundaries are Periodic**
- **ROBIN TYPE Bottom and Top Boundaries Conditions**

$$a\phi_s + b\left.\frac{\partial \phi}{\partial z}\right|_s = c \qquad (40)$$

Where a, b and c are constants.

- **BC is Dirichlet when a=1, b= 0**
- **BC is Neumann when a=0, b=1**
- **BC is Mixed type when a, b ≠ 0**

Building Blocks for Spatial Discretization Based on Finite Difference Method

Comments on Boundary Conditions:

- ***<u>Ghost Cells</u>*** **are used in order to avoid the BAISED SCHEMES for Interpolation or gradient operators near the walls.**

Ghost Cells for Dirichlet BC:

$$\phi_{-\frac{1}{2}} = 2c - \phi_{\frac{1}{2}} \tag{41}$$

Ghost Cells for Neumann BC:

$$\phi_{-\frac{1}{2}} = -c\left(-z_{-\frac{1}{2}} + z_{\frac{1}{2}}\right) + \phi_{\frac{1}{2}} \tag{42}$$

Building Blocks for Spatial Discretization Based on Finite Difference Method

Comments on Boundary Conditions:

- ***Ghost Cells*** **are used in** ***FOURTH*** **order to avoid the BAISED SCHEMES for Interpolation or gradient operators near the walls.**

Ghost Cells for Dirichlet BC:

$$\phi_{-\frac{1}{2}} = \frac{8c - 6\phi_{\frac{1}{2}} + \phi_{\frac{3}{2}}}{3} \qquad (43)$$

$$\phi_{-\frac{3}{2}} = 8c - 6\phi_{\frac{1}{2}} + \phi_{\frac{3}{2}},$$

Ghost Cells for Neumann BC:

$$\phi_{-\frac{1}{2}} = -c\frac{z_{-\frac{3}{2}} - 27z_{-\frac{1}{2}} + 27z_{\frac{1}{2}} - z_{\frac{3}{2}}}{24} + \phi_{\frac{1}{2}}, \qquad (44)$$

$$\phi_{-\frac{3}{2}} = -3c\frac{z_{-\frac{3}{2}} - 27z_{-\frac{1}{2}} + 27z_{\frac{1}{2}} - z_{\frac{3}{2}}}{24} + \phi_{\frac{3}{2}}$$

- **Very Brief Detail on Parametrization (LES) in MicroHH**

  - **Monin-Obukhov surface Model**
    - **Constrained to rough surfaces and high Reynolds Numbers, which is typical for atmospheric flows**
    - **Computes surface fluxes of horizontal momentum components and scalars using Monin-Obukhov Similarity Theory (Wyngaard, 2010)**

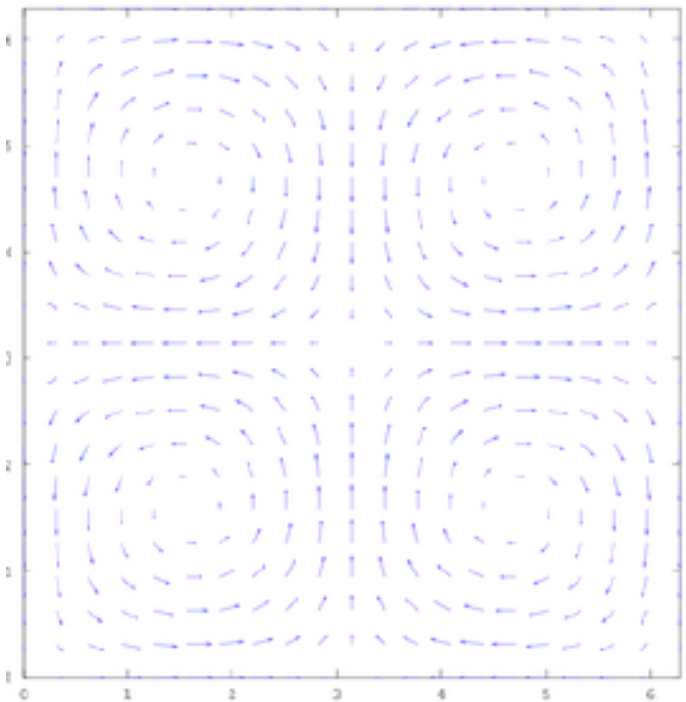
  - **(Non-Dynamic) Smagorinksy-Lilly Subgrid Diffusion**

  - **Warm 2-moment Bulk Microphysics**

Validation of Dynamical Core - 1

Case A: Taylor Green Vortex

- **2-Dimensional Unsteady Flow of Decaying Vortex with Exact Solution**



$$u(x,z,t) = \sin(2\pi x)\cos(\pi z)\, f(t),$$
$$w(x,z,t) = \cos(2\pi x)\sin(\pi z)\, f(t),$$
$$p(x,z,t) = \frac{1}{4}\left(\sin(4\pi x) + \sin(4\pi z)\right) f(t)^2,$$

where $f(t) = 8\pi^2 \nu t$.

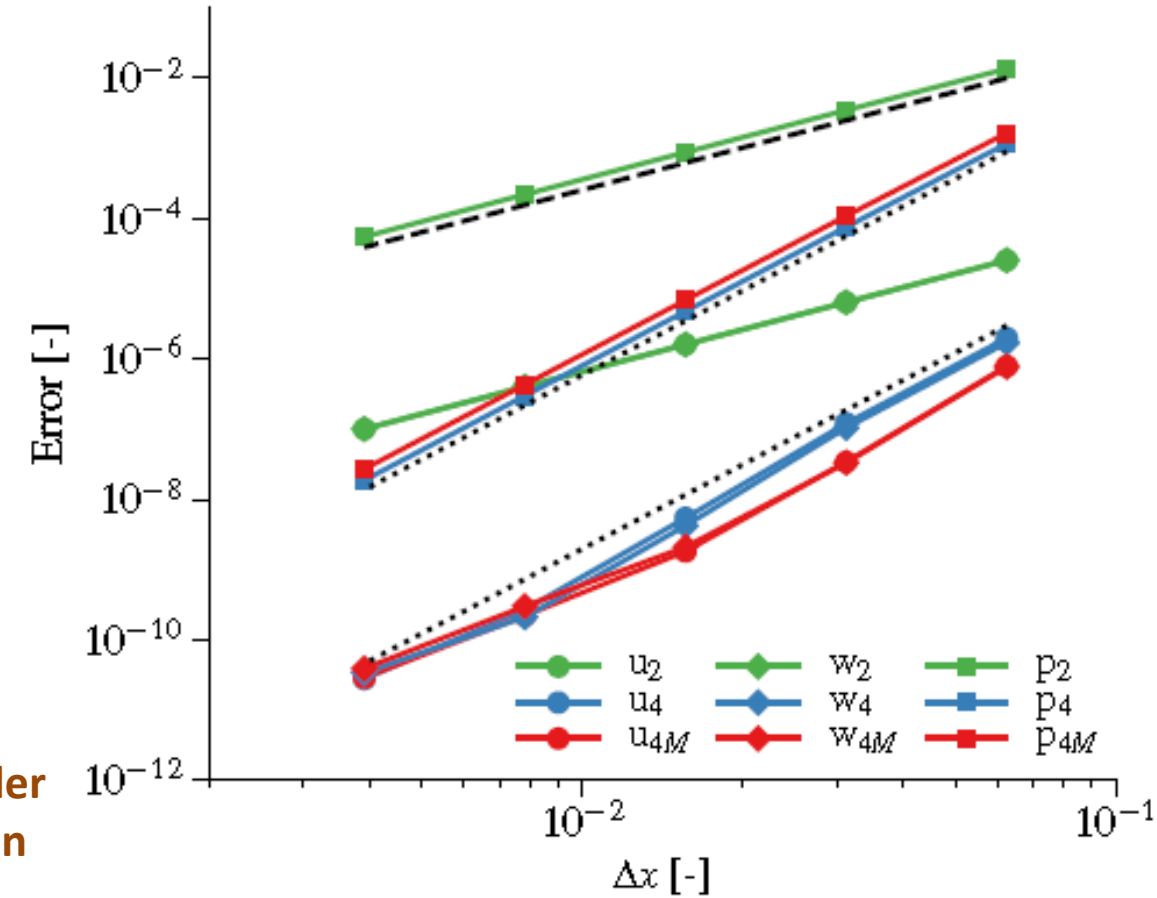
Use analytical form at t=0 and run for one vortex rotation t=1 and compare the result against the analytical solution for

$$\nu = (800\pi^2)^{-1}$$

Error:

$$\sum \Delta x \, \Delta z \left| \phi_{i,k} - \phi_{\mathrm{ref},i,k}, \right|$$

All variables converge to the order of the scheme but for 4th order on fine grids.



Convergence of Spatial Discretization Error in 2D Taylor Green Vortex

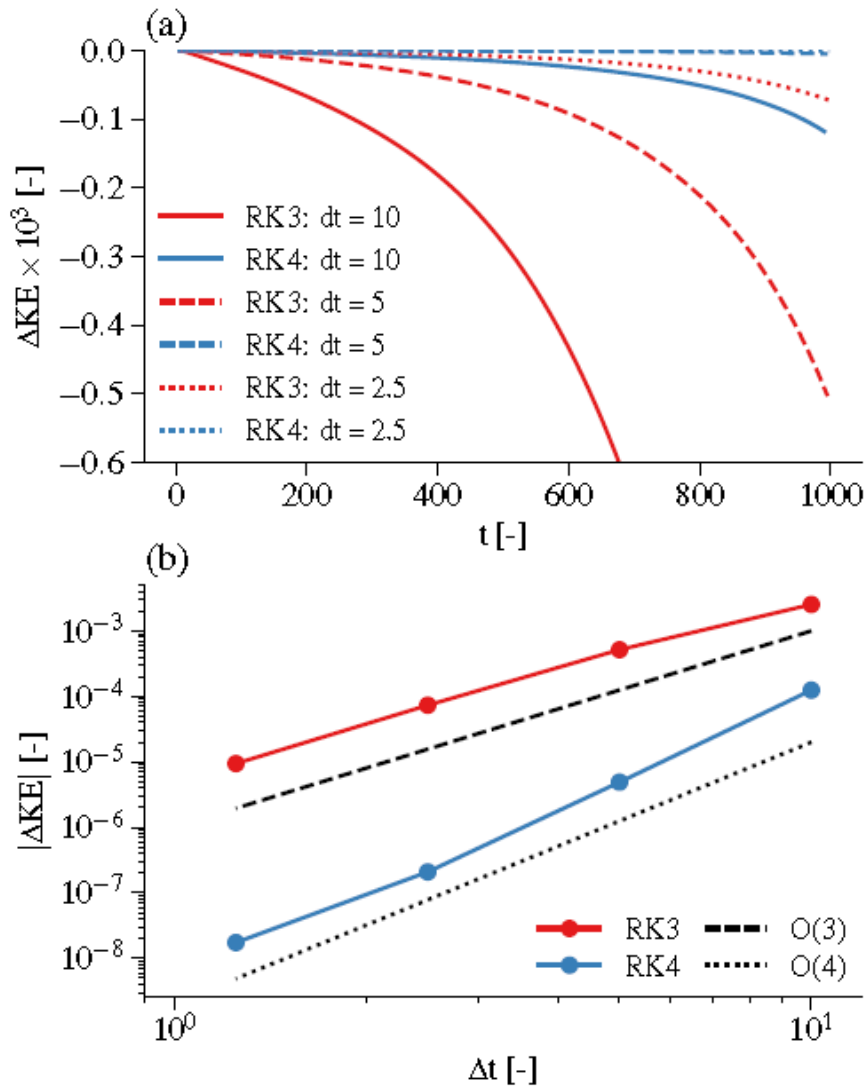
- Subscript 2 indicates the 2nd order scheme
- Subscript 4 the most accurate 4th order scheme
- Dashed Black Line is the reference for 2nd order convergence
- The Dotted black lines indicate the 4th order convergence

Validation of Dynamical Core - 2

Case B: Kinetic Energy Conservation and Time Accuracy

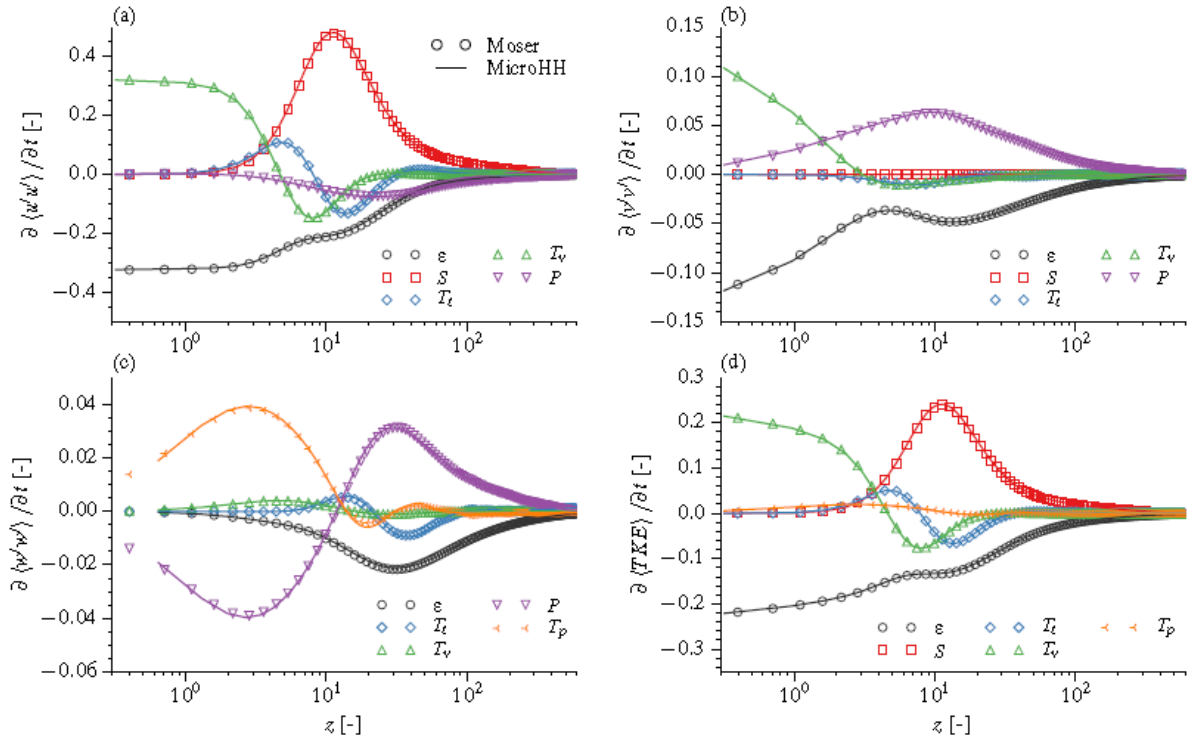
Time evolution of the kinetic energy change Δ KE during 1000 time units of random noise advection for the RK3 and RK4 time integration schemes with three different time steps (a).

Kinetic energy change convergence of the temporal discretization for the RK3 and RK4 schemes (b).



Validation of Dynamical Core - 3

Case C: Turbulent Channel Flow (768 x 384 x 256)



Budgets of Variances and Turbulence KE compared with against Moser et al (1999)'s reference data at Re_τ=590 . Height Z , variance and TKE budget are normalized with u_τ / ν and ν / u_τ^4 respectively.

(Van Heerwaarden et al, GMD, 10., 2017

Validation of Atmospheric LES - 1

Case D: Dry Convective Boundary Layer with Strong Inversion

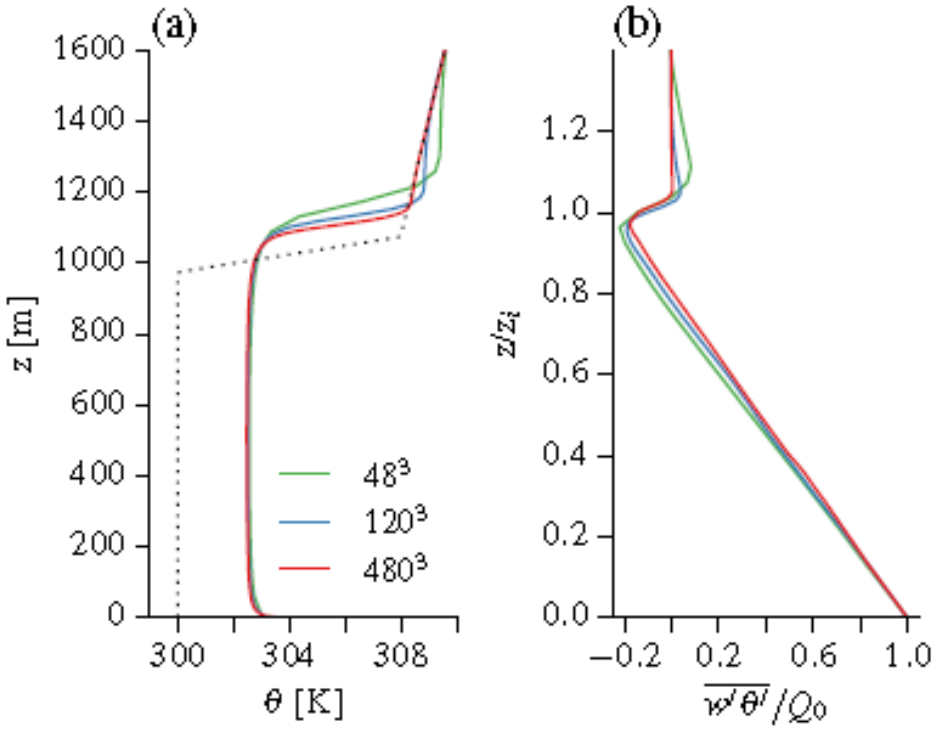
Problem Description:

- A dry CBL that grows into a linearly stratified atmosphere with a very strong capping inversion.
- The system is heated from the bottom by applying a constant Kinetic heat flux of 0.24 Km/s
- The domain size is 5120 x 5120 x 2048 m
- Gravity damping has been applied in the top 25% of the domain.
- Simulation is run for 3 hrs. with three different spatial resolutions.

Validation of Atmospheric LES - 1

Case D: Dry Convective Boundary Layer with Strong Inversion

- A well mixed layer with an overlaying capping inversion is seen
- Linear heat flux with –ve flux values in the entrainment zone
- Resolving BL poses challenge
- Strong inversion at coarse level leads to unphysical overshoot of potential temperature flux above BL top



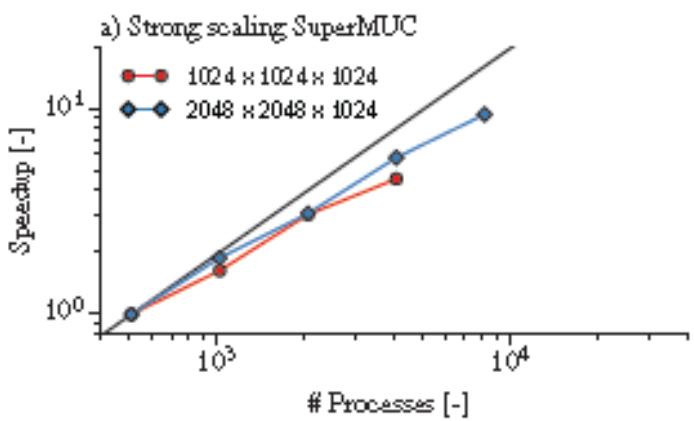
(Van Heerwaarden et al, GMD, 10., 2017

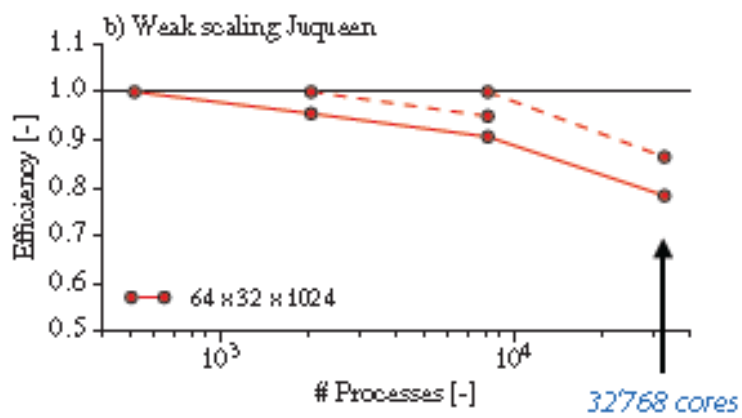
Vertical Profiles of horizontally averaged potential temperature (a) and normalized Kinematic heat flux. The boundary depth Zi is the location of the maximum vertical gradient in the potential temperature profile in (a)

(Van Heerwaarden et al, GMD, 10., 2017

Performance, efficiency and scaling

- Performance: well optimized code
  - 2.5 - 5.5 times faster than DALES / UCLA-LES, similar performance to PALM (for dry CBL)
  - GPU implementation: 30x speedup over single core, ~64 cores needed to match performance GPU
- Memory efficient: low storage Runge-Kutta schemes
  - Requires 2 x 3D field per prognostic variable + pressure (+ viscosity) + 4 x temporary field
  - Important for GPU's, where memory is limited
- Scales well over 2 orders of magnitude increase in cores
  - DNS of dry CBL:





Validation of Atmospheric LES - 2

Barbados Oceanographic and Meteorological Experiment
(The BOMEX Shallow Cumulus case)

(Van Heerwaarden et al, GMD, 10., 2017

- Produces non-precepitating shallow cumulus
- It has large-scale cooling applied that represents radiation, as well as large scale drying to allow the atmosphere to relax to a steady state.
- In addition a large scale vertical velocity is applied over a certain height range to reproduce the approximate synoptic conditions
- Simulation is run for 6 hrs
- All results compared well within 1 standard deviation of those described in Siebesma et al 2003.

Validation of Atmospheric LES - 2

(Van Heerwaarden et al, GMD, 10., 2017

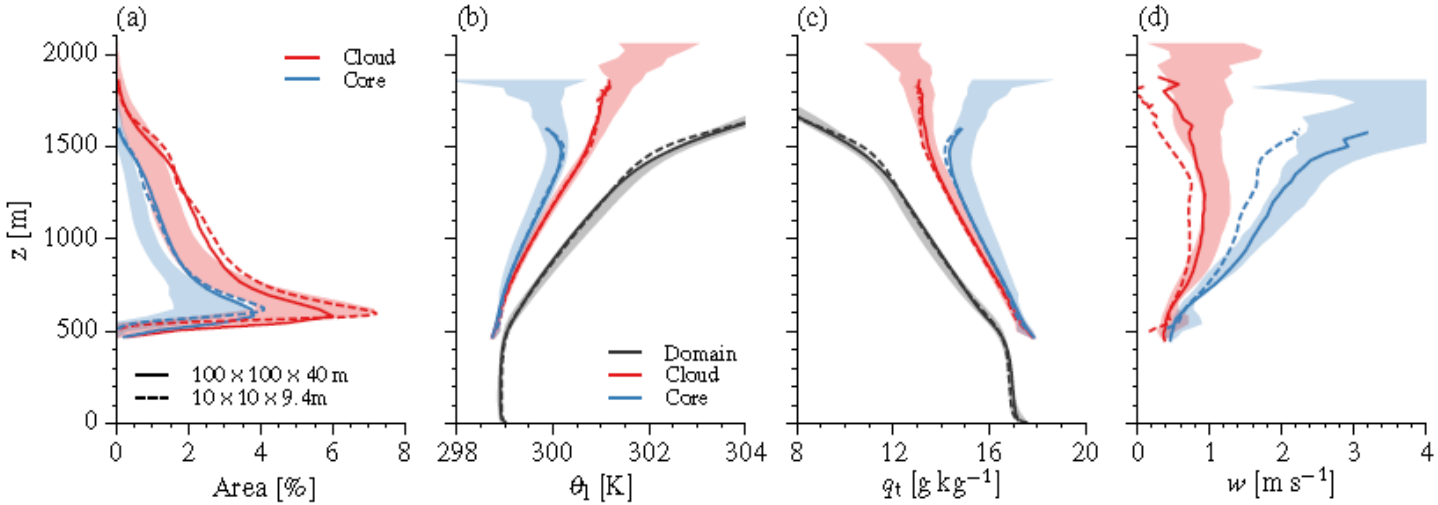


Figure 10. BOMEX LES intercomparison (S03). Shown are the domain mean, and conditionally sampled cloud ($q_l > 0$) and cloud core ($q_l > 0$ and $b - \langle b \rangle > 0$) vertical profiles of (**a**) area coverage of cloud and cloud core, (**b**) liquid water potential temperature, (**c**) total specific humidity, and (**d**) vertical velocity. The results are averaged over $t = 18\,000$–$21\,600$ s. The shaded area denotes the mean ± 1 standard deviation of the participating models from S03; the solid and dashed lines the results from MicroHH, using the original (solid) and a higher-resolution (dashed) setup.