Large-Eddy Simulation of Stratified Turbulence. Part I: A Vortex-Based Subgrid-Scale Model

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ABSTRACT

The stretched-vortex subgrid-scale (SGS) model is extended to enable large-eddy simulation of buoyancy-stratified turbulence. Both stable and unstable stratifications are considered. The extended model retains the anisotropic form of the original stretched-vortex model, but the SGS kinetic energy and the characteristic SGS eddy size are modified by buoyancy subject to two constraints: first, the SGS kinetic energy dynamics is determined by stationary and homogeneous conditions, and second, the SGS eddy size obeys a scaling analogous to the Monin–Obukhov similarity theory. The SGS model construction, comprising an ensemble of subgrid stretched-vortical structures, naturally limits vertical mixing but allows horizontal mixing provided the alignment of the SGS vortex ensemble is favorable, even at high nominal gradient Richardson numbers. In very stable stratification, the model recovers the \( z \)-less limit, in which a vortex-based Obukhov length controls the SGS dynamics, while in very unstable stratification, the model recovers the free-convection limit, in which a vortex-based Deardorff velocity controls the SGS dynamics. The efficacy of the present SGS model is demonstrated by simulating the canonical stationary and homogeneous, stratified sheared turbulence at high Reynolds numbers and moderately high Richardson numbers. In the postprocessing, the SGS dynamics of the stretched-vortex model is further interrogated to yield predictions of buoyancy-adjusted one-dimensional SGS spectra and SGS root-mean-square velocity-derivative fluctuations.

1. Introduction

The immense range of scales encountered in many flows of practical importance render direct numerical simulation (DNS) of the Navier–Stokes equations prohibitively expensive. In the atmospheric boundary layer, for instance, the largest eddies that scale with the boundary layer height are six orders of magnitude larger than the smallest Kolmogorov scales (e.g., Wyngaard 2010). By contrast, only a meager fraction of this dynamical range can be captured, even if we take into account the anticipated future increase in computing power. Therefore, numerical investigations of turbulence in the atmosphere have in the past and will for the foreseeable future rely on large-eddy simulation (LES) (e.g., Siebesma et al. 2003; Stevens et al. 2005; Beare et al. 2006), in which large eddies are resolved while small eddies are modeled. In flow regimes in which buoyancy stratification enhances or inhibits turbulence, as is common in the ocean and atmosphere (e.g., Ivey et al. 2008; Fernando and Weil 2010), a faithful subgrid-scale (SGS) model must capture this buoyancy effect when it reaches the subgrid-scale range. This last point is the subject of the present subgrid-scale model development. In this paper, we will use the terms “model” and “turbulence closure” interchangeably because we are only concerned with the effects of unresolved turbulent motions.

Since an LES derives much of its predictive capacity from directly simulating the dynamically important large scales (which determine the turbulent fluxes, for example), it seems reasonable to dismiss the SGS model as a convenient device that replaces the dissipative action of the small scales. Energy would otherwise accumulate at the scale of the grid spacing and eventually destabilize the computation. However, this line of reasoning...
calls into question the fidelity of the smallest resolved scales that directly interact with the SGS model (e.g., Domaradzki et al. 1993; Aluie and Eyink 2009). For instance, in a resolution sensitivity study, Matheou et al. (2011) show that the smallest resolved scales may not exhibit the expected inertial scaling and that the convergence of certain integrated statistics requires no less than a costly eightfold increase in resolution. Thus, a strong incentive exists for the development of SGS models that would better preserve or otherwise restore the fidelity of the full simulated dynamical range and accelerate convergence of statistics. This is a motivation behind the present model development.

A factor central to the success of the LES–SGS methodology is the notion that most of the turbulent kinetic energy, typically 80%, is resolved, leaving the SGS model to account for the remaining 20% residing below the cutoff scale (Pope 2004; Matheou et al. 2010). As anticipated in Matheou et al. (2010), this rule of thumb does not always hold because stable stratification, if it exists, may limit the size of energetic eddies. In a given stable stratification, larger eddies need to expend more kinetic energy in overturning motions, bringing heavier fluid from below upward and lighter fluid from above downward, implying a stratification-controlled scale-selection mechanism. If $L$ is the buoyancy-affected scale, above which overturning motion is strongly suppressed, then, as stratification increases, $L$ approaches the cutoff scale $\Lambda$ and the energetic motions concentrate around $\Lambda$. A common choice for $L$ is the Ozmidov scale (e.g., Dalaudier and Sidi 1990), but the Obukhov scale is also possible since they become proportional to each other as stratification increases (Chung and Matheou 2012). The accurate modeling of this interaction between the imposed smallest resolved scale in LES and the physical buoyancy-affected scale of a stably stratified turbulent flow is a central theme of the current study.

In very stable stratifications, there can be instances when $L$ is smaller than $\Lambda$ such that the energetic motions are too small to be resolved by the grid—a situation more akin to the Reynolds-averaged Navier–Stokes (RANS) modeling approach. In an LES, this can cause the SGS model to predict nearly zero SGS fluxes. This effect is manifested as a numerical discontinuity, such as that found at a sharp inversion (e.g., Stevens et al. 2005), and a successful LES must include considerations for both a faithful SGS model and a numerical method that handles numerical discontinuities gracefully without being overly dissipative (cf. Hill and Pullin 2004). Presently, we focus on the SGS model but do not directly address the numerical method.

There are many SGS models that account for buoyancy effects, both explicitly (e.g., Lilly 1962; Deardorff 1980; Moeng 1984; Mason 1985; Canuto and Minotti 1993; Cuijpers and Duynkerke 1993) and implicitly (e.g., Bou-Zeid et al. 2010), but these are tailored for the Smagorinsky (1963) closure and its variants. Most of these models are based on an eddy-viscosity formulation with various levels of complexity (e.g., evolution equations for the turbulent kinetic energy and perhaps higher-order moments). In the present investigation, we develop and evaluate a rather different buoyancy adjustment that relies on the structure-based stretched-vortex SGS model. We will nevertheless employ concepts often used in the development of buoyancy-adjusted eddy viscosity models—namely, use of the equilibrium SGS kinetic energy equation and dimensional reasoning for determining the modified SGS eddy size.

This study is documented in two parts. In the Part I (present paper), the SGS model is developed and assessed on a conceptually simple flow. In Matheou and Chung (2013, manuscript submitted to J. Atmos. Sci.), hereafter Part II, the novel turbulence closure is evaluated on large-eddy simulations of the atmospheric boundary layer—a problem of practical significance. The two parts complement each other and span the entire scope of this work from theory to model formulation and application. We develop the SGS model in section 2, beginning with a review of the stretched-vortex model in sections 2a and 2b, followed by the framework for stratification adjustment in section 2c. The cases of unstable (section 2d) and stable (section 2e) stratification are considered separately, and then the full buoyancy-adjusted model is summarized (section 2g) and interpreted (section 2h). Because a scaling ansatz is adopted for the energetic length scale in stable stratification, a constant is introduced and its numerical value is determined in section 2i via DNS data. In section 3, we discuss the subgrid-scale modeling of various SGS statistics consistent with the present stretched-vortex model description of SGS motions, including one-dimensional SGS-continued spectra (section 3a), the buoyancy-adjusted SGS energy spectrum (section 3b), and the root-mean-square (rms) of velocity-derivative fluctuations (section 3c). In section 4, LES of stationary homogeneous sheared turbulence is presented to demonstrate the capability of the SGS model and the conclusions of the present investigation are given in section 5.

2. Subgrid-scale model development

In LES, an SGS model is required for the unfiltered terms in the filtered Navier–Stokes equations (Leonard 1974). These unclosed terms are

$$\tau_{ij} = \Pi_i \Pi_j - \Pi_i \Pi_j \approx u'_i u'_j,$$  \hspace{1cm} (1)
\[ \sigma_i = \overline{\delta u_i} - \overline{\phi u_i}, \]  
\[ T = \gamma \Delta K^{1/2}, \]

(respectively, the SGS stress and the SGS scalar flux). In (1) and (2), \( u_i \) is the velocity, \( \phi \) is a scalar, the overbar denotes the LES spatial filter, and the prime denotes the SGS fluctuations. In the following, we develop a structure-based SGS model suitable for use in both stably and unstably stratified turbulent flows. The main idea is to use the SGS turbulent kinetic energy equation to constrain the SGS turbulent kinetic energy and SGS eddy length scale while retaining the anisotropic tensorial form of the original stretched-vortex model for the SGS stress and the SGS buoyancy flux. As noted in the introduction, the term model here is synonymous with turbulence closure. This is a notation that is typically adopted in the LES literature (e.g., Pope 2004, and references therein), where “SGS model” refers to a suitable expression of the unclosed terms, (1) and (2), of the Navier–Stokes equations.

a. Review of the stretched-vortex model

The stretched-vortex SGS model for LES (Misra and Pullin 1997; Pullin 2000) models the unclosed terms, (1) and (2), by a physical description of the SGS field constructed from an ensemble of stretched-vortical structures, each of which satisfies the Navier–Stokes equations asymptotically (Lundgren 1982). Once this physical description is in place, statistics such as correlations, spectra, and high-order statistics can be calculated (Pullin and Saffman 1994, Lundgren 2001; O’Gorman and Pullin 2003). The stretched-vortex model performs well in a variety of flows (Misra and Pullin 1997; Pullin 2000; Voelkl et al. 2000; Kosović et al. 2002; Faddy and Pullin 2005; Hill et al. 2005; Pantano et al. 2006, 2007, 2008; Chung and Pullin 2009; Chung and Lundgren 2001; O’Gorman and Pullin 2003). The specific forms for the SGS stress and SGS scalar flux are respectively given by

\[ \tau_{ij} = \langle \delta_{ij} - \epsilon_{ij}^e \epsilon_{ij}^n \rangle K, \]  
\[ \sigma_i = -\left( \frac{\gamma}{2} \right) \hat{\Delta} K^{1/2} \langle \delta_{ij} - \epsilon_{ij}^e \epsilon_{ij}^n \rangle \partial \phi \partial \alpha_j, \]

where \( K \) is the SGS turbulent kinetic energy; \( \hat{\Delta} \) is the filter cutoff width, also identified as the SGS eddy length scale; \( \partial \phi \partial \alpha_j \) is the resolved scalar gradient; \( \epsilon_{ij}^e \) is the unit vector aligned with SGS vortices; the angle brackets denote averaging over the probability density function (pdf) of SGS vortex orientations; and \( \gamma \) is an \( O(1) \) constant that relates the eddy-turnover time \( T \) to \( K^{1/2} \) and \( \Delta \) via where \( \gamma \) is typically set to unity (Pullin 2000). In (3), \( \tau_{ij} \) models the full SGS stress tensor, including the anisotropic component. Using a single-vortex ensemble, for instance, \( \tau_{11} = (1 - \epsilon_{1e}^e \epsilon_{1e}^n)K, \tau_{12} = -\epsilon_{1e}^e \epsilon_{2e}^nK, \) and the trace, \( \tau_{ii} = \tau_{11} + \tau_{22} + \tau_{33} = (3 - 1)K = 2K, \) twice the SGS kinetic energy, as required. In contrast, the isotropic component of the standard Smagorinsky model is absorbed into the pressure, which is not the case in this SGS model. The cutoff-scale is often set equal to the effective grid spacing, \( \hat{\Delta} = (\Delta x \Delta y \Delta z)^{1/3} \). By definition, subgrid scale is considered any quantity on scales less than \( \hat{\Delta} \), regardless of the actual grid spacing. The basic form of the model, (3) and (4), originates from the expression for SGS stress tensor in a homogeneous anisotropic turbulent flow consisting of a collection of straight axisymmetric vortex structures [Pullin and Saffman 1994, their (8); Pullin 2000, his (24)].

Typically, a single orientation for SGS vortical structures is used for each grid cell, and therefore the orientation distribution is a delta function pdf and the angle brackets in (3) and (4) can be replaced by parentheses. The most often used orientation alignment is with the most extensional eigenvector of the resolved strain-rate tensor, \( \mathbf{S}_c = (\langle \partial \phi / \partial \alpha_j \rangle + \langle \partial \phi / \partial \alpha_j \rangle)/2 \) (Voelkl et al. 2000; Pantano et al. 2008), which is also employed in this study.

The SGS turbulent kinetic energy is determined by integrating the energy spectrum \( E(k) \); that is,

\[ K = \int_{\pi \Delta}^{\infty} E(k) \, dk, \]

associated with such an SGS field of stretched vortices. Even though (6) implies a sharp cutoff spectral filter, the LES filtering operation is formal and never employed; it is merely an indication that scales smaller than \( \Delta \) are to be treated as subgrid and need to be modeled, regardless of whether or not they are resolvable by the grid. The vortical structures are Lundgren (1982) spiral vortices with a three-dimensional energy spectrum given by

\[ E(k; \lambda_v) = K_0 e^{2/3} \lambda_v^{5/3} \exp(-k^2 \lambda_v^2), \]

where \( \lambda_v^2 = [2\nu/(3S_v)] \) (Pullin 2000), \( K_0 \) is the Kolmogorov prefactor, \( \epsilon \) is the local cell-averaged dissipation rate, \( \nu \) is the kinematic viscosity of the fluid, and

\[ S_v = -\langle \delta_{ij} - \epsilon_{ij}^e \epsilon_{ij}^n \rangle \partial \phi / \partial \alpha_j \]

is the strain aligned with the ensemble SGS vortex axis. The final step in determining the expressions for the subgrid terms is to estimate the product \( K_0 \epsilon^{2/3} \). This
provides closure and determines the value of the subgrid kinetic energy using the local, resolved-scale, second-order velocity structure function $F_2(r, x)$ (Metais and Lesieur 1992; Voelkl et al. 2000),

$$K_0^{2/3} = \frac{F_2}{A \Delta^{2/3}},$$

where

$$A = 4 \int_0^\pi s^{-5/3} \left(1 - \frac{\sin s}{s}\right) ds \approx 1.90695.$$  

A local (discrete) spherical average is used to estimate $F_2$,

$$F_2(\Delta; x) = \frac{1}{6} \sum_{i=1}^3 [(\delta u_1^x)^2 + (\delta u_2^x)^2 + (\delta u_3^x)^2] + [(\delta u_1^y)^2 + (\delta u_2^y)^2 + (\delta u_3^y)^2],$$

where

$$[\delta u^x_i] = \pi_i(x \pm \Delta x) - \pi_i(x)$$

is the velocity difference of component $u_i$ in direction $x_i$ at $x$. This allows the SGS terms to be estimated dynamically using only the local instantaneous resolved fields without performing any temporal or spatial averages. Note that all operations needed to evaluate the SGS terms are local in space and time, and the model is dynamic and without any free parameters.

b. On the relation between flow physics and model construction

Before we consider the necessary modifications for stratified flows, we comment on the relation between flow physics and the stretched-vortex SGS model construction. Turbulence is not composed of a collection of nearly axisymmetric noninteracting spiral vortices. However, similar to all turbulence closures, the stretched-vortex model is a framework, or construct, through which we can incorporate flow physics in order to accurately account for the unresolved motions. For instance, the vortex construct allows for SGS flow anisotropy. Moreover, the anisotropy, or the preferred SGS flow direction, is related to the dynamics of the large-scale flow (e.g., Yeung and Brasseur 1991) with observed preferential alignment between vorticity and strain (She et al. 1990; Bou-Zeid et al. 2010; Xu et al. 2011). This leads to a tensor eddy diffusivity model [(4)], where the SGS scalar flux is not necessarily aligned with the resolved gradient. The misalignment between the resolved gradient and the SGS flux is often observed in turbulent flows (Corrsin 1974; Sreenivasan et al. 1982). The classical Kolmogorov cascade dynamics are included through the structure of the Lundgren spiral vortex ($-5/3$-power inertial-subrange decay of the kinetic energy and scalar variance spectra).

The structure function matching, which determines the value of the SGS kinetic energy, corresponds to the self-similarity assumption that relates the dynamics of the flow above (resolved) and below (unresolved) $\Delta$. As we discuss in the following sections, these model attributes enable a stratification adjustment that is faithful to the flow physics. In summary, the stretched-vortex model is sufficiently versatile to allow physics to be incorporated but at the same time not overly complex such that too much empiricism is required to constrain a large number of degrees of freedom.

c. Framework for stratification adjustment

Consider the SGS turbulent kinetic energy equation, written without the storage and transport terms as is appropriate for a stationary and homogeneous SGS flow,

$$\frac{1}{2} \frac{\partial u_i u_i'}{\partial t} = b \theta' \frac{\partial u_i}{\partial x_i} - \epsilon_{\text{sgs}} - \frac{\partial u_i'}{\partial x_i} \frac{\partial u_i}{\partial x_i},$$

where the prime denotes SGS fluctuations so that $(1/2)u_i u_i'$ is identified as the SGS turbulent kinetic energy; $b \theta'$ is the SGS buoyancy flux representing the reversible conversion from potential energy to kinetic energy; $3$ is the direction opposing gravity; $\epsilon_{\text{sgs}}$ is the SGS irreversible viscous dissipation, $\nu (\partial u_i/\partial x_i)^2$; and $-\frac{\partial u_i'}{\partial x_i} \frac{\partial u_i}{\partial x_i}$ represents the production of SGS turbulent kinetic energy by the SGS flow working against the resolved gradient. The symbol for buoyancy $b$ is presently used as a generic buoyancy variable. For dry air, $b = g \theta' / \theta_{\text{ref}}$, where $\theta'$ is the perturbation potential temperature (Stevens 2005).

In neutrally stratified free-shear flows (Mason 1994; Pope 2004), the length scale characterizing the energy of the SGS flow field is set by $\Delta$ by designing simulations such that $\Delta$ lies within the inertial subrange of turbulence. However, this may no longer be the case in stable stratification in which the SGS flow may set its own smaller length scale. We expect reductions to both the SGS kinetic energy and SGS eddy size in stable stratification. In unstable stratification, we only expect an increase in the SGS kinetic energy but not the SGS eddy size since the largest eddies remain confined by the grid. To formalize, we anticipate a new SGS turbulent kinetic energy,

$$K_s = K_f K,$$

and a new SGS eddy length scale,
\( \hat{\Delta}_s = \hat{\Delta}_s f_{\hat{\Delta}}, \)  

(15)

where \( f_K \) and \( f_{\hat{\Delta}} \) are stratification-adjustment factors—to be determined—subject to the constraint in (13). The value \( K \) is known and can be computed as described in section 2a. The subscript \( s \) in \( K_s \) and \( \Delta_s \) stands for the values in stratified conditions. In the following model for stratification adjustment, we shall assume that stratification only modifies the kinetic energy \( K \) and, possibly, the characteristic length scale, but not the tensorial forms of (3) and (4). This is tantamount to assuming that, if mixing of the buoyancy field occurs, it occurs in the plane normal to the ensemble SGS vortex axis. Further, we shall assume that the SGS vortex alignment does not depend on stability. This assumption is supported by measurements of strain–vorticity alignments in the stably stratified surface layer (Bou-Zeid et al. 2010).

The first step in determining \( f_K \) and \( f_{\hat{\Delta}} \) is to substitute \( K_s \) and \( \Delta_s \) for \( K \) and \( \Delta \) in (3) and (4), with \( \phi = b \), and then identifying \( \tau_b \) and \( \sigma_1 \), respectively, with \( \overline{u_i^3 u_j^3} \) and \( \overline{u_i u_j} \) in (13) with \( \phi = b \), to obtain

\[ 0 = -(\gamma/2)\hat{\Delta}_s K_s^{1/2} N_v^2 - \epsilon_{\text{sgs}} + K_s S_v, \]  

(16)

where

\[ N_v^2 = \langle \delta_{ij} - e_i^s e_j^s \rangle \overline{\partial b/\partial x_j} \]  

(17)

is the resolved buoyancy gradient in the plane normal to the ensemble SGS vortex axis (see also discussion in section 2b). The term \( S_v \) is defined in (8). Both \( N_v \) and \( S_v \) are known from the resolved field. For reference, \( S_v > 0 \) implies \( -\overline{u_i^3 u_j^3/\partial x_j} > 0 \), corresponding to the stretching of the ensemble SGS vortex by the resolved-scale strain—an action that produces SGS turbulent kinetic energy, also known as forward scatter. Also, \( N_v^2 > 0 \) implies \( \overline{\partial b/\partial x_j} < 0 \), corresponding to the conversion of SGS kinetic energy to SGS potential energy when the buoyancy field is overturned by the SGS vortex ensemble. The magnitude of this conversion depends on both the local resolved-scale stratification \( \overline{\partial b/\partial x_j} \) and the alignment of the subgrid vortex \( e_i^s \) relative to gravity—a feature unique to the stretched-vortex SGS model. In setting \( \phi = b \) in the SGS turbulent kinetic energy equation [see (16)], we have converted the inactive scalar \( \phi \) into the active scalar \( b \) that is capable of modifying the SGS flow.

We now recast \( \epsilon_{\text{sgs}} \) in terms of \( K_s \) and \( \hat{\Delta}_s \) by introducing \( \kappa_v \), a coefficient similar to the von Kármán constant, associated with the SGS flow:

\[ \epsilon_{\text{sgs}} = K_s^{3/2}/(\kappa_v \Delta_s), \]  

(18)

originally due to Taylor (1935), often referred to as the zeroth law of turbulence (e.g., Rollin et al. 2011; Nedić et al. 2013). With respect to determining the stability-correction functions, \( f_K \) and \( f_{\hat{\Delta}} \), no assumptions have been made so far: \( \epsilon_{\text{sgs}} \) is merely recast in dimensionless form using \( \kappa_v \). Upon substitution into (16), we obtain

\[ 0 = -(\gamma/2)\hat{\Delta}_s K_s^{1/2} N_v^2 - K_s^{3/2}/(\kappa_v \hat{\Delta}_s) + K_s S_v. \]  

(19)

Now, the value of \( \kappa_v \) is determined from neutral stratification at large Reynolds numbers; that is, set \( N_v^2 = 0, \hat{\Delta}_s = \hat{\Delta}, K_s = K, \) and \( S_v \Delta^2/\nu \gg 1 \) to find

\[ (\kappa_v \hat{\Delta}/K_s^{1/2})S_v = 1, \]  

(20)

which dynamically defines \( \kappa_v \) in terms of the known \( S_v \) and \( K_s \) independent of stratification. This can be compared with its counterpart in Monin–Obukhov theory that \( (\kappa z/\langle u_d \rangle) d\tau/\langle z \rangle = 1 \), where \( \kappa \) is the von Kármán constant and \( z \) the distance from the surface (i.e., the characteristic eddy size). One can interpret \( \Delta \) as playing the role of a confinement scale in neutral stratification that scales the largest SGS eddies in a way that is analogous to the height \( z \) in the surface layer. In this sense, \( \kappa_v \) is a vortex-based von Kármán constant that scales the largest eddies with the velocity scale \( K_s^{1/2} \) in a neutral flow configuration defined by \( \Delta \) subject to background straining \( S_v \) of the vortex ensemble. The high Reynolds number condition is required to ensure consistency with the interpretation that \( \kappa_v \) is related to quantities associated with the geometry of turbulence production as opposed to quantities influenced by viscosity. Hereafter, \( \kappa_v \) is known from (20). The remaining unknowns of (19) are \( K_s \) and \( \Delta_s \).

Next, we define a vortex-based Obukhov length \( L_v \) by identifying \( u_a \) with \( K_s^{1/2} \) and substituting for \( \overline{b u_i^3} \) from (4):

\[ L_v = K_s^{3/2}/(-\kappa_v \overline{b u_i^3}) = K_s \kappa_v (\gamma/2) \Delta_s N_v^2 \]  

(21)

[cf. the usual Obukhov length \( L = u_a^3/(-\kappa b \overline{u_i^3}) \)]. The definition in (21), which comes from the stretched-vortex closure for scalar flux [see (4)], implies that \( \Delta_s^{1/2} L_v^{1/2} \propto K_s^{1/2}/N_v \)—a vortex-based buoyancy length scale. This relationship is consistent with the scaling relationship between the mixing length \( l_m \), the Obukhov length \( L \), and the buoyancy length \( l_b = u_b \nu /N \) that \( l_m^{1/2} L^{1/2} \propto l_b \) (Chung and Matheou 2012). Stratification is stable when \( L_v > 0 \), unstable when \( L_v < 0 \), and neutral when \( L_v = \infty \). Substituting (21) into (19) along with (20) reduces the stationary and homogeneous SGS turbulent kinetic energy equation to

\[ \left( \frac{K}{K_s} \right)^{1/2} \Delta_s^{1/2} S_v = L_v + \Delta_s. \]  

(22)
As often encountered in the study of stratified turbulence, this is one equation for two unknowns: \( K_s \) and \( \Delta_s \). We will use a scaling ansatz to close this system when we consider the case of stable stratification.

The parameters of the stratification-adjustment problem for the stretched-vortex model intrinsically suggest a length-scale stratification parameter that is similar to the Obukhov length. The choice of the stratification parameter is not critical. However, the Monin–Obukhov framework for sheared stratified turbulence of Chung and Matheou (2012) is particularly appropriate here.

d. Unstable stratification

The simpler case of unstable stratification is considered first. In this case, \( \Delta_s / L_v < 0 \). However, \( \Delta_s = \Delta_s \Delta = \hat{\Delta}; f_\Delta = 1 \). That is, the largest SGS scales remain confined by \( \Delta \), and accordingly no adjustment is needed for the eddy length scale. Then, with no further assumptions, (22) immediately simplifies to

\[
K_s = Kf_K = K/(1 + \xi_v)\,^2, \tag{23}
\]

where

\[
\xi_v = \hat{\Delta}/L_v \tag{24}
\]

is the vortex-based dimensionless height, used as the stability parameter in the buoyancy-correction functions. Note that \( \xi_v \) depends implicitly on the ensemble orientation of the SGS vortices—an important aspect of the SGS model that we will explore in section 2h. We have determined \( f_K(\xi_v) \) and \( f_\Delta(\xi_v) \) for unstable stratification. It remains to determine \( \xi_v \) in terms of known quantities measured on the grid. Combining (21), \( \Delta_s = \Delta \), (23), and (20), we find that

\[
R_i/(\kappa_v/\gamma) = 2\xi_v/(1 + \xi_v)^2, \quad \xi_v < 0, \tag{25}
\]

where

\[
R_i = N^2/\nu^2, \tag{26}
\]

the vortex-based gradient Richardson number. In the case of unstable stratification, \( R_i \) is negative. We now consider the limit of very unstable conditions \( R_i \to -\infty \), \( \xi_v \to -1 \), which is the pure buoyancy-driven (no mean shear) confined mixing regime, also known as free, or unforced, convection. In this free-convection regime, buoyancy forcing is entirely balanced by dissipation, the first two terms on the right-hand side of (19), and \( K_s^3/(\kappa_v \Delta_v) = U^3/\nu^2 \) recovers \( K_s^{1/2} = (\kappa_v \Delta_v/\nu^2)^{1/3} \), the generalized Deardorff velocity, which is the velocity scale traditionally used for free convection capped by an inversion (Deardorff 1970). This limit can be verified by inspecting (22), putting \( \Delta_s = \Delta = -L_v \), and noting that the shear production must drop out.

e. Stable stratification

We now consider stable stratification. In this case, we can no longer expect a fixed \( \Delta \) to lie within the inertial subrange of the energetic SGS eddies. Indeed, unlike SGS eddies in neutral and unstable stratification that interact actively and directly with the resolved eddies through the Richardson–Kolmogorov cascade, the energetic SGS eddies in strong stratification can be small relative to \( \Delta \) such that their dynamics become less coupled to the resolved flow. The decoupling of the scale dynamics is similar to the z-less scaling of stably stratified turbulence in the surface layer, with a continuum of eddy sizes from large to small scales. Presently, we introduce a scaling ansatz, borrowing from a well-established relationship in atmospheric surface layers (Kaimal et al. 1972) and reinforced by DNS (Chung and Matheou 2012), that \( 1/\Delta_s = 1/\Delta + (\alpha - 1)/L_v \); that is,

\[
\hat{\Delta}_s = \Delta_s \Delta = \Delta[1 + (\alpha - 1)/\xi_v], \tag{27}
\]

where \( \alpha \) is a model constant. This is a robust functional form for the parameterization of the characteristic length scale in stably stratified turbulence that has been extensively used in the past since Brost and Wyngaard (1978) and Nieuwstadt (1984).

Equation (27) implies that the SGS eddies scale as the weighted harmonic average of \( \Delta \) and \( L_v \). In terms of the dimensionless height, \( \xi_v \gg 1 \) (very stable) means \( \Delta_s = L_v/(\alpha - 1) \). For \( \Delta_s \), one can formally write \( f(\hat{\Delta}_s, \Delta_s, L_v) = 0 \). In very stable stratification, \( \Delta \) becomes inconsequential and \( \Delta_s \propto L_v \), and similarly, in neutral stratification, \( L_v \) is irrelevant and so \( \Delta_s \propto \Delta \). The harmonic average in (27) simply amalgamates the two limits. We can interpret \( 0 < \xi_v < 1 \) as the weakly stable regime where the largest eddies are still resolved by the LES, but the damping effects of stratification are nevertheless felt by the SGS field. On the other hand \( \xi_v > 1 \Leftrightarrow L_v < \Delta \) means that the most energetic SGS eddies that scale with \( L_v \) are no longer resolvable by the LES. In other words, the SGS flow is deemed strongly stratified relative to \( \Delta \).

Combining the length-scale ansatz in (27), to close (22), we obtain

\[
\frac{\nu^2}{K_s^{1/2}} S_v = 1 + \alpha \xi_v, \quad \text{i.e., } K_s = Kf_K = \frac{K}{(1 + \alpha \xi_v)^2}. \tag{28}
\]

We have now determined \( f_K(\xi_v) \) and \( f_\Delta(\xi_v) \) for stable stratification. Compare (28) with its counterpart in Monin–Obukhov theory that \( \phi_f(\xi) = (\kappa z/\nu) d\tau/d\xi = 1 + \beta_\infty \xi \). It
overturning motions are damped by stable stratification instead, its role is to describe how quickly turbulent activities on the stretched-vortex model, we simply multiply $K$ and $\Delta$ by $f_K(\zeta_v)$ and $f_\Delta(\zeta_v)$ in (3) and (4), where $K$ is determined by the usual structure-function matching procedure (Voelkl et al. 2000) as if the SGS flow were unstratified and $\Delta$ is the LES filter width. For convenience, we explicitly summarize the stratification adjustment as follows:

$$\tau_i = (\delta_{ij} - e_i^e e_j^e)K_s,$$

$$\sigma_i = -(\gamma/2)\dot{\Delta}K_s^{1/2}(\delta_{ij} - e_i^e e_j^e)\partial\bar{\theta}/\partial x_j,$$

where $e_i^e$ is defined in section 2a, $K_s = Kf_K(\zeta_v)$, $\Delta_s = \Delta f_\Delta(\zeta_v)$.

FIG. 1. DNS (dots) suggests that the model constant, given by $\alpha = Rf_i^{-1} = \lim_{Rf_i \to \infty} Rf_i^{-1}$, is approximately 5.0 (line).

remains to determine $\zeta_v$ in terms of $Ri_v$. To this end, we combine (21), (27), (28), and (20):

$$Ri_v/(\kappa_v/\gamma) = 2\zeta_v[1 + (\alpha - 1)\zeta_v]/(1 + \alpha\zeta_v)^2, \quad \zeta_v > 0.$$  

(29)

f. Determination of model constant

The only model constant is $\alpha$, and it is only used in stable stratification. Note that $\alpha$ in (27) does not play a role in describing the dynamics of weak stratification; instead, its role is to describe how quickly turbulent activities on the stretched-vortex model gives $(\kappa_v/\Delta/K_s^{1/2})S_v \sim \alpha\Delta/L_w$, or upon rearranging,

$$\alpha \sim \kappa_v/K_s^{1/2}S_vL_w \sim \frac{K_sS_v}{-b^3u'_3} \sim \frac{-b^3u'_3}{-b^3u'_3} = Rf_i^{-1},$$

(30)

the stable limit of the negative production-to-buoyancy-flux ratio, or simply the inverse critical flux Richardson number $Rf_i^{-1}$. Note that the final expression in (30) is independent of the geometry of turbulence production, and hence independent of the choice of $e_i^e$. If $Rf_i \approx 0.2$, as is common in the atmospheric surface layer (e.g., Businger et al. 1971), then $\alpha \approx 5.0$. Using DNS data of Chung and Matheou (2012), we determine the value of $\alpha$ as $\lim_{Ri_v \to \infty} Rf_i^{-1}$, which is consistent with $\alpha = 5.0$ (see Fig. 1).

g. Model summary

To use the stratification adjustment in the stretched-vortex SGS model, we simply multiply $K$ and $\Delta$ by $f_K(\zeta_v)$ and $f_\Delta(\zeta_v)$ in (3) and (4), where $K$ is determined by the usual structure-function matching procedure (Voelkl et al. 2000) as if the SGS flow were unstratified and $\Delta$ is the LES filter width. For convenience, we explicitly summarize the stratification adjustment as follows:

$$\tau_i = (\delta_{ij} - e_i^e e_j^e)K_s,$$

$$\sigma_i = -(\gamma/2)\dot{\Delta}K_s^{1/2}(\delta_{ij} - e_i^e e_j^e)\partial\bar{\theta}/\partial x_j,$$

where $e_i^e$ is defined in section 2a, $K_s = Kf_K(\zeta_v)$, $\Delta_s = \Delta f_\Delta(\zeta_v)$.

$\alpha \approx 5.0$, $\gamma \approx 1.0$, and $\zeta_v$ is determined by inverting (25) and (29):

$$\xi_v = \begin{cases} \frac{g}{2} \left[ 1 + (\alpha - 1)\zeta_v \right], & \zeta_v > 0 \\ 1, & \zeta_v \leq 0 \end{cases},$$

(34)

$$Ri_v = Ri_v/(\kappa_v/\gamma),$$

(36)

where

$$Ri_v = \frac{N_s^2}{S_v} = \frac{(\delta_{ij} - e_i^e e_j^e)\partial\bar{\theta}/\partial x_j}{(-\delta_{ij} - e_i^e e_j^e)\partial\bar{\bar{\Pi}}/\partial x_j)^2},$$

(37)

$$\kappa_v = K_s^{1/2}\frac{S_v}{S_v^{1/2}} = \frac{S_v^{1/2}}{S_v^{1/2}}.$$

(38)

The piecewise functions are continuous through $\xi_v = 0$. See Fig. 2 for plots of $Ri_v$ and the stability functions $[f_K(\xi_v) \text{ and } f_\Delta(\xi_v)]$.

h. Physical interpretation of stratified model

A novel feature of the buoyancy adjustment is that $Ri_v$ depends on $e_i^e$ through (37). The dependence of SGS turbulent activity upon $e_i^e$ can be interpreted as a model for intermittent patches of turbulence frequently observed in very stable high-$Ri$ environments (e.g., Pardyjak et al. 2002; Fernando and Weil 2010). This is because the SGS model allows for SGS turbulence activity even if...
the nominal Ri is large, since it does not necessarily follow that Ri is, large because Ri ≠ Ri. Ri captures an important feature of a vertically stratified environment: that it is easier to stir in the horizontal than in the vertical. This is achieved in a local and dynamic fashion without any flow-adjustable parameters. Using the choice for SGS vortex orientation \( \mathbf{e}^v = \mathbf{e}_3 \) (most extensional eigenvector of the strain-rate tensor), we illustrate the link between the anisotropic character of the SGS model and the physics of stratified turbulence with two cases: first, vertically axisymmetric straining flow, and second, vertically shear eddies.

In the first case, the SGS flow is subjected to a vertically axisymmetric incompressible background strain described by \( \partial \mathbf{u}_i / \partial x_j = S \delta_{ij} \), and background stratification \( \partial \mathbf{b}_i / \partial x_j = \delta_{ij} N^2 \) such that the choice \( \mathbf{e}^v = \mathbf{e}_3 \) now gives \( e_i^v = \delta_{i3} \) (Fig. 3b). Then \( S_v = S/2 \) and \( N_v^2 = N^2/2 \); that is, we have \( \text{Ri}_v = 2N_v^2/S_v^2 = 2\text{Ri} \), which is twice the usual gradient Richardson number. For weak stratification, (29) can be expanded for small \( \zeta_v \) to give \( \text{Ri}_v/(\kappa_v/\gamma) \approx 2\zeta_v \); that is, \( \text{Ri}_v \sim (\kappa_v/\gamma)\zeta_v \).

The vortex-based von Kármán constant is dynamically determined as part of the running simulation, and an estimate can be found if we identify the eddy-turnover time as \( T_s = K_s/\epsilon_{\text{gs}} \). We then eliminate \( \epsilon_{\text{gs}} \) via (18), giving \( T_s = \kappa_v T_s/\kappa_s \), where \( \kappa_s \) can be compared with (5) to get \( \kappa_s/\gamma \approx 1 \). And thus, \( \text{Ri} \sim \zeta_v \), which is comparable to measurements of the atmospheric surface layer in weak stratification that indicate \( \text{Ri} \sim 0.74\zeta \) (Businger et al. 1971). On the other hand, when the stratification is strong, (29) gives \( \text{Ri}/(\kappa_v/\gamma) \sim 2(\alpha - 1)/\alpha^2 \approx 0.32 \) for \( \alpha \approx 5.0 \), or using the previous estimates that \( \kappa_v/\gamma \approx 1 \) and that \( \text{Ri}_v = 2\text{Ri} \) in vertically shear eddies, we obtain \( \text{Ri} \sim 0.16 \) again, comparable to atmospheric-surface-layer measurements in strong stratification that indicate \( \text{Ri} \sim 0.21 \).

When \( \text{Ri}/(\kappa_v/\gamma) > 2(\alpha - 1)/\alpha^2 \approx 0.32 \) (Fig. 2a), the flow is strongly stratified and so a stationary SGS flow can no longer be sustained, leading to \( f_K = f_\Delta = 0 \). If \( \text{Ri}_v < 0 \), the flow is unstably stratified and the SGS buoyancy adjustment is thought to be unnecessary since the
energetic scales are likely to be in the resolved scales (Chung and Pullin 2010), but the adjustment is included in the present model extension, as it may be needed if the flow is far from equilibrium.

3. Subgrid-scale statistics
   a. SGS-continued one-dimensional spectra

   One-dimensional spectra are the type most often encountered in the study of turbulent flows, especially in measurements. By construction, LES provides a limited range of scales. However, here we utilize the multiscale character of the stretched-vortex SGS model to recover information about the unresolved scales to augment the resolved-scale statistics. We consider how to construct the one-dimensional spectrum $\Theta_{ij}(k_3)$ that contains contributions from the SGS motion as implied by the SGS model of stretched vortices. The direction indicated by the subscript $3$ in $k_3$ is chosen, without loss of generality, as the dimension onto which the full three-dimensional spectrum $F_{ij}(k)$ is collapsed. At any $k_3$, the one-dimensional spectrum comprises not only contributions from the resolved scales $\Theta_{ij}^{res}(k_3)$ but also contributions from the subgrid scales $\Theta_{ij}^{sgs}(k_3)$ (Pullin and Saffman 1994; Mattner 2011) even for $k_3 < k_c$; the latter aliasing contribution is an artifact of the one-dimensional spectrum. The decomposition is formally written as

   $$\Theta_{ij}(k_3) = \Theta_{ij}^{res} + \Theta_{ij}^{sgs} = \int_{k<k_c} \Phi_{ij}(k) dk_1 dk_2 + \int_{k>k_c} \Phi_{ij}(k) dk_1 dk_2,$$

where $k = (k_1^2 + k_2^2 + k_3^2)^{1/2}$ and $\Phi_{ij}(k)$ is the usual three-dimensional velocity spectrum tensor (Batchelor 1953). Presently, we shall only be concerned with principal spectra—namely, $\Theta_{11}$, $\Theta_{22}$, and $\Theta_{33}$. In the context of the stretched-vortex SGS model, the forms of the SGS contribution to one-dimensional spectra are known (Pullin and Saffman 1994; Chung and Pullin 2009; Mattner 2011), summarized as follows:

   $$\Theta_{11}^{sgs}(k_3) = \left( \frac{2}{\pi} \left( \frac{I_1 \cos^2 \theta \cos^2 \phi + I_2 \sin^2 \phi}{\sin \theta} \right) \right),$$
   $$\Theta_{22}^{sgs}(k_3) = \left( \frac{2}{\pi} \left( \frac{I_1 \cos^2 \theta \sin^2 \phi + I_2 \cos^2 \phi}{\sin \theta} \right) \right),$$
   $$\Theta_{33}^{sgs}(k_3) = \left( \frac{2}{\pi} \left( \frac{I_1 \sin^2 \theta}{\sin \theta} \right) \right),$$

where

   $$I_1 = \int_{0}^{\pi} E_{1}(k_3 \sin \theta | s)(s^{-2} - 1)^{1/2} ds,$$

...
where \( s_a = \min\{1, |k_3\sin\theta|/|k_c|\} \) and \( \theta \) and \( \phi \) are the Euler angles, relative to the 3 frame, of subgrid vortices that contribute to the ensemble implied by the orientation average given by the angle brackets. As a check, one can integrate (40)–(42) and (43) and (44) to further show that

\[
K_s = \frac{1}{2} \int_{-\infty}^{\infty} \Theta_{sgs}^3(k_3) \, dk_3 = \int_{k_c}^{\infty} E_s(k) \, dk,
\]

where \( E_s(k) \) is the SGS energy spectrum containing the stratification adjustment, described next in section 3b. The computation of SGS spectra is part of the post-processing step. Because numerical quadrature is expensive, the integrals in (43) are sampled and averaged randomly in homogeneous directions over a smaller section \( 2g \). By definition, the integrals in (40)–(42) and (43) and (44) to further show that 

\[
I_2 = \int_{0}^{s_a} E_s(|k_3\sin\theta|/s)(s^2 - 1)^{1/2} \, ds,
\]

Fig. 4. Stability correction for various \( \zeta_v = \pi/(k_c L_w) \) to SGS energy spectrum for fixed \( k_c L_w = 0.01 \) shown for subgrid wavenumbers \( k/k_c > 1 \). Clockwise: \( \zeta_v = -0.5, -0.2, -0.1, 0, 0.1, 0.2, 0.5, 1 \).

damping the large scales (low wavenumbers) through \( f_E \). That is, stable stratification introduces its own energetic peak, which may be smaller than \( \Delta \); this picture is consistent with DNS (Chung and Matheou 2012).

c. Subgrid-scale contribution to the root-mean-square of velocity-derivative fluctuations

A salient feature of the stretched-vortex SGS model is its detailed physical description of SGS motion, which allows, in principle, the calculation of any SGS statistic of interest. Presently, we describe the procedure for computing the SGS contribution to the root-mean-square of velocity-derivative fluctuations \( \langle u_{\alpha,\beta}^2 \rangle \) (no summation implied over \( \alpha \) or \( \beta \)). These quantities are used to compute dissipation-related statistics, such as the Taylor Reynolds number. To begin, these quantities can be formally expressed as

\[ u_{\alpha,3} u_{\alpha,3} = \int_{-\infty}^{\infty} k_3^2 \Theta_{\alpha a}^{sgs}(k_3) \, dk_3, \]

(no summation implied over \( \alpha \)). Substituting (40)–(42), exchanging the order of integration, and changing variables, this simplifies to

\[
\frac{u_{1,3}^2 u_{1,3}}{u_{1,3}} = \frac{2}{J_1} \left( J_1 \cos^2 \theta \cos^2 \phi + J_2 \sin^2 \phi \right),
\]

\[
\frac{u_{2,3}^2 u_{2,3}}{u_{2,3}} = \frac{2}{J_1} \left( J_1 \cos^2 \theta \sin^2 \phi + J_2 \cos^2 \phi \right),
\]

\[
\frac{u_{3,3}^2 u_{3,3}}{u_{3,3}} = \frac{2}{\sin \theta} \left( J_1 \sin^2 \theta \right),
\]
Table 1. LES parameters. The parameter $c(N^2)$ is often referred to as the buoyancy Reynolds number; $Rf$ and $Ri$ are the flux and gradient Richardson numbers; $\Delta$ is the LES cutoff scale; $\Delta x$ is the grid spacing; $N$ is the number of grid points; and $L$ is the domain length. For all cases, $L_x/N_x = L_y/N_y = L_z/N_z = \Delta x$ and $Pr = 0.7$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$c(N^2)$</th>
<th>$Rf$</th>
<th>$Ri$</th>
<th>$\Delta/\Delta x$</th>
<th>$N_x$</th>
<th>$N_y$</th>
<th>$N_z$</th>
<th>$L_x/L_z$</th>
<th>$L_y/L_z$</th>
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</thead>
<tbody>
<tr>
<td>A0</td>
<td>$4.0 \times 10^8$</td>
<td>0.09</td>
<td>0.075</td>
<td>1</td>
<td>256</td>
<td>128</td>
<td>128</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>A1</td>
<td>$4.0 \times 10^8$</td>
<td>0.09</td>
<td>0.082</td>
<td>2</td>
<td>512</td>
<td>256</td>
<td>256</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>A2</td>
<td>$4.0 \times 10^8$</td>
<td>0.09</td>
<td>0.081</td>
<td>4</td>
<td>1024</td>
<td>512</td>
<td>512</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>$1.1 \times 10^8$</td>
<td>0.13</td>
<td>0.119</td>
<td>1</td>
<td>512</td>
<td>256</td>
<td>256</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

where

$$J_1 = \int_{-\infty}^{\infty} k_3^3 I_1 dk_3 = \frac{\pi}{8} \sin^3 \theta \int_{k_c}^{\infty} k^2 E_s(k) dk, \quad (53)$$

$$J_2 = \int_{-\infty}^{\infty} k_3^2 I_2 dk_3 = \frac{3\pi}{8} \sin^2 \theta \int_{k_c}^{\infty} k^2 E_s(k) dk. \quad (54)$$

As a check for consistency, one can sum over all the velocity components,

$$\overline{u_{j,k}^{'}u_{j,k}^{'}} = \int_{-\infty}^{\infty} k_3^2 \Theta_{jk}^{\text{gs}}(k_3) dk_3 = \sin^2 \theta \int_{k_c}^{\infty} k^2 E_s(k) dk. \quad (55)$$

Now, put $\sin^2 \theta = 1 - \cos^2 \theta$ and sum over three directions, recalling that the square of the direction cosines sum to unity, to recover

$$\overline{u_{j,k}^{'}u_{j,k}^{'}} = 2 \int_{k_c}^{\infty} k^2 E_s(k) dk, \quad (56)$$

as required. For numerical computation, we rewrite the SGS dissipation integral as

$$\int_{k_c}^{\infty} k^2 E_s(k) dk = k_c^2 \int_1^{\infty} x^2 E_s(xk_c) dx$$

$$= k_c^3 \int_0^1 y^{-4} E_s(k_c/y) dy, \quad (57)$$

where the final form is computed using numerical quadrature. Again, as with SGS spectra, we sample this quantity randomly over a small fraction of the volume in homogeneous directions.

### 4. Stationary homogeneous stratified sheared turbulence

To assess the performance of the newly developed stratification adjustment of the stretched-vortex SGS model, we perform an LES of a stably stratified flow. Because LES modeling of stably stratified turbulence has been more challenging than the unstable/convective cases, the scope of Part I is limited to stable stratification. In Part II, we thoroughly assess both stable and unstable stratification using more complex setups.

The case considered presently is the canonical configuration of a homogeneous stably stratified turbulent flow that is driven by shear. The spatially uniform shear, the means by which turbulence is produced, is dynamically adjusted at each time step such that the kinetic energy and all turbulence statistics remain stationary. Similar to the mean shear, the mean density profile varies linearly with height but is constant in time. Accordingly, triply periodic boundary conditions are used to enforce homogeneity. The Boussinesq approximation is used to account for the effects of density stratification. The flow has been the subject of a previous DNS investigation (Chung and Matheou 2012). The current numerical solution methodology and method of analysis of the turbulence statistics are identical to those in Chung and Matheou (2012).

We run two cases corresponding to very high Reynolds numbers and moderately high stratification. (As discussed in the introduction, the case of very high stratification requires a tailored numerical method that can gracefully handle discontinuities without being overly dissipative—an area beyond the scope of the present study.) To assess the robustness of the SGS model, case A is run for three grid resolutions. Table 1 lists the parameters of the simulations and Table 2 lists statistics of the simulations, including the fraction of SGS contribution to the various statistics, calculated using the techniques described in section 3. In Tables 1 and 2 only the buoyancy Reynolds number $R = c(N^2)$ is prescribed. These Reynolds numbers are chosen to be as large as possible so that the resulting predictions can be attributed to the performance of the SGS model alone. Because the flow is homogeneous, the nondimensional bulk statistics of Tables 1 and 2 completely characterize the flow. Figures 5 and 6 show instantaneous snapshots of the density fluctuation (without the mean) field on three planes [cf. images in Chung and Matheou (2012) and Matheou and Chung (2012)]. The reduction of the vertical energetic motion scale is noticeable in the more-stratified case B compared to case A.
As required in LES, most of the turbulent kinetic energy is resolved (SGS motion contributes about 10% in both cases), but virtually all of the turbulent dissipation is modeled (occurs subgrid). Note that the stretched-vortex model is “aware” of the flow Reynolds number since the fluid’s molecular viscosity explicitly enters the model through (7). An estimate for the Taylor Reynolds number is available because the SGS contribution to quantities like \((\hat{u}'\hat{u}'/\hat{x})^2\) can be computed (see section 3c). In this section, the postprocessed SGS statistics are computed using the grid-independent form of the local subgrid energy spectrum [(6)] by putting \(S_\nu = \left[\epsilon_{\text{sgs}}/(15\nu)\right]^{1/2}\) in (6) so that \(\lambda_\nu = (20/3)^{1/4}\eta_{\text{sgs}}\), where \(\eta_{\text{sgs}} = (\nu^3/\epsilon_{\text{sgs}})^{1/4}\) (cf. Chung and Pullin 2010 and Mattner 2011).

A distinctive feature of the stretched-vortex SGS model is that, because of the structural nature of the turbulence closure, many subgrid-scale statistics can be estimated. In addition to bulk (scalar)-flow quantities, such as SGS velocity-derivative statistics, subgrid-scale spectra can be computed using the technique described in section 3a. One-dimensional spectra, resolved and SGS continued, are shown in Fig. 7. The composite spectra are plotted in Monin–Obukhov coordinates on the horizontal axis and Kolmogorov coordinates written in Monin–Obukhov variables on the vertical axis, which is a convenient scaling for this flow (cf. Kaimal et al. 1972 and Chung and Matheou 2012). If the resolved spectra were plotted alone, it would appear that the smallest resolved scales do not exhibit the expected inertial scaling. It appears from Fig. 7 that the missing energy near \(\Delta\) has been transferred to the subgrid scales, explained in the following. The scales smaller than \(\Delta\) should be treated by

### Table 2. Taylor statistics, including SGS contributions: \(\text{Re}_\lambda = \lambda u_{\text{rms}}/\nu, \lambda = u_{\text{rms}}/(\hat{u}'\hat{x})_{\text{rms}}\)

<table>
<thead>
<tr>
<th>Case</th>
<th>(\nu(V^3))</th>
<th>(\text{Re}_\lambda)</th>
<th>SGS fraction of (u'^2_{\text{rms}})</th>
<th>SGS fraction of (\hat{u}'\hat{x}'_{\text{rms}}^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A0</td>
<td>(4.0 \times 10^8)</td>
<td>(3.9 \times 10^7)</td>
<td>0.13</td>
<td>0.999</td>
</tr>
<tr>
<td>A1</td>
<td>(4.0 \times 10^8)</td>
<td>(4.0 \times 10^7)</td>
<td>0.13</td>
<td>0.999</td>
</tr>
<tr>
<td>A2</td>
<td>(4.0 \times 10^8)</td>
<td>(4.0 \times 10^7)</td>
<td>0.13</td>
<td>0.999</td>
</tr>
<tr>
<td>B</td>
<td>(1.1 \times 10^8)</td>
<td>(1.9 \times 10^7)</td>
<td>0.10</td>
<td>0.999</td>
</tr>
</tbody>
</table>

FIG. 5. Snapshots of density fluctuations on three planes from case A0 of stratified homogeneous sheared turbulence.
the SGS model, regardless of whether these scales are resolvable by the grid. The SGS model is designed to actively dissipate resolvable modes \( k = \sqrt{k_x^2 + k_y^2 + k_z^2} > \pi/\Delta \). Because the SGS model is implemented in physical space, the dissipation does not occur over a narrow range in spectral space. In addition, the one-dimensional spectra collects all energies at a given \( k_x \), regardless of \( k \). Near the cutoff range, the number of modes that are actively dissipated \( (k > \pi/\Delta) \) but resolvable \( (k_x > \pi/\Delta) \) is significant leading to the drop in resolved-energy contribution as shown in Fig. 7. This interpretation is reinforced by the somewhat smooth composite spectra near the cutoff region, clearly showing that the dissipated energy transferred to the subgrid scale can be “reconstituted” by the SGS model. That the SGS motion contributes energy to the one-dimensional spectra even at low wavenumbers (large scales) is an artifact of the one-dimensional spectrum, as discussed in section 3a [see also section 8.1 in Tennekes and Lumley (1972)]. The small kink of the spectrum at the LES resolution scale is due to minor numerical aliasing at the highest resolved wavenumbers in the LES. This is commonly observed in simulations using pseudospectral methods (e.g., Kaneda et al. 2003; Yeung et al. 2005).

It is important to note that even though most of the turbulent kinetic energy is resolved, the flow is far from being an underresolved DNS, but a fully developed turbulent flow with a Taylor Reynolds number \( O(10^7) \)—a value that far exceeds those found in the atmosphere and ocean (cf. Brethouwer et al. 2007). Figure 7 corroborates this fact by showing that the smallest flow scale is \( 10^5 \) times smaller than the LES grid resolution.

Insensitivity to grid resolution is a good SGS model test. Grid convergence of LES statistics (e.g., mean profiles) does not imply a “flawless” prediction, but it is a necessary condition for a predictive model and a self-consistency check of the implementation. When considering an LES resolution parameter study, the two relevant parameters are \( \Delta \) and \( \Delta x \), and two types of resolution studies are possible: (i) the ratio \( \Delta/\Delta x \) can be fixed and \( \Delta x \) varied, or (ii) \( \Delta \) can be fixed and \( \Delta x \) varied. Here, we follow the latter procedure because our main interest is to investigate the pure behavior of the SGS model in the absence of numerical artifacts. This is especially needed in a physical LES of a stably stratified flow in which the SGS motion (and hence dissipation) can be smaller than “resolvable” by the grid if \( \Delta/\Delta x = 1 \). The ratio \( \Delta/\Delta x \) is varied from 1 to 4 for cases A0–A2. Tables 1 and 2 show
that the gradient and flux Richardson numbers and Taylor Reynolds number remain unchanged as $\Delta x$ is decreased. Comparison of these quantities is a rigorous test, as they strongly depend on SGS and second-order turbulence statistics. Figure 8 shows the grid independence of the resolved-scale and SGS spectra. An important implication of the collapse of the resolved-scaled spectra is that the smallest scales are accurate when $\Delta = \Delta x$, as it is typically used in LES. Further, the minor aliasing kink in the spectra near the cutoff scale for the lowest-resolution LES vanishes once the resolution is increased (Fig. 8). This supports the idea that the same kinks seen in Fig. 7 are merely numerical artifacts.

5. Conclusions

We developed and evaluated an SGS model suitable for use in large-eddy simulation of stably and unstably stratified turbulence. This represents a step forward in extending the capability of the methodology known as large-eddy simulation with subgrid-scale modeling (LES–SGS). A novel aspect of the present SGS model construction is the encapsulation of the anisotropic character of stably stratified turbulence. This is achieved by exploiting the structural character of the stretched-vortex SGS model, which, by design, accounts for the anisotropy of unresolved motions.

The extension of the stretched-vortex model to stratified turbulent flows is accomplished by appropriate modifications, or adjustments, to the SGS kinetic energy and characteristic length scale. The stability-correction
functions are based on an assumption that the SGS flow is statistically stationary within each grid cell for the duration of the time step—a common approximation in SGS modeling—and on a scaling ansatz that controls the reduction of the energetic length scale as the very stable regime is approached. This is a robust scaling that is analogous to the Monin–Obukhov similarity theory. In fact, the stability-adjustment formulation is founded on the Monin–Obukhov interpretation of homogeneous stratified turbulence (Chung and Matheou 2012). In very stable stratification, the model recovers the $z$-less limit, in which a vortex-based Obukhov length controls the SGS dynamics, while in very unstable stratification, the model recovers the free-convection limit, in which a vortex-based Deardorff velocity controls the SGS dynamics.

A key feature of the buoyancy-adjusted stretched-vortex model is that the adjustment depends both on the resolved flow and on the SGS flow structure. The stability adjustment limits vertical mixing when the subgrid vortical axes lie in the horizontal but allows horizontal mixing when the subgrid vortical axes lie in the vertical, even at high gradient Richardson numbers. The SGS model formulation remains local and dynamic, without any flow-adjustable parameters.

Large-eddy simulation of stationary and homogeneous stratified sheared turbulence is performed to assess the performance of the SGS model. The prediction for high Reynolds number ($Re_a \approx 10^7$) homogeneous stratified sheared turbulence is augmented by evaluation of the SGS contributions to one-dimensional spectra and rms of fluctuations.

In Part II, we demonstrate use of the buoyancy-adjusted stretched-vortex SGS model for LES of a variety of geophysical flows.

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