A high order finite difference solver for massively parallel simulations of stably stratified turbulent channel flows

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Abstract

Investigation of stably stratified turbulent flows in the atmosphere is challenging owing to its nonstationarity and heterogeneity, especially in very stable conditions. In recent years, numerical simulation is becoming a powerful tool to complement the understanding of fundamental characteristics of strongly stratified flows. Owing to its highly accurate representation of small-scale turbulence structures, the direct numerical simulation (DNS) is shown to be the most effective numerical approach for strongly stratified flows. However, due to the limitation of the traditional parallel strategy, the existing DNS studies on stratified channel flows are limited to relatively low Reynolds numbers. In order to make the DNS studies more relevant to the atmospheric boundary layer flows, in this paper, a high-order finite-difference DNS solver is developed for simulating stably stratified turbulent channel flows at relatively high Reynolds numbers. Utilizing the advanced two dimensional domain decomposition technique, the DNS solver is shown to be competent for petascale simulations with excellent scalability tested up to 32768 CPU cores. Using this newly developed solver, two stably stratified open-channel simulations are conducted with the highest Reynolds number being approximately 10^5 . The fundamental characteristics of strongly stratified turbulent flows, e.g., spatio-temporal variation of global intermittency, are compared with those previously reported at relatively low Reynolds numbers, and their similarities and discrepancies are also discussed. In addition, the DNS-based Monin-Obukhov similarity relationships are compared with those proposed based on observational data to evaluate their relevance to atmospheric flows. The source code and the simulation results are available at <http://sites.google.com/site/scdnscode/>

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1. Introduction

In the nocturnal atmospheric boundary layer (ABL), the surface is cooled and the turbulence is typically stably stratified. For weakly stable conditions, the turbulence structures are commonly stationary and horizontally homogeneous, and they are relatively well described by the classic ABL theories, e.g., see the textbooks [1, 2, 3, 4]. However, in very stable conditions, turbulence transport and mixing are significantly modulated by buoyancy, resulting in strongly heterogeneous and nonstationary turbulence activities, e.g., gravity waves, intermittent turbulence. Although numerous studies have been conducted to investigate the behaviors of the very stable ABL, its fundamental characteristics are still far from fully understood (please refer to Mahrt [5] for a review of current challenges in the very stable ABL). From a practical standpoint, investigation of stably stratified flows is related to various industrial, environmental, and geophysical applications, e.g., wind energy estimation [6, 7], transport of pollutants in the ABL [8, 9, 10], mixing parameterization for numerical weather prediction models [11].

In recent years, numerical simulation is becoming a powerful tool to complement the understanding of the underlying dynamics and physics of the very stable ABL. The large-eddy simulation (LES) is one of the most efficient computational techniques for high Reynolds number turbulent flow simulations. However, its applicability for strongly stratified flow simulations remains an unsettled issue [12]. Furthermore, it is well-known in the literature that the LES-based flow characteristics are strongly dependent on the employed subgrid-scale (SGS) model, spatial resolution, filter type, etc. To circumvent these ad-hoc numerical influences, a viable alternative, i.e., the direct numerical simulation (DNS) approach, can be utilized. In this approach, the Navier-Stokes (NS) equations are solved without any averaging, any filtering, or any other approximations for turbulence. The true benefit of using the DNS approach, lies in its ability to capture the small-scale turbulence structure in strongly stratified conditions. In recent years, a number of DNS studies have been conducted to investigate the fundamental characteristics of strongly stratified turbulent channel flows. Research topics include, but not limited to, criteria for turbulence decaying [12, 13, 14], impact of stratification on turbulence structures [15, 16, 17, 18], spatio-temporal characteristics

30 of intermittent turbulence [19, 20, 21, 22], similarity theories [18, 21, 23, 24].

Despite the benefits afforded by DNS for analyses of very stably stratified flows, the Reynolds number (Re) in DNS studies is quite limited due to the exorbitant computational cost. To the best of the author’s knowledge, so far, the highest Re reported in DNS of stably stratified channel flows is on the order of 10^4 [12, 17, 18, 21, 23, 24], significantly lower than
 35 the typical Re in the ABL (10^7 or more). A critical question is: Is the low- Re DNS-based results relevant to the atmospheric flows? According to the Re -similarity theory in Townsend [25], the low- Re DNS simulations can reproduce the atmospheric flow conditions as long as the Re is high enough. Recent DNS studies have found encouraging indications of the Re -similarity theory by comparing the DNS-based and observational-based similarity
 40 relationships [21, 23, 24]. However, due to the limitation of Re , the range of stabilities is relatively short in those DNS studies. For example, the highest stability parameter (z/Λ with z being the height and Λ being the local Obukhov length) reported in van de Wiel et al. [23], and He and Basu [24] is approximately 5, much lower than the typical values observed in the very stable ABL (z/Λ on the order of 10s, e.g., see Sorbjan and Grachev [26]). In
 45 order to probe the very stably stratified turbulent flows using the DNS-based results, there is a need to push Re to a higher level (10^5 or more). Fortunately, with the tremendous advance in computational techniques, such large-scale DNS simulations can be performed using the petascale computer system (systems capable of performing 10^{15} or more operations per second). In terms of accuracy, the spectral method is considered to be the most efficient
 50 option for DNS [27, 28]. However, the ability to handle complicated geometric boundary [29], e.g., complex topography, makes the finite-difference DNS approach a competitive option. It is noted that finite-difference DNS of stably stratified channel flows at petascale raises a number of issues.

- Fractional time-step method [30, 31] has found widespread usage in finite-difference
 55 DNS of channel flows. In order to eliminate the numerical viscous stability restriction, the semi-implicit scheme, i.e., explicit treatment for convective terms and implicit treatment for viscous terms, is a favorable choice for time advancement. The viscous stability restriction can be quite severe, especially in high Re simulations where dense near-wall grids are used, and in strongly stratified flows where drastically nonstationary and bursting conditions are present, e.g., wave-motions, intermittent turbulence.
 60 For the second order spatial schemes, the resulting discretization equations can be

efficiently solved using the factorization approximation [31]; however, the extension of factorization for higher order of spatial accuracy is cumbersome (see detailed discussion in Section 2). In recent years, a few high-order finite-difference DNS solvers have been developed for simulating turbulent channel flows [21, 32, 33]; however, all of them used an explicit time-advancement scheme. In order to enhance the numerical stability (decrease the computational costs), there is a need to develop a high order finite-difference DNS solver using semi-implicit scheme for simulating strongly stratified flows at high Re .

- At present, petascale computer systems commonly have more than 10^5 CPU cores and several of them have more than 10^6 cores [34]. However, the traditional parallel simulations, which utilize a 1D domain decomposition technique, significantly restrict the maximal number of CPU cores that a simulation can use. For example, in Laizet and Vassilicos [35], a five billion grids DNS simulation took more than 47 days using 1024 cores. Obviously, it is hard to conduct productive scientific investigation at this rate. In order to circumvent this limitation, 2D domain decomposition was recently adopted in a handful of DNS solvers to simulate neutrally stratified channel flows [32, 36] using more than 10^5 CPU cores. However, for stably stratified channel flows, no such massively parallel solver was previously reported.

In summary, the motivation of this study is to develop a high-order finite-difference DNS solver for simulating strongly stratified turbulent channel flows at relatively high Re . To be more specific, in this work, a semi-implicit scheme is utilized for time-advancement, and the spatial derivatives are discretized using the fourth-order central differential scheme in the horizontal direction and the second-order central differential scheme in the vertical (wall-normal) direction. The resulting discretization equations, including the momentum, temperature, and pressure equations, are then directly solved using the Fourier analysis approach. The 2D domain decomposition technique is utilized for parallel communication, and the scalability of the newly developed DNS solver is tested with up to 32768 CPU cores. The DNS solver is verified using the benchmark data in Moser et al. [37], and García-Villalba and del Álamo [17] for neutrally and stably stratified channel flows. Moreover, two stably stratified open-channel simulations are conducted and analyzed with the highest Reynolds number being approximately 10^5 . We would like to highlight that the current DNS solver

uses a non-slip boundary condition at the bottom wall to mimic the sheared boundary layer flows, which is different from the massively parallel DNS solvers for isotropic stratified
95 turbulent flows, such as those reported in Rosenberg et al. [38], and de Bruyn Kops [39], to name a few.

The structure of this paper is as follows: in Section 2, we introduce the details of numerical method and summarize the computational configurations. The simulated profiles of mean flows and turbulence statistics are shown in Section 3. In this section, we also discuss
100 the spatio-temporal characteristics of strongly stratified flows. Moreover, the simulated similarity relationships are compared with the observational-based ones to evaluate the relevance of the DNS-based results. Conclusion and future directions are given in Section 4. Finally, the verification of the newly developed DNS solver is presented in the Appendix.

2. Method

105 2.1. Governing equations

Under the Boussinesq approximation, the governing Navier-Stokes and the temperature equations for incompressible flows are presented in Equations 1–3. The governing equations are normalized by h and u_τ , where h is the channel height, and $u_\tau = \sqrt{\tau_w/\rho_0}$ is the friction velocity with ρ_0 being the reference density and τ_w being the shear stress at walls. The
110 friction Reynolds number and Richardson number are defined as $Re_\tau = u_\tau h/\nu$ and $Ri_\tau = (\theta_{top} - \theta_{bot})gh/\theta_{top}u_\tau^2$, respectively. Here ν is the kinematic viscosity, g is the gravitational acceleration, and the subscripts *top* and *bot* represent the top and bottom walls, respectively. We consider stably stratified air flows, so the Prandtl number (Pr) is set to 0.7. ΔP is the streamwise pressure gradient driving the flow and p is the dynamic pressure.

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial(u_i u_j)}{\partial x_j} = \frac{1}{Re_\tau} \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} + \Delta P \delta_{i1} + Ri_\tau \theta \delta_{i3}, \quad (2)$$

$$\frac{\partial \theta}{\partial t} + \frac{\partial(\theta u_j)}{\partial x_j} = \frac{1}{Re_\tau Pr} \frac{\partial}{\partial x_j} \left(\frac{\partial \theta}{\partial x_j} \right). \quad (3)$$

115 2.2. Time advancement

Following Kim and Moin [31], the fractional time step method is utilized for the time advancement. First, the momentum equation (Eq. 2) is discretized by a semi-implicit scheme in time. The Crank-Nicolson scheme is used for the viscous terms. For the convective terms, either Adams-Bashforth or Runge-Kutta scheme can be used. For easy presentation, the second order Adams-Bashforth scheme is presented here and the detailed implementation of the Runge-Kutta scheme can be seen in Orlandi [40]. An intermediate velocity field, e.g., u_i^* , is then calculated based on the flow fields from the current (n) and previous ($n - 1$) time steps:

$$u_i^* = u_i^n + \frac{1}{2}\Delta t(3N_i^n - N_i^{n-1}) + \frac{\Delta t}{2Re_\tau}L(u_i^* + u_i^n) - \Delta t \frac{\delta p^n}{\delta x_i}. \quad (4)$$

Here N_i is the discretization of the nonlinear convective terms, i.e., $-\frac{\delta}{\delta x_j}(u_i u_j)$. The external body force terms, i.e., $\Delta P \delta_{i1}$ and $Ri_\tau \theta \delta_{i3}$, are also included in N_i . The discretization of the linear viscous terms is given by $L(u_i) = \frac{\delta}{\delta x_j} \left(\frac{\delta u_i}{\delta x_j} \right)$. Note that the resulting intermediate velocity u_i^* does not satisfy the continuity equation (Eq. 1). To enforce continuity, a pseudo pressure (ϕ) is defined to “project” u_i^* to a divergence-free velocity field (u_i^{n+1}):

$$\frac{u_i^{n+1} - u_i^*}{\Delta t} = -\frac{\delta \phi}{\delta x_i}. \quad (5)$$

Taking the divergence of Eq. 5 and enforcing $\frac{\delta u_i^{n+1}}{\delta x_i} = 0$, one obtains the pressure Poisson equation:

$$\frac{\delta}{\delta x_i} \left(\frac{\delta \phi}{\delta x_i} \right) = \frac{1}{\Delta t} \frac{\delta u_i^*}{\delta x_i}. \quad (6)$$

Solving Eq. 6 for ϕ , and substituting it into Eq. 5, one obtains a new velocity field u_i^{n+1} at time step $n + 1$ which satisfies both continuity and momentum equations. The pressure at the new time step is updated by:

$$p^{n+1} = p^n + \phi - \frac{\Delta t}{2Re_\tau}L(\phi). \quad (7)$$

For the temperature equation (Eq. 3), a similar semi-implicit scheme is utilized for time advancement:

$$\theta^{n+1} = \theta^n + \frac{1}{2}\Delta t(3N^n - N^{n-1}) + \frac{\Delta t}{2Re_\tau Pr}L(\theta^{n+1} + \theta^n), \quad (8)$$

Figure 1: Schematic of fully staggered grids. A 2D case is shown for reference. Here u and v are stored at the cell surfaces while p is stored in the cell centers.

where $N = -\frac{\delta}{\delta x_j}(\theta u_j)$ is the discretization of the nonlinear convective terms.

2.3. Spatial discretization

Spatial derivatives in Eqs. 4 to 8 are discretized on fully staggered grids [41] for a strong coupling of velocity and pressure fields, as illustrated in Fig. 1. Note that a 2D staggered grid schematic is shown for reference. Here u and v represent the velocity components in the x and y directions, respectively. The velocity components (u , v) are stored at the cell surfaces, whereas the pressure and temperature are stored in the cell centers. For channel flow simulations, the horizontal grids are uniformly spaced, while in the wall-normal direction, a stretched grid is used for a better representation of flows near the walls. The horizontal and vertical derivatives are discretized using the fourth order central differential scheme and the second order central differential scheme, respectively.

Specifically, in the horizontal direction, the nonlinear convective terms are casted in the divergence form and then discretized using the fourth order central differential scheme. For example, for the $\frac{\delta(uu)}{\delta x}$ and $\frac{\delta(uv)}{\delta y}$ terms:

$$\frac{\delta(uu)_{i+\frac{1}{2},j,k}}{\delta x} = \frac{-u_{i+2,j,k}^2 + 27u_{i+1,j,k}^2}{24\Delta x} + \frac{-27u_{i,j,k}^2 + u_{i-1,j,k}^2}{24\Delta x}. \quad (9)$$

$$\frac{\delta(uv)_{i+\frac{1}{2},j,k}}{\delta y} = \frac{-(uv)_{i+\frac{1}{2},j+\frac{3}{2},k} + 27(uv)_{i+\frac{1}{2},j+\frac{1}{2},k}}{24\Delta y} + \frac{-27(uv)_{i+\frac{1}{2},j-\frac{1}{2},k} + (uv)_{i+\frac{1}{2},j-\frac{3}{2},k}}{24\Delta y}. \quad (10)$$

150 Note that extra interpolation is needed due to the staggered grid configuration. For example, $u(i, j, k)$ and $u(i+1/2, j+1/2, k)$ are obtained by using the fourth order interpolation scheme:

$$u_{i,j,k} = \frac{-u_{i+\frac{3}{2},j,k} + 9u_{i+\frac{1}{2},j,k}}{16} + \frac{9u_{i-\frac{1}{2},j,k} - u_{i-\frac{3}{2},j,k}}{16}, \quad (11)$$

$$u_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{-u_{i+\frac{1}{2},j+2,k} + 9u_{i+\frac{1}{2},j+1,k}}{16} + \frac{9u_{i+\frac{1}{2},j,k} - u_{i+\frac{1}{2},j-1,k}}{16}. \quad (12)$$

Note that a similar fourth order central differential scheme for the convective terms in staggered grids was previously reported in Kampanis and Ekaterinaris [42], and Vreman and Kuerten [33]. As discussed in Morinishi et al. [43], the convective terms can be casted in
 155 several alternative forms, e.g., advective, skew-symmetric, and rotational forms. Compared with these alternative options, the current converge form for the convective terms is the most straightforward and computationally efficient approach. Moreover, its truncation error was found to be less compared with the other options. For example, the rotational form can induce large truncation errors if the second order central differential scheme is used in the
 160 vertical direction [44]. In addition, it was reported that the skew-symmetric form has much larger truncation error than the divergence form [33]. By using the divergence form for the convective terms, the momentum is conserved. As can be seen in Section. 2.4, the continuity is also conserved to machine accuracy at the discretization level. It is important to aware that the current divergence form does not strictly conserve kinetic energy, as pointed out
 165 in Morinishi et al. [43]. Nevertheless, the divergence form is still a robust option as the error produced by the convective discretization scheme was found to be significantly (three to four orders of magnitude) smaller than that dissipated by viscosity in DNS [33].

For the viscous terms and the pressure term, the fourth order central differential scheme is straightforward to implement and no extra interpolation is needed. For example, for the
 170 $\frac{\partial}{\partial x}(\frac{\partial u}{\partial x})$ term in u equation:

$$\frac{\delta}{\delta x} \left(\frac{\delta u_{i,j,k}}{\delta x} \right) = \frac{-u_{i+2,j,k} + 16u_{i+1,j,k} - 30u_{i,j,k} + 16u_{i-1,j,k} - u_{i-2,j,k}}{12(\Delta x)^2}. \quad (13)$$

In the vertical direction, a stretched grid is used, and the variation of grid points is defined by the following hyperbolic tangent function:

$$z_i = h - \frac{h}{\tanh(2\alpha)} \tanh\left(\frac{2\alpha}{1 - N_1}(i - N_1)\right), \quad (14)$$

where α is a parameter to control the refinement of grids near the wall and N_1 is the grid number in the vertical direction. For the vertical derivatives, the second order central differential scheme is used, for example:

$$\frac{\delta u_{i+\frac{1}{2},j,k}}{\delta z} = \frac{u_{i+\frac{1}{2},j,k+\frac{1}{2}} - u_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z(k)}, \quad (15)$$

$$\frac{\delta^2 u_{i+\frac{1}{2},j,k}}{\delta z^2} = \frac{\frac{u_{i+\frac{1}{2},j,k+1} - u_{i+\frac{1}{2},j,k}}{\Delta z_t(k)} - \frac{u_{i+\frac{1}{2},j,k} - u_{i+\frac{1}{2},j,k-1}}{\Delta z_b(k)}}{\Delta z(k)}, \quad (16)$$

where $\Delta z_t(k) = \frac{\Delta z(k) + \Delta z(k+1)}{2}$ and $\Delta z_b(k) = \frac{\Delta z(k) + \Delta z(k-1)}{2}$. The velocity $u_{i+\frac{1}{2},j,k+\frac{1}{2}}$ can be obtained by linear interpolation in the z direction.

2.4. Solution of the momentum, temperature, and pressure equations

As can be seen in Eq. 4, to obtain the intermediate velocity u^* , one needs to solve the Helmholtz equation in the following form:

$$u^* - \frac{\Delta t}{2Re_\tau} L(u^*) = u^n + \frac{1}{2} \Delta t (3N^n - N^{n-1}) + \frac{\Delta t}{2Re_\tau} L(u^n) - \Delta t \frac{\delta p^n}{\delta x} = Q^u. \quad (17)$$

Substituting the spatial discretization in Section 2.3 into Eq. 17, one obtains the linear algebraic equations for u^* . As mentioned in the introduction, the factorization approximation, introduced in the original fractional time step approach in Kim and Moin [31], was shown to be quite efficient in solving the linear algebraic equations for the second order spatial discretization. However, for the fourth order spatial schemes, the factorization approximation method becomes hard to implement since the factorization still results in a five diagonal matrix in the x and y directions, which is quite cumbersome to inverse. To mitigate this issue, in this paper, the Fourier analysis approach is utilized to solve the Helmholtz equation for velocity fields. Let the intermediate velocity (u^*) and the source term (Q^u) be represented by the discrete Fourier transform:

$$u_{i,j,k}^* = \sum_{l=0}^{N_x-1} \sum_{m=0}^{N_y-1} \tilde{u}_{l,m,k}^* W_x^{il} W_y^{jm}, \quad (18)$$

$$Q_{i,j,k}^u = \sum_{l=0}^{N_x-1} \sum_{m=0}^{N_y-1} \tilde{Q}_{l,m,k}^u W_x^{il} W_y^{jm}, \quad (19)$$

defined in $i=1, 2, \dots, N_x$, $j=1, 2, \dots, N_y$. Here N_x and N_y are the cell numbers in the x and y directions, respectively, and $W_x = e^{I2\pi/N_x}$, $W_y = e^{I2\pi/N_y}$ with $I = \sqrt{-1}$. Substituting Eqs. 18 and 19 into Eq. 17, one obtains a tridiagonal system of equations, which can be easily solved by Thomas algorithm:

$$A\tilde{u}_{l,m,k-1}^* + B\tilde{u}_{l,m,k}^* + C\tilde{u}_{l,m,k+1}^* = \tilde{Q}_{l,m,k}^u. \quad (20)$$

195 Here the coefficients are given by: $A = -\frac{\Delta t}{2Re_\tau \Delta z(k) \Delta z_b(k)}$, $C = -\frac{\Delta t}{2Re_\tau \Delta z(k) \Delta z_t(k)}$,
 $B = 1 - k_x - k_y - A - C$, and $k_x = \frac{\Delta t(-W_x^{2l} + 16W_x^l - 30 + 16W_x^{-l} - W_x^{-2l})}{24Re_\tau(\Delta x)^2}$, $k_y =$
 $\frac{\Delta t(-W_y^{2m} + 16W_y^m - 30 + 16W_y^{-m} - W_y^{-2m})}{24Re_\tau(\Delta y)^2}$ are the modified wavenumbers. u^* can then be calcu-
 200 lated using the inverse discrete Fourier transform of $\tilde{u}^*$. The Fourier analysis approach
 can also be applied for the v , w , and T equations, which results in similar coefficients and
 modified wavenumbers.

Once the intermediate velocity fields are known, one can solve the pressure Poisson
 equation (Eq. 6) for the pseudo pressure (ϕ). Similar to that shown in Section 2.3, the Pois-
 son equation is discretized using the fourth order and the second order central differential
 schemes in the horizontal and vertical directions, respectively. As a result, a fifteen-point
 205 stencil is obtained for the Poisson equation. By utilizing a similar Fourier analysis and sub-
 stituting the corresponding discrete Fourier transform into Eq. 6, the following tridiagonal
 system of equations are obtained for ϕ :

$$A\tilde{\phi}_{l,m,k-1} + B\tilde{\phi}_{l,m,k} + C\tilde{\phi}_{l,m,k+1} = \tilde{Q}_{l,m,k}^p, \quad (21)$$

where $A = \frac{1}{\Delta z(k) \Delta z_b(k)}$, $C = \frac{1}{\Delta z(k) \Delta z_t(k)}$, $B = k_x + k_y - A - C$, and $k_x = (W_x^{3l} - 54W_x^{2l} +$
 $783W_x^l - 1460 + 783W_x^{-l} - 54W_x^{-2l} + W_x^{-3l})/576(\Delta x)^2$, $k_y = (W_y^{3m} - 54W_y^{2m} + 783W_y^m -$
 210 $1460 + 783W_y^{-m} - 54W_y^{-2m} + W_y^{-3m})/576(\Delta y)^2$ are the modified wavenumbers. Once the
 pseudo pressure is obtained, the pressure and velocity fields at the new time step can be
 calculated using Eqs. 7 and 5, respectively.

As shown above, a generalized Fourier analysis approach is used for solving the velocity
 and temperature Helmholtz equations, as well as the pressure Poisson equation. We would
 215 like to highlight that an important advantage of using the generalized Fourier solver is

that the implementation for massive parallelism is quite straightforward (please see detailed discussion in Section 2.6).

2.5. Boundary conditions

In the DNS of open-channel flows, the computational domain is a rectangular box. The domain is periodic in the horizontal direction and is bounded by two walls in the vertical direction. Periodic boundary conditions are prescribed along the streamwise (x) and spanwise (y) boundaries. A non-slip boundary condition ($u, v, w = 0$) is specified at the bottom wall ($z = 0$), whereas at the top wall ($z = h$), a free-slip boundary condition is imposed ($\partial u/\partial z = 0, \partial v/\partial z = 0, w = 0$). In order to impose stratification in the channel, fixed normalized temperatures ($\theta_{\text{top}} = 0, \theta_{\text{bot}} = -1$) are also prescribed along the top and the bottom walls. The pressure boundary condition at the bottom and top walls is zero-gradient ($\partial p/\partial z = 0$).

Similar boundary conditions are also needed when solving the velocity, temperature, and pressure equations using the Fourier analysis method. For example, for Eq. 20, the same non-slip and free-slip boundary conditions are applied for the Fourier coefficients $\tilde{u}^*$, i.e., $\tilde{u}^* = 0$ at the bottom wall and $\partial \tilde{u}^*/\partial z = 0$ at the top wall. For the temperature equation, the fixed temperature condition is imposed by keeping the Fourier coefficient $\tilde{\theta}_{l=0,m=0} = -1$ and other Fourier coefficients to be zero at the bottom wall (similar treatment is applied for the top wall). For the pressure Poisson equation, we set $\tilde{p}_{l=0,m=0} = 0$ at the bottom wall to remove the null space. No such treatment is needed for the velocity and temperature Helmholtz equations.

As shown in Eq. 2, a streamwise pressure difference (ΔP) is imposed in the u equation to drive the flow. A constant friction condition can be imposed if the pressure difference is set to be invariant during the simulations, i.e., $\Delta P = 1$. Alternatively, ΔP can vary during the simulation to adjust a constant mass flow rate. As discussed in Brethouwer et al. [20], compared with the constant pressure difference approach, the constant mass flow rate condition has a better performance in reducing low-frequency temporal oscillations for the very stable cases, especially if a small computational domain is used. However, its limitation is that the friction is not controlled and the grid resolution in wall-unit is not known in advance. This can be an issue for the finite-difference solver since a relatively fine grid resolution is needed. Given this motivation, the constant pressure difference condition is used in this study.

2.6. 2D domain decomposition for parallel computation

In this study, a 2D “pencil” domain decomposition method is used for parallel computation on distributed-memory systems. As mentioned in the introduction, compared with the 1D domain decomposition, the 2D decomposition configuration significantly increases the CPU cores that a simulation can use, which is essential for petascale DNS simulations. Moreover, the serial algorithm used in the current DNS solver can be directly applied for parallel simulations (see the detailed discussion in the following). This is a quite favorable feature for the implicit time advancement scheme as the original serial algorithm and code programming logic for the linear algebraic equations remain the same.

Figure 2: Illustration of 2D pencil decomposition and transposition for the computational domain. (a), (b), and (c) are for the X, Y, and Z pencil arrangements, respectively. Here the computational domain is divided into $12 \times 12 \times 8$ cells (black thin lines) in the x , y , and z directions, respectively. The domain is then decomposed into 4 rows and 3 columns ($P_{\text{row}} = 4$, $P_{\text{col}} = 3$; red thick lines) in the Z pencil arrangement for parallel simulations. The Z pencil arrangement can be further transposed to the Y or X pencil for parallel communication.

We present the detailed implementation of the 2D decomposition in our DNS solver by showing a simplified example in Fig. 2. Here the computational domain is divided into $12 \times 12 \times 8$ cells (black thin lines) in the x , y , and z directions, respectively. The domain is then decomposed into 4 rows and 3 columns of pencils ($P_{\text{row}} = 4$, $P_{\text{col}} = 3$; red thick lines), so that each Message Passing Interface (MPI) process can work on one pencil in parallel. Fig. 3 summarizes the flow chart of the current DNS solver using the 2D pencil decomposition technique. Initially, the domain is divided using the Z pencil arrangement (Fig. 2c). Parallel communication is needed when: (i) calculating the spatial discretization for the convective, viscous, pressure terms, etc; (ii) performing the 2D Fast Fourier Transform (FFT), e.g., Eqs. 18 and 19, for the solution of the velocity, temperature, and pressure equations. For

the calculation of spatial discretization, standard MPI blocking communication is used in the horizontal direction between each pencil. In order to perform 2D FFT at horizontal planes, the Z pencil arrangement is transposed to Y pencil arrangement (Fig. 2b) and 1D FFT is conducted along the y direction. Then, the Y pencil arrangement is further transposed to the X pencil arrangement (Fig. 2a) and another 1D FFT is performed along the x direction to obtain the 2D FFT coefficients. Finally, the calculated 2D FFT coefficients in the X pencil is transposed back to the Z pencil. Once the 2D FFT coefficients are known (e.g., $\tilde{u}^*$, $\tilde{Q}^u$), parallel solution of Eq. 20 using Thomas algorithm in the Z pencil arrangement can be easily done and no extra parallel communication is needed. Note that by using the global data transposition, the implementation of parallel computation in the current solver is quite straightforward and one does not need to change the original serial coding logic.

Figure 3: Flow chart of the current DNS solver using the 2D pencil decomposition technique. The pencil transposition operations at each step are also shown for reference.

As shown above, the data transposition is a critical step for parallel communication. Essentially, the data transposition is implemented through the `MPI_ALLTOALL` function. In this function, all the data assigned to the MPI processes are globally exchanged to each other. It is clear that this operation can cause significant communication delay, and one should minimize its usage for a better parallel efficiency. As shown in Fig. 3, a total of 12 transpositions are needed for each time-iteration. It is also noted that the efficient 2D data transposition using the `MPI_ALLTOALL` function is probably a purely computer-science related topic, and its detailed implementation can be quite cumbersome. Fortunately, at present, several high-performance data transposition libraries are readily available, e.g., P3DFFT [45], 2DECOMP&FFT [46]. In the current DNS solver, the 2D transposition is performed using the 2DECOMP&FFT library v1.5.847 and the FFT is conducted with the FFTW library v3.3.4 [47].

Table 1: Evaluation of the strong scalability of the current DNS solver on ARL HPC Excalibur, AFRL HPC Lightning, and TACC Stampede. The parallel efficiency is calculated as $E_1 = \frac{P_0}{P} \frac{T_0}{T}$. Here P and T are the number of cores and the elapsed time per step, respectively. The subscript 0 denotes the case using smallest number of cores.

Excalibur												
Grids	2048×2048×256					4096×4096×512				8192×8192×512		
Cores	512	1024	2048	4096		4096	8192	16384		16384	32768	
Time/Step (s)	13.58	7.00	3.55	1.70		17.18	8.58	4.13		28.17	14.86	
Efficiency	100%	97%	96%	100%		100%	100%	104%		100%	95%	
Lightning												
Grids	1024×1024×128					2048×2048×256				4096×4096×512		
Cores	128	256	512	1024	2048	512	1024	2048	4096	4096	8192	16384
Time/Step (s)	4.12	2.29	1.15	0.55	0.32	9.99	5.12	2.72	1.57	14.17	6.72	4.34
Efficiency	100%	90%	90%	94%	80%	100%	98%	92%	80%	100%	105%	82%
Stampede												
Grids	1024×1024×128					2048×2048×256				4096×4096×512		
Cores	128	256	512	1024	2048	512	1024	2048	4096	4096	8192	16384
Time/Step (s)	3.76	1.89	1.06	0.52	0.30	8.07	4.77	2.41	1.30	10.80	6.18	3.40
Efficiency	100%	99%	89%	90%	78%	100%	85%	84%	78%	100%	87%	79%

2.7. Parallel efficiency

The parallel efficiency, or the scalability, is essential for large-scale DNS simulations. The current DNS solver has been tested on the following HPC platforms: ARL HPC Excalibur, AFRL HPC Lightning, and TACC Stampede. Excalibur is a Cray XC40 system equipped with Intel Xeon E5-2698 v3 processors clocked at 2.3 GHz. The total number of nodes in Excalibur is 3098 with 32 CPU cores per node, and they are interconnected using the Cray Aries with Dragonfly topology. Excalibur has a peak PFLOPS of 3.7. Lightning is a Cray XC30 system populated with Xeon E5-2697 v2 processors clocked at 2.7 GHz. In total, Lightning has 2370 computational nodes with 24 cores per node, connected through the Cray Aries network. Lightning is rated at 1.2 peak PFLOPS. Stampede is a Dell Linux Cluster configured with more than 6400 nodes, and each is outfitted with two Intel Xeon E5-2680 processors clocked at 2.7 GHz. The Mellanox FDR InfiniBand technology is used for interconnection. The peak PFLOPS of Stampede is approximately 2.

First, the strong scalability of the current DNS solver is tested. The strong scalability is defined as the variation of the simulation speed (elapsed time per step) when increasing the CPU cores for a fixed grid number. A perfect strong scalability implies that simulation

speed increases by a factor of two if the CPU cores are doubled. Table 1 shows the strong
 scalability test results using the three HPC systems. Here four stably stratified open-channel
 flow cases, with the grid points being 0.13, 1.1, 8.6, and 34.4 billion, are simulated using
 various numbers of CPU cores. The parallel efficiency for strong scalability is calculated
 310 as $E_1 = \frac{P_0}{P} \frac{T_0}{T}$. Here P and T are the number of cores and the elapsed time per step,
 respectively. The subscript 0 denotes the case using smallest number of cores. Overall,
 the current DNS solver manifests reasonably good parallel efficiency on these three HPC
 platforms with Excalibur having the best performance. Selectively, the scalability data for
 Excalibur is shown in Fig. 4 along with the ideal scalability line for reference. Remarkably,
 315 we observe a 95% parallel efficiency when increasing the CPU cores from 16384 to 32768
 for the 34.4 billion grid case. This high parallel efficiency is probably attributed to the
 dragonfly topology employed in the Cray Aries interconnection, which provides significantly
 improved bandwidth for the MPI_ALLTOALL function. However, it is also noted that for
 a given number of grids and CPU cores, the simulation speed for Excalibur is the slowest
 320 among the three HPC platforms. This is expected since Excalibur has 32 CPU cores per
 node, as a trade-off, the CPU frequency is relatively low (2.3 GHz). We would like to point
 out that a few super-linearity scalability results are observed in Table 1 (parallel efficiency
 is slightly larger than 100%). Similar super-linearity results were also previously reported
 in the scalability tests in Laizet and Li [32], and Lee et al. [48]. This is not unexpected
 325 given the fact that the parallel efficiency is known to be sensitive to the performance of
 network and the 2D mapping strategy, i.e., the choice of P_{row} and P_{col} . The optimal values
 for P_{row} and P_{col} vary depending on the architecture of the HPC platforms, as well as the
 interconnection layout. In principle, P_{row} should not be much larger than P_{col} to ensure an
 efficient usage of memory cache for distributed 3D arrays (please refer to Laizet and Li [32]
 330 for detailed discussion). However, in practice, some trial and errors are needed to ensure a
 maximal parallel efficiency.

In addition to the strong scalability, the weak scalability is tested (Table 2). The weak
 scalability is defined as the variation of the simulation speed when increasing the CPU cores
 with the number of grids per core fixed. In this paper, the number of grids per core is
 335 set to be approximately 1 million. In other words, the grid number for the 128-core case
 is approximately 0.54 billion, whereas for the 16384-core case, the grid number is about
 17.2 billion. One can see that, with increasing the number of cores, the elapsed time per

Table 2: Evaluation of the weak scalability of the current DNS solver on ARL HPC Excalibur, AFRL HPC Lightning, and TACC Stampede. The number of grid per core is set to be approximately 1 million. The parallel efficiency is calculated as $E_2 = \frac{T_0}{T}$. Here T is the the elapsed time per step. The subscript 0 denotes the case using smallest number of cores.

Excalibur						
Cores	512	1024	2048	4096	8192	16384
Time/Step (s)	6.91	7.00	7.48	7.93	7.88	7.30
Efficiency	100%	99%	92%	87%	88%	95%
Lightning						
Cores	512	1024	2048	4096	8192	16384
Time/Step (s)	5.89	5.40	5.93	6.68	6.44	6.99
Efficiency	100%	109%	99%	88%	91%	84%
Stampede						
Cores	512	1024	2048	4096	8192	16384
Time/Step (s)	4.08	4.24	4.42	5.14	5.22	5.84
Efficiency	100%	96%	92%	79%	78%	70%

step globally decreases. This is expected since the increasing grid number causes excessive network communication which consequently decreases the parallel efficiency. Overall, the weak scalability performance is quite reasonable with Excalibur having the best parallel efficiency.

Given the good scalability, the current DNS solver is shown to be competent to perform petascale DNS simulations for stratified channel flows with grid number on the order of 10 billion. In order to further test its ability to capture the turbulence characteristics of strongly stratified flows, two DNS simulations are conducted and analyzed in detail at a relatively high Re in the following sections.

2.8. Simulation configurations

Table 3 summaries the simulation configurations used in the study. Two stably stratified open-channel simulations (S1: weakly stratified, $Ri_\tau = 100$; S2: strongly stratified, $Ri_\tau = 10^4$) are performed at $Re_\tau = 1000$ for detailed analyses. For the strongly stratified case, the bulk Reynolds number, i.e., $Re_b = u_b h / \nu$, is about 10^5 , and the corresponding bulk Richardson number, i.e., $Ri_b = (\theta_{top} - \theta_{bot})gh / \theta_{top} u_b^2$, is approximately 1.0. Here the bulk velocity u_b is defined as the averaged velocity in the channel. It is important to note that the

Figure 4: Scalability test for the current DNS solver on Excalibur. Platform: Cray XC40. CPU: Intel Xeon E5-2698 v3; Interconnection: Cray Aries / Dragonfly. Compiler: Intel Fortran v15.0.1; MPI library: Cray-MPICH v7.1.0.

open-channel flow is equivalent to a z -symmetrized (closed-channel) plane Poiseuille flow; however, the definitions of Ri_τ in these two cases are slightly different. The conventional definition for Ri_τ in closed-channel flows [17, 49] is two times larger than the definition used here for open-channel flows. In other words, the stratification level with $Ri_\tau = 10^4$ in an open-channel is similar to that in a closed-channel with $Ri_\tau = 2 \times 10^4$.

As mentioned above, the grids are uniformly spaced in the horizontal direction and stretched in the vertical. The grid resolutions are set to be $\Delta x^+ = 8.9$ and $\Delta y^+ = 4.9$, where Δx^+ and Δy^+ are the normalized grid resolutions in inner units (e.g., $\Delta x^+ = \Delta x u_\tau / \nu$). To fully resolve turbulence in near-wall regions, the first grid level near the bottom wall is located at $z^+ < 0.4$, and more than 20 grids are set within $z^+ < 10$, where z^+ is the normalized grid distance from the bottom wall, $z^+ = z u_\tau / \nu$. The horizontal and vertical spatial-derivatives are discretized using the fourth order and second order central differential schemes, respectively, as shown in Section 2.3. For S1, the coupled Adams-Bashforth and Crank-Nicolson scheme is used for time advancement, whereas for S2 the coupled Runge-Kutta and Crank-Nicolson scheme is used in order to obtain better numerical stability. The boundary conditions for the stably stratified open-channel flows were introduced in Section 2.5.

According to García-Villalba and del Álamo [17], Brethouwer et al. [20], and Ansorge

Table 3: Summary of the computational configurations for the neutrally and stably stratified channel flows in this study. The cases S1 and S2 (open-channel configuration) are for detailed analyses, and the cases V1 to V7 (closed-channel configuration) are for solver verification. Re_b and Re_τ are the bulk and the friction Reynolds numbers, respectively; Ri_b and Ri_τ are the bulk and the friction Richardson numbers, respectively; h/L is stability parameter with L being the Obukhov length and h being the open-channel height (h is set to be 1.0 for the current study); L_x and L_y are the domain lengths in the streamwise (x) and spanwise (y) directions, respectively; N_x, N_y, N_z are the cell numbers in the x, y, z directions, respectively; $\Delta x^+, \Delta y^+, \Delta z^+$ are the normalized grid resolutions (e.g., $\Delta x^+ = \Delta x u_\tau / \nu$). The smaller and larger Δz^+ represent the vertical grid resolution at the bottom and the top walls, respectively. tu_τ/h is the non-dimensional averaging time for the calculations of turbulence statistics.

Case	Re_b	Re_τ	Ri_b	Ri_τ	h/L	L_x	L_y	N_x	N_y	N_z	Δx^+	Δy^+	Δz^+	tu_τ/h
S1	23200	1000	0.19	100	0.41	$25h$	$10h$	2816	2048	256	8.9	4.9	0.4–8.8	10
S2	100500	1000	0.99	10^4	6.90	$25h$	$10h$	2816	2048	256	8.9	4.9	0.4–8.8	5
V1	2800	180	0	0	0	$4\pi h$	$4\pi h/3$	256	192	128	8.8	4.4	0.3–6.1	20
V2	6900	395	0	0	0	$2\pi h$	πh	288	288	288	8.8	4.3	0.3–6.1	20
V3	11000	590	0	0	0	$2\pi h$	πh	432	432	432	8.6	4.3	0.3–6.1	20
V4	2800	180	0	0	0	$8\pi h$	$4\pi h$	512	512	128	8.8	4.4	0.3–6.3	20
V5	3100	180	0.03	18	0.06	$8\pi h$	$4\pi h$	512	512	128	8.8	4.4	0.3–6.3	20
V6	3800	180	0.13	120	0.23	$8\pi h$	$4\pi h$	512	512	128	8.8	4.4	0.3–6.3	20
V7	5400	180	0.27	480	0.64	$8\pi h$	$4\pi h$	512	512	128	8.8	4.4	0.3–6.3	20

and Mellado [21], a large computational domain is needed to accommodate the spatial-temporal variation of stably stratified flows, especially for very stable cases. In the current study, the domain size is chosen to be $L_x \times L_y \times L_z = 25h \times 10h \times h$. In order to obtain initial conditions for the simulations, coarse-resolution cases are run for about 50 non-dimensional time (i.e., $tu_\tau/h \approx 50$) to obtain quasi-stationary flow fields. Then the flow variables are interpolated to fine-resolution initial fields. Finally, 10 and 5 non-dimensional times are run to calculate the turbulence statistics for S1 and S2, respectively. The S2 case took about 90 hours using 8192 cores on AFRL HPC Lightning.

In order to verify the current DNS solver, seven simulations (V1-V7, see Table 3) are performed for both neutrally and stably stratified flows and the simulations results are compared with the benchmark data reported in Moser et al. [37], and García-Villalba and del Álamo [17], as can be seen in the Appendix. The simulations results are shown to be in reasonably good agreement with the benchmark DNS data. These results demonstrate the success of the current DNS solver and build confidence for the simulations and analyses

reported in the rest of the paper.

3. Results and Discussion

The simulation results for S1 and S2 are reported in this section to demonstrate the ability of the newly developed DNS solver for simulating stably stratified channel flows at a relatively high Reynolds number. We would like to highlight that only a few characteristics of high Re stably stratified channel flows are analyzed and compared with the existing DNS results at relatively low Re . Systematic investigation of such topic is beyond the scope of the current study, and will be conducted in a separate paper. Specifically, in this section, the impacts of stratification on the mean flows and turbulence statistics are investigated, and the spatio-temporal characteristics of turbulence structures under different stratification levels are illustrated. At last, the simulated similarity relationships are compared with the well-known Monin-Obukhov similarity theory to evaluate their relevance to the atmospheric flow conditions.

3.1. Profiles of mean flows and turbulence statistics under stably stratified conditions

Under stably stratified conditions, the vertical motion of turbulence is suppressed by buoyancy, resulting in significant modification of turbulence structures compared with the neutral case. Such topic has been investigated in a number of LES and DNS studies, e.g., Armenio and Sarkar [49], and García-Villalba and del Álamo [17], based on stratified closed-channel flows at relatively low Reynolds numbers ($Re_\tau < 550$) and stratification levels ($Ri_\tau < 1920$). In this section, the impacts of stratification on the profiles of mean flows and turbulence statistics at $Re_\tau = 1000$ are documented, and the highest stratification level considered here is $Ri_\tau = 10^4$.

Fig. 5 shows the vertical profiles of mean variables and turbulence statistics for stably stratified open-channel flows at $Re_\tau=1000$. Here S1 ($Ri_\tau = 100$) and S2 ($Ri_\tau = 10^4$) correspond to the weakly and strongly stratified cases, respectively. As can be seen in Fig. 5a, with increasing the stratification level, the mean velocity variation is modified significantly. For S1, a relatively flat (well-mixed) velocity profile is observed in the channel, whereas for S2, the velocity accelerates drastically, especially near the top wall. The ratio of the velocities between the strongly stratified and the weakly stratified cases is approximately 9 at the top channel, which is significantly larger than the ratio (~ 2) reported in Armenio

Figure 5: Vertical profiles of mean variables and turbulence statistics for stably stratified open-channel flows at $Re_\tau=1000$. —: S1 ($Ri_\tau = 100$); —·—: S2 ($Ri_\tau = 10^4$). (a) $\bar{u}$, (b) $\bar{\theta}$, (c) $\overline{u'w'}$, and (d) $\overline{w'\theta'}$.

and Sarkar [49] ($Re_\tau = 180$) and García-Villalba and del Álamo [17] ($Re_\tau = 550$). It is noted that the maximal amount of velocity acceleration can be obtained when Ri_τ exceeds the laminarization threshold; a parabolic velocity profile is formed in this case. According to the linear stability theory in Gage and Reid [50], for $Re_\tau = 1000$, the Ri_τ threshold is $\sim 4.4 \times 10^4$. The current Ri_τ value for S2 is still four times smaller than the laminarization threshold. This can be further confirmed by the fact that the maximal velocity for S2 is $u_{max}/u_\tau \approx 185$, smaller than the maximal value from the parabolic profile at $Re_\tau = 1000$, i.e., $u_{max}/u_\tau = Re_\tau/2 = 500$.

The acceleration of velocity is attributed to the drastic decrease of vertical momentum flux (reduced mixing), as can be seen in Fig. 5c. The peak $-\overline{u'w'}$ decreases from ~ 0.8 (S1) to ~ 0.35 (S2). Moreover, the $-\overline{u'w'}$ value for S2 decreases substantially in $z/h > 0.3$, implying a full laminarization of the flow. Quite interestingly, the current result indicates

a coexistence of turbulent flows and fully laminarized flows, located in the lower and the upper part of the channel, respectively (see detailed illustration in Section 3.2). Note that in
430 Armenio and Sarkar [49], and García-Villalba and del Álamo [17], the turbulent momentum flux was also found to be significantly suppressed by the stratification. However, the decaying of turbulence was found to be transient and intermittent and no full (steady) laminarization was reported.

The mean temperature profile is also modified by the stratification as shown in Fig. 5b.
435 The temperature gradient decreases significantly near the bottom wall, indicating a substantial reduction of surface heat-flux as a result of the stable stratification. The Nusselt number (Nu) is a useful metric which reflects how close the flow is to a laminar state. Nu is defined as the ratio between heat transfer due to turbulence and pure conduction (laminar state): $Nu = \frac{h}{\theta_{\text{top}} - \theta_{\text{bot}}} \left(\frac{\partial \theta}{\partial z} \right)_{\text{bot}}$. The Nu for S1 is 7.2 and it becomes 1.2 for S2, implying
440 that the flow is becoming closer to laminar. Note that a linear mean temperature profile will be formed in a laminar state. Similar to those reported for the momentum flux, the turbulent heat flux is also found to be significantly suppressed by stratification, and a full laminarization is observed in the upper channel.

3.2. Spatio-temporal characteristics of global intermittency

445 The existence of global intermittency, or turbulent burst, in the very stable boundary layer is well-known in the literature. This intriguing phenomenon is typically characterized as an observed time-series alternating between quiescent (laminar) and bursty (turbulent) state. This type of intermittent time-series has been widely observed in various regions of the world [51, 52, 53, 54, 55, 56], to name a few. It is also documented in the literature that
450 the globally intermittent turbulence portrays intriguing spatio-temporal correlations [57]. A number of studies have been conducted to investigate the generation and dynamics of global intermittency in the ABL [54, 55, 58, 59, 60], among others. In recent years, the global intermittency was successfully reproduced by a number of DNS studies [12, 17, 20, 21, 22], which complements the understanding of its spatio-temporal characteristics. In this section,
455 we document the spatio-temporal variations of global intermittency at $Re_\tau = 1000$. The similarity and discrepancy between the previously reported results and the current results are discussed.

A number of monitor points are placed in various vertical locations of the channel to document the time-variations of the stratified turbulent flows. Fig. 6 shows the time-series

Figure 6: Time-series of vertical velocity at different locations in the channel. (a) S1 ($Ri_\tau = 100$), and (b) S2 ($Ri_\tau = 10^4$).

460 of vertical velocity at different locations in the channel. For S1, the turbulent flow is continuous and no intermittency is observed. However, for S2, alternating turbulent and laminar flows are clearly identified in the time-series, especially in the lower channel. In the vertical direction, the turbulent bursting event is triggered slightly earlier near the upper channel than the bottom wall. These features coincide with those reported in He and
 465 Basu [22] for low Re flows. However, in contrast to He and Basu [22] that the turbulence sustained in the upper channel, in the current case the turbulence is totally laminarized in $z/h > 0.3$. Based on their DNS results, Ansorge and Mellado [21] showed that the turbulence laminarization is not an on-off process. Instead, the turbulence first becomes steadily intermittent and then fully laminarized with increasing the stratification level. This

470 statement is well corroborated by the current DNS results. Moreover, the current results indicate that the full laminarization process is not synchronous in the vertical direction; this process first occurs in the upper channel due to the dominant buoyancy while the intermittent turbulence can still sustain in the lower channel at the same time.

Figure 7: Contour of vertical velocity at the x - y plane located at $z/h = 0.1$. (a) S1 ($Ri_\tau = 100$), and (b) S2 ($Ri_\tau = 10^4$).

According to Coulter and Doran [57], the intermittent time-series was found to be spatially correlated in the ABL, implying that the turbulent bursting event may not be a fully localized phenomenon. The spatial correlation of temporal intermittency was further corroborated by the DNS study in He and Basu [22]. In their study, the coexisting laminar–turbulent flows were found to be advecting with mainstream and triggering intermittent time-series signal. Investigation of the spatial pattern of coexisting laminar–turbulent flows is important for the understanding of temporal intermittency. Furthermore, to what extent does the temporal intermittency spatially correlate with each other has implication for turbulence parameterization in mesoscale modeling [57].

Fig. 7 shows the contour of vertical velocity at the x - y plane located at $z/h = 0.1$. A horizontally homogeneous turbulent field is found for S1, whereas for S2, a coexistence of

Figure 8: Premultiplied (a) streamwise and (b) spanwise spectra of u at $z/h = 0.1$. Here E_{uu}^x and E_{uu}^y are the 1D energy spectra of u in the x and y directions, respectively. The corresponding wavenumbers are k_x and k_y , and the corresponding wavelengths are λ_x and λ_y . —: S1 ($Ri_\tau = 100$); -·-: S2 ($Ri_\tau = 10^4$).

laminar–turbulent bands is observed. Note that similar spatial intermittency was previously reported in DNS studies [12, 17, 20, 21, 22] at relatively low Re . It would be interesting to evaluate if the spatial patterns of the coexisting laminar–turbulent flows have scaling features at a relatively high Re . For this purpose, we calculate the premultiplied streamwise and spanwise spectra of u at $z/h = 0.1$, as shown in Fig. 8. Here E_{uu}^x and E_{uu}^y are the 1D energy spectra of streamwise velocity in the x and y directions, respectively. The corresponding wavenumbers are k_x and k_y , and the corresponding wavelengths are λ_x and λ_y . Note that λ_x and λ_y are normalized in inner units, e.g., $\lambda_x^+ = \lambda_x u_\tau / \nu$. The premultiplied spectra represent the contribution of streamwise velocity variance from an infinitesimal logarithmic wavelength interval at λ_x or λ_y . One can see that, for the weakly stratified case (S1), a single spectral peak is observed at $\lambda_x^+ \approx 1000$ and $\lambda_y^+ \approx 400$ for the streamwise and spanwise spectra, respectively. This peak corresponds to the alternating low- and high-speed

streaks, i.e., the near-wall coherent structures, with characteristic lengths $\lambda_x^+ \approx 1000$ and $\lambda_y^+ \approx 400$. For the very stable case (S2), the characteristic lengths for the near-wall streaks decrease as a result of the suppression of buoyancy. This trend coincides well with that
500 observed in the stably stratified closed-channel flows at $Re_\tau = 550$ [17]. Moreover, for S2, another spectral peak is found at much larger characteristic wavelengths, i.e., $\lambda_x^+ \approx 1.4 \times 10^4$ and $\lambda_y^+ \approx 3.3 \times 10^3$. This large-scale peak is clearly associated with the spatial pattern of global intermittency. Note that in Brethouwer et al. [20], similar double-peak spectra were reported for strongly stratified open-channel flows. The corresponding wavelengths for inter-
505 mittent pattern in the spanwise direction are $\lambda_y^+ \approx 4.5 \times 10^3$ at $Re_\tau = 192$ and $\lambda_y^+ \approx 2.5 \times 10^3$ at $Re_\tau = 334$. Although the current Re_τ is much larger than those reported in Brethouwer et al. [20], we do not observe clear dependence of intermittent pattern wavelengths on Re_τ . It is suggested that the magnitude of intermittent pattern wavelength scales in inner units in $Re_\tau < 1000$. This result implies that the pattern wavelengths decrease in outer units with
510 increasing Re_τ , i.e., $\lambda_y/h \approx 23.4, 7.5$, and 3.3 for $Re_\tau = 192, 334$, and 1000 , respectively. It is important to note that the indication of the scaling behavior is only based on three Re_τ , systematic evaluation of this topic at wider ranges of Re_τ is needed in the future work.

3.3. Relation to Monin-Obukhov similarity theory

The Monin-Obukhov similarity theory (MOST) is widely used to describe the flux-
515 gradient relationships in the ABL. In the past decades, a number of similarity relationships for wind speed and temperature have been proposed based on observational data [61, 62, 63, 64], to name a few. In order to evaluate the relevance of the current DNS results to realistic atmospheric flow conditions, we compare the simulated flux-gradient similarity relationships with those observed in the ABL. According to the MOST, the normalized
520 gradients of velocity and temperature can be related to the stability parameter (ζ) as:

$$\frac{\kappa z}{u_*} \frac{\partial \bar{u}}{\partial z} = \Phi_m(\zeta), \quad (22)$$

$$\frac{\kappa z}{\theta_*} \frac{\partial \bar{\theta}}{\partial z} = \Phi_h(\zeta). \quad (23)$$

Here $\kappa = 0.4$ is the von Karman constant, $u_* = (\overline{u'w'^2} + \overline{v'w'^2})^{1/4}$ is the local friction velocity, $\theta_* = -\overline{w'\theta'}/u_*$ is the local temperature scale, and $\zeta = z/\Lambda$ with Λ being the local Obukhov length defined as $\Lambda = -\overline{\theta}u_*^3/\kappa g \overline{w'\theta'}$. Fig. 9 shows the dependence of Φ_m and Φ_h

Figure 9: Dependence of (a) Φ_m and (b) Φ_h as a function of stability parameters. The symbols are the ensemble results constructed from the DNS data. $\bullet$: S1 ($Ri_\tau = 100$); $\blacksquare$: S2 ($Ri_\tau = 10^4$). The lower and higher error bars represent 25 and 75 percentile value of the ensemble results, respectively. The lines are the similarity relationships proposed in Dyer [61] (—) and Duynkerke [62] (—·—).

as a function of the stability parameter. The symbols are the ensemble results based on the
 525 DNS data. For each simulation, the ensemble samples are based on the horizontal-plane
 averaged variables at different vertical locations and times (please refer to He and Basu
 [24] for more details of DNS-based similarity relationships). In order to avoid the impact
 of molecular viscosity at the bottom wall and the boundary condition at the top wall, the
 similarity relationships are constructed using the DNS data in $0.1 < z/h < 0.9$ for S1.
 530 For S2, an even shorter data range ($0.1 < z/h < 0.3$) are used since the flows are fully
 laminarized in $z/h > 0.3$. The lines are the existing similarity relationships, i.e., the linear
 functions: $\Phi_m = 1 + 5z/\Lambda$, $\Phi_h = 1 + 5z/\Lambda$ proposed in Dyer [61] (D74), and the nonlinear
 functions: $\Phi_m = 1 + 5z/\Lambda(1 + 6.25z/\Lambda)^{-0.2}$, $\Phi_h = 1 + 7.5z/\Lambda(1 + 9.375z/\Lambda)^{-0.2}$ proposed
 in Duynkerke [62] (D91). Although the weakly and strongly stratified cases (S1 and S2)

cover different range of stability, they all agree reasonably well with those proposed based on the observational data, especially for D74. We do point out that there is a noticeable overestimation of Φ_m in the lower stability region ($0.1 < z/\Lambda < 0.6$ in Fig. 9a). Overall, the good agreement between the DNS-based similarity relationships and those proposed using observational data demonstrates the relevance of DNS results to atmospheric flow conditions. It is also noted that the stability parameter covers a much wider range, i.e., $(z/\Lambda)_{\max} \approx 20$, compared to the previous results using the low- Re DNS data, as reported in van de Wiel et al. [23], and He and Basu [24]. This feature highlights the advantage of using the current massively parallel DNS solver for simulating high- Re stably stratified flows.

4. Conclusions

In this paper, a high-order finite-difference direct numerical simulation (DNS) solver is developed for massively parallel simulations of incompressible stably stratified turbulent flows in open channels. The semi-implicit fractional time step method is used for time advancement, and the spatial derivatives are discretized using the fourth-order and second-order central differential schemes in the horizontal and vertical directions, respectively. The resulting discretization equations, including the momentum, temperature, and pressure equations, are then directly solved using the Fourier analysis approach. The 2D domain decomposition technique is utilized for parallel communication, and a reasonably good scalability is obtained with up to 32768 CPU cores.

The newly developed DNS solver is then verified using the benchmark data in Moser et al. [37], and García-Villalba and del Álamo [17] for neutrally and stably stratified flows, and a reasonably good agreement is found. Moreover, two stably stratified open-channel simulations are conducted with a weak and a very strong stratification level. The bulk Reynolds number for the strongly stratified case is approximately 10^5 . The characteristics of strongly stratified flows are compared with those previously reported at relatively low Reynolds numbers, and several discrepancies are observed. For example, the acceleration of mean velocity is found to be much higher than the low Reynolds number cases. In addition, the laminarization process is found to be asynchronous in the vertical direction; this process first occurs in the upper channel due to the dominant buoyancy while the intermittent turbulence can still sustain in the lower channel at the same time. In addition

to the discrepancies, we observe intriguing scaling behavior for the spatial pattern of global intermittency. That is to say, the pattern wavelength is found to scale in inner units in $Re_\tau < 1000$. In order to evaluate the relevance of the DNS-based results to the atmospheric flows, the DNS-based similar relationships are compared with those proposed using observational data, and a reasonably good agreement is found. It is also observed that the range of the stability parameter, i.e., $(z/\Lambda)_{\max} \approx 20$, from the current high- Re DNS-based similarity relationships is much wider compared with the existing low- Re DNS-based results, i.e., $(z/\Lambda)_{\max} \approx 5$.

Above all, the newly developed DNS solver is shown to be competent for massively parallel simulations of stably stratified channel flow at relatively higher Reynolds numbers. In the future, this solver will be used to generate a DNS dataset with a wide range of Reynolds numbers and Richardson numbers. Using this comprehensive dataset, various flux- and gradient-based similarity relationships will be constructed and compared with the existing similarity functions [2, 65, 66] to further evaluate the relevance of DNS-based results. Moreover, new similarity relationships will be developed based on this DNS dataset, and systematic investigations will be conducted to document the turbulence characteristics in the “very stable” regime.

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595 Appendix A. Solver verification

In this appendix, the solver verification is performed. Seven closed-channel simulations (both neutrally and stably stratified; V1-V7 in Table 3) are conducted and the simulation results are compared with the benchmark data [17, 37]. The boundary conditions and domain sizes are chosen to be identical to those used in Moser et al. [37], and García-Villalba and del Álamo [17]. The grid resolutions are set to $\Delta x^+ \leq 8.8$ and $\Delta y^+ \leq 4.4$. The horizontal and vertical spatial-derivatives are discretized using the fourth order and second order central differential schemes, respectively, and a coupled Adams-Bashforth and Crank-Nicolson scheme is used for time advancement. The simulations are run for 20 non-dimensional time (i.e., $tu_\tau/h = 20$) for the calculation of turbulence statistics.

605 First, the simulation results produced by the current DNS solver are compared against the well-cited DNS benchmark (neutrally stratified case) from Moser et al. [37]. Fig. A.10 shows the vertical profiles of mean flows and turbulence statistics at $Re_\tau = 180, 395$, and 590. One can see that the results from the current solver agree well with those from Moser et al. [37]. We do point out that the momentum flux $\overline{u'w'}$ for $Re_\tau = 395$ is underestimated at $z/h \approx 0.3$, see Fig. A.10d.

Next, the DNS results for the stably stratified flows are compared with the data (extracted by a digitizer) in García-Villalba and del Álamo [17]. Vertical profiles of mean flows and turbulence fluxes are shown in Fig. A.11. Again, the results from the current solver agree well with those from García-Villalba and del Álamo [17] for all the stratification levels. 615 The maximal discrepancy is found for $\overline{w'\theta'}$ at $z/h \approx 1.0$.

Although some differences are observed between the results from the current DNS solver and those from Moser et al. [37], and García-Villalba and del Álamo [17], this level of discrepancy is not unexpected from different DNS solvers (please refer to the code verification in Kasagi et al., [67], Laizet and Lamballais [68], to name a few). In summary, the current solver accurately simulates the mean flows and turbulent statistics for the neutral and stratified cases. Without any doubt, these solver verification results build confidence for the simulations and analyses reported in the paper.

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Figure A.10: Vertical profiles of mean variables and turbulence statistics for neutrally stratified closed-channel flows at $Re_\tau=180$, 395, and 590. (a) $\bar{u}$, (b) $\overline{u'u'}$, (c) $\overline{w'w'}$, and (d) $\overline{u'w'}$. The lines are the simulation results from the current DNS solver. —: $Re_\tau=180$; — —: $Re_\tau=395$; — · —: $Re_\tau=590$. The symbols are the benchmark data from Moser et al. [37]. □: $Re_\tau=180$; △: $Re_\tau=395$; ○: $Re_\tau=590$.

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Figure A.11: Vertical profiles of mean variables and turbulence statistics for stably stratified closed-channel flows at $Re_\tau=180$. (a) $\bar{u}$, (b) $\bar{\theta}$, (c) $\overline{u'w'}$, and (d) $\overline{w'\theta'}$. The lines are the simulation results from the current DNS solver. —: $Ri_\tau=0$; —: $Ri_\tau=18$; —: $Ri_\tau=120$; —: $Ri_\tau=480$. The symbols are the benchmark data from García-Villalba and del Álamo [17]. $\circ$: $Ri_\tau=0$; $\square$: $Ri_\tau=18$; $\triangle$: $Ri_\tau=240$; $\diamond$: $Ri_\tau=480$.

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