Large-eddy simulation of conditionally neutral boundary layers:
a mesh resolution sensitivity study

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ABSTRACT

Large-eddy simulation (LES) is used to model turbulent winds in a nominally neutral atmospheric boundary layer at varying mesh resolutions. The boundary layer is driven by wind shear with zero surface heat flux and is capped by a stable inversion. Because of entrainment the boundary layer is in a weakly stably stratified regime. The simulations use meshes varying from $128^2 \times 64$ to $1024^2 \times 512$ gridpoints in a fixed computational domain of size $(2560, 2560, 896)$ m. The subgrid-scale (SGS) parameterizations used in the LES vary with the mesh spacing. Low-order statistics, spectra, and structure functions are compared on the different meshes and are used to assess grid convergence in the simulations. As expected, grid convergence is primarily achieved in the middle of the boundary layer where there is scale separation between the energy containing and dissipative eddies. Near the surface second-order statistics do not converge on the meshes studied. The analysis also highlights differences between one-dimensional and two-dimensional velocity spectra; differences are attributed to sampling errors associated with aligning the horizontal coordinates with the vertically veering mean wind direction. Higher-order structure functions reveal non-Gaussian statistics on all scales, but are highly dependent on the mesh resolution. A generalized logarithmic law and a $k^{-1}$ spectral scaling regime are identified with mesh dependent parameters in agreement with previously published results.
1. Introduction

Large-eddy simulation (LES) has become an essential tool for studying a wide range of societal pertinent atmospheric boundary layer (ABL) applications (e.g., wind energy meteorology, Calaf et al. 2010; Abkar and Porté-Agel 2013; Churchfield et al. 2012; Sørensen et al. 2015; Allaerts and Meyers 2015) where accurate simulation and representation of near surface processes are needed. Hence the community needs to thoroughly investigate the numerous assumptions, components, and choices underpinning LES.

Although the fundamentals underpinning LES remain similar to their original formulation introduced numerous years ago (Lilly 1967; Deardorff 1970, 1972), recent advances in high performance computing allows for larger domains and higher resolutions such that LES can now simulate a sufficiently wide inertial range to provide important insight into turbulence beyond second-order statistics (Stevens et al. 2014). Since the physical sub-grid-scale model (SGS) used to close the equations depends on resolution, mesh size is a crucial factor. Increasing the number of grid points for simulations using similar domain lengths implies that finer turbulent structures are resolved. In the atmospheric surface layer, i.e. the portion of the ABL directly influenced by the underlying ground surface, the characteristic length scale of turbulence grows as $\kappa z$, where $\kappa$ is the von Kármán constant $\sim 0.4$ and $z$ is the distance from the surface. Thus close to the surface high resolution is needed. The inherent problem of resolving the surface layer and capturing the logarithmic law describing the mean wind speed is well described by Brasseur and Wei (2010) and will also be discussed later in this paper.

A target of the present work is to examine the impact of mesh resolution, $\Delta$, on neutral ABL turbulence generated by LES. In typical LES applications, the SGS model utilizes a turbulent eddy viscosity prescription $\nu_t \sim \sqrt{e \Delta}$ where $e$ is the SGS energy and $\ell$ is a length scale; the SGS
parameterization is made scale aware by choosing $\ell \sim \Delta$. Thus, variations in mesh spacing or equivalently turbulent eddy viscosity change the large-eddy Reynolds number $Re_\ell$ of the simulation (see section 4a). The impact of Reynolds number on turbulence is a traditional focus of direct numerical simulation (DNS) studies (e.g., Moin and Mahesh 1998), but its impact in atmospheric LES is rarely studied (e.g., Sullivan and Patton 2011; Bou-Zeid 2015).

In general, studying the effect of mesh resolution across the entire ABL is also relevant for applications where realistic turbulence profiles are needed, e.g., wind turbines operate in the lowest couple of hundred meters of the ABL and the turbulence is responsible for the loading and hence fatigue on the turbines. When deciding where to position a wind turbine, i.e. choosing the correct turbine class to match the local site conditions (International Electrotechnical Commission 2005), any uncertainty in predicting turbulence levels will manifest itself as an increased uncertainty of the turbine’s life expectancy and operation window.

The ABL can be naturally divided into three main canonical classes: the 1) neutral, 2) convective (or unstable) and 3) stable boundary layer, which can largely be characterized by zero, positive and negative surface heat fluxes, respectively. The effect of mesh resolution on turbulence simulated by large-eddy simulation in the latter two ABL classes has been carefully studied by Sullivan and Patton (2011, convective) and Sullivan et al. (2016, stable) with the same pseudo-spectral model utilized here. Both of those studies found that second-order turbulence statistics can be strongly affected by mesh size. In those studies, the ABL was also capped by potential temperature inversion creating a region through which warm air entrains from above by eddies of decreasing size as the turbulence interacts with the overlying stratification. Since increasing resolution alters the range of turbulent structures resolved, high resolution also potentially impacts the region surrounding the capping inversion and hence the ability to properly simulate ABL growth. We therefore use a similar set-up to the previous two aforementioned studies but examine the asymptotic situation.
of negligible heat flux at the surface, *i.e.* the neutral boundary layer in which production of turbulent kinetic energy primarily occurs through shear but where heat entrained at the top of the ABL ensures weak stable stratification throughout the ABL. This type of canonical boundary layer has been called an *inversion capped neutral* boundary layer or a *conditionally neutral* boundary layer in contrast to the Neutral Ekman boundary layer where temperature effects are completely absent. Neutral Ekman boundary layers were also recently studied with the same LES model as in our study (Jiang et al. 2018), and it was found that increased horizontal grid resolution has a profound effect on the size of the logarithmic layer near the ground by thinning the layer closest to the surface where the most energetic eddies are under-resolved by the LES.

Several studies have focused on LES of conditionally neutral boundary layers: Lin et al. (1996) focuses mainly on the momentum flux and vorticity balance, Pedersen et al. (2014) showed the development of boundary layers from looking at the terms in the turbulent kinetic energy equation (TKE), and Otte and Wyngaard (2001) primarily focused on the interfacial layer around the capping inversion, while Moeng and Sullivan (1994) compared the overall structure in relation to stable and convective boundary layers. Furthermore wind farm studies have been presented by Abkar and Porté-Agel (2013) and Allaerts and Meyers (2015, 2017) focusing on how the strength of the inversion affects wind turbine performance within farms as a result of altered momentum fluxes in the wake regions. Pollard et al. (1972) and Zilitinkevich et al. (2007) showed that the height of the boundary layer also depend on the Brunt-Väisälä frequency, thus adding another time scale to the problem in addition to that introduced by the Coriolis force. Common for all the studies just mentioned is that all the simulations discussed use fairly coarse resolution compared to those examined by Sullivan and Patton (2011) and Sullivan et al. (2016). Pedersen et al. (2014) claimed to observe mesh independence when it comes to capturing the log-law at the surface and when estimating the boundary layer growth rate, $w_e$ (in the absence of subsidence); but
we will show mesh-dependencies for statistics even down to second order for simulations using similar domain sizes but resolved by up to $1024^2 \times 512$ grid points on a domain with physical size $(2560 \text{ m})^2 \times 896 \text{ m}$. It should also be noted that Pan and Chamecki (2016) found a resolution dependence in the logarithmic layer of a canopy ABL when looking at non-Gaussian effects at the smallest scales through velocity structure functions.

The paper is organized as follows: Section 2 presents a description of the LES and its configuration. Section 3 provides an overview of the suite of LES simulations studied including the ABL development and sampling/averaging procedure considerations. Section 4 contains the analysis and discussions, and Section 5 provides a summary of the findings.

2. LES equations

We use the National Center for Atmospheric Research (NCAR) pseudo-spectral LES code (Sullivan and Patton 2011; Sullivan et al. 2016), mimicking a dry atmospheric boundary layer (ABL) under the Boussinesq approximation over a flat lower boundary with constant roughness length, $z_0$. The origin of the model goes back to the original work of Deardorff (1970) with the novel modifications introduced by Moeng (1984); Moeng and Wyngaard (1988).

The LES equations are formulated in a right-handed Cartesian coordinate system, $x = (x_1, x_2, x_3) = (x, y, z)$, for the spatial filtered variables, $\tilde{u}(x, t), \tilde{\theta}(x, t), \tilde{\pi}(x, t)$ and $e(x, t)$, which are the velocity, potential temperature, modified hydrodynamic pressure (normalized by a reference
density) and sub-grid-scale (SGS) kinetic energy, respectively:

\[ \partial_t \tilde{u}_i + \tilde{u}_i \partial_j \tilde{u}_j = -\partial_i \tilde{\pi} + \varepsilon_{ij3} f (\tilde{u}_i - U^G_i) + \beta \tilde{\theta} \delta_i3 - \partial_j \tau_{ij} \]  

(1)

\[ \partial_i \tilde{u}_i = 0 \]  

(2)

\[ \partial_i \tilde{\theta} + \tilde{u}_i \partial_i \tilde{\theta} = -\partial_i \tau_{i\theta} \]  

(3)

\[ \partial_i e + \tilde{u}_i \partial_j e = \mathcal{P} + \mathcal{B} + \mathcal{D} - \mathcal{E}. \]  

(4)

The incompressibility condition listed in eq. 2 leads to a Poisson equation for the pressure variable \( \tilde{\pi} \). The advection term in eq. 1 is written in rotational form, and the vertical momentum equation \((i = 3)\) is solved only for the part deviating from hydrostatic balance and the horizontal mean, i.e. \( \langle \tilde{u}_3 \rangle = 0 \) at all heights (Moeng 1984). The model is forced by a geostrophic relationship with a constant height independent geostrophic velocity \( U^G_i \) and Coriolis parameter \( f \), i.e. mimicking barotropic conditions. The buoyancy parameter, \( \beta = g/\theta_0 \), is held constant with gravitational acceleration \( g = 9.81 \text{ ms}^{-2} \) and reference potential temperature \( \theta_0 = 290 \text{ K} \). Where appropriate we will use explicit variable naming; \((u, v, w)\) instead of the more compact Einstein notation \((u_1, u_2, u_3)\) for the velocity vector.

We use Deardorff’s (1980) SGS model with a stability-corrected length scale. Details of the right-hand-side terms in eq. 4 representing shear production \( \mathcal{P} \), buoyancy \( \mathcal{B} \), diffusion \( \mathcal{D} \) and dissipation \( \mathcal{E} \) as well as the SGS terms in eqs. 1-4

\[ \tau_{ij} = u_i u_j - \tilde{u}_i \tilde{u}_j - \frac{\delta_{ij}}{3} (u_k \tilde{u}_k - \tilde{u}_k \tilde{u}_k) \]  

(5)

\[ \tau_{i\theta} = \tilde{u}_i \tilde{\theta} - \tilde{u}_i \tilde{\theta} \]  

(6)

\[ e = \frac{1}{2} (u_i \tilde{u}_i - \tilde{u}_i \tilde{u}_i). \]  

(7)

can be found in Deardorff (1980), Moeng (1984), Moeng and Wyngaard (1988). Near the surface we use the two-part SGS eddy-viscosity model extension which explicitly accounts for the
near-surface mean flow (Sullivan et al. 1994). For all simulations discussed, the scale at which the equations are filtered falls at scales at least decades larger $O(1 - 10m)$ than the Kolmogorov micro-scale $O(1mm)$, therefore the viscous terms that would otherwise appear in eq. 1 have been neglected. As in both Sullivan and Patton (2011) and Sullivan et al. (2016) the focus in this paper is on the dependence of mesh resolution given a specific SGS model. Results may therefore differ when applying SGS models of other types (such as the different Dynamic Smagorinsky models introduced and discussed in Porte-Agel et al. 2000; Meneveau and Katz 2000; Bou-Zeid et al. 2005, 2008).

We apply rough wall boundary conditions at the lower bottom 'surface' through specification of Monin-Obukhov similarity functions (Moeng 1984; Moeng and Sullivan 1994). At the upper boundary a radiation condition is applied (Klemp and Durran 1983). We use periodic boundary conditions at all lateral walls. Broad details regarding code parallelization and use of Fast Fourier Transforms to solve the Poisson equation for the non-local pressure can be found in Sullivan and Patton (2011).

Time is advanced through a third-order Runge-Kutta scheme, where the time step is dynamically calculated each iteration based upon a constant Courant-Friedrichs-Lewy (CFL) number of 0.5. We take advantage of the Galilean invariance of the governing equations and hence move the mesh with a speed equal to half the geostrophic speed $U^G$, which permits approximately a factor of two larger time step.
3. Design of LES experiments

a. Grid mesh

The focus is on mesh dependence of shear driven boundary layers under weakly stable stratification, hence a series of simulations have been conducted with varying mesh resolution from $128^2 \times 64$ to $1024^2 \times 512$ (Table 1). All simulations use the same domain size $(L_x, L_y, L_z) = (2560, 2560, 896)$ m, however the simulation duration $T$ differs slightly across simulations. $\Delta t_{avg}$ denotes the average time step in the simulations. As is common practice in pseudo-spectral codes in order to avoid aliasing effects, the top one-third wave numbers are ignored (Orszag 1971), meaning that the spatial resolution, i.e. the effective LES filter width is $\Delta_f = \left(\frac{3}{2} \Delta x \frac{3}{2} \Delta y \Delta z\right)^{1/3}$. Due to the doubling of resolution at each simulation level the aspect ratio, $\Delta x/\Delta z = \Delta y/\Delta z$ is held constant in our study. Brasseur and Wei (2010) discuss possible implications of grid aspect ratio for the “overshoot” problem in the logarithmic layer, and Ercolani et al. (2017) finds an optimal value of 4 (it is $\sim 1.4$ in our study and thus closer to the isotropy assumption in the SGS model) although it is not clear whether that result applies to incompressible pseudo-spectral solvers like the NCAR LES code.

b. Imposed parameters

The externally imposed parameters defining the canonical ABL are held constant for all runs, these include: surface heat flux $Q_0 = 0$ K m s$^{-1}$, geostrophic velocity $(U^G, V^G) = (5, 0)$ m s$^{-1}$, Coriolis parameter $f = 10^{-4}$ s$^{-1}$, and surface roughness length $z_0 = 0.05$ m. All simulations are initialized with constant potential temperature gradient, $\frac{\partial \theta_f}{\partial z} = 0.003$ K m$^{-1}$, throughout the domain. The subscript $f$ refers to the “free” atmosphere, i.e. the non-turbulent atmosphere into which the boundary layer develops. As time advances, boundary layer growth occurs as turbulent kinetic

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energy is produced by shear production at the surface and entrainment of potential temperature at the top. The stable stratification capping the ABL from above is characterized by a Brunt-Väisälä frequency $N^2 = \beta \frac{\partial \tilde{\theta}}{\partial z} = 10^{-4} \text{s}^{-2}$. The coordinate system is aligned with $i = 1$ in the direction of the geostrophic wind, $U^G$, which has consequences for one-dimensional spectral properties (see Section 4.c).

The velocity fields are initialized with the geostrophic wind profile. Incompressible velocity and temperature fluctuations initiate turbulence in the lowest 50 m. Following Beare et al. (2006), horizontally-homogeneous vertical profile of SGS kinetic energy is initialized in the lowest 250 m as: $e(z) = 0.4(1 - z/250)$.

c. Averaging procedures

Due to horizontal homogeneity we approximate ensemble averaging, $\langle \rangle$, with horizontal averaging, which then becomes only a function of the vertical direction $z$. We denote the local fluctuations in a variable, $\chi(x, y, z, t)$ as departures from the horizontal average according to:

$$\tilde{\chi}(x, y, z, t) = \tilde{\chi}(x, y, z, t) - \langle \tilde{\chi} \rangle (z, t),$$ (8)

where the time dependence has been kept in order to emphasize the inherent statistical non-stationarity of the flow. We use the longest duration simulation (Run B) to identify a pseudo-stationary time period for comparison of the different mesh-resolution simulations.

At every time step, we estimate the boundary layer height using two different methods: 1) the “maximum gradient method” applied to potential temperature (Sullivan et al. 1998) leading to $z_i$, and 2) finding the height, $h$, at which the square root of the total Reynolds stress $\left( \langle \tilde{u}'\tilde{v}' + \tau_{13} \rangle^2 + \langle \tilde{v}'\tilde{w}' + \tau_{23} \rangle^2 \right)^{1/4}$ falls to 5% of its surface value $u_*$ (Kosovic and Curry 2000). $u_*$ is evaluated at $z = \Delta z/2$, i.e. in the first grid point from the resolved horizontal velocities, $\tilde{u}$.
and $\tilde{\nu}$, through the logarithmic law. Figure 1 compares $z_i$ and $h$ for times larger than $35T_E$ for Run B, i.e. at times after the initial spin-up. We observe a linear relationship with a ratio, $z_i/h = 1.12$.

Since absolute numbers are not relevant, from here onward we will refer to $z_i$ as our ABL height estimate.

To compare the four simulations, we define a large-eddy turn-over time scale as $T_E = z_i/u_\star$. Figure 2 shows profiles of mean wind speed, $S = \left( \langle \tilde{u} \rangle^2 + \langle \tilde{v} \rangle^2 \right)^{1/2}$ and the total Reynolds Stress as a function of time, where we present profiles for the longest simulation Run B averaged over intervals ranging from between $\{5-15\}T_E$ to between $\{125-135\}T_E$. In both panels we see that the profiles each approach a limiting profile as time advances. At $\{55-65\}T_E$ we conclude that the profile shapes are similar to the limiting shapes and that a pseudo stationary state has been reached.

Figure 3 shows the growth rate (or alternatively the entrainment rate) $w_e = \partial z_i/\partial t$ as a function of the eddy turn over time $T_E$. At $\{55-65\}T_E$, the growth rate reach a constant value $w_e \sim 0.85 \text{ m s}^{-1}$ and the variation in $w_e$ among the four simulations is less than 5%. This time interval ($\{55-65\}T_E$) can therefore be assumed quasi-stationary and is used from here forward as our averaging interval. Figure 4 shows that the friction velocity $u_\star$ also converges by $\{55-65\}T_E$; $u_\star$ actually converges much earlier, at around $30T_E$, since $u_\star$ is by definition governed by surface processes in contrast to $z_i$.

### 4. Results

This section presents mesh resolution sensitivity results. Bulk parameters from the simulations are calculated using averages over the interval $\{55-65\}T_E$. The numbers are presented in Table 2.
a. Large-eddy Reynolds number and SGS dissipation

In Sullivan and Patton (2011) on convective boundary layers the ratio $z_i/\Delta_f$ was used as a measure of the ABL resolution as it represents the separation between the largest possible energy containing eddy in the flow and the scales of motion nearest to the LES cut-off. In Figure 1 we have shown that in our conditional neutral boundary layer $z_i \sim 1.12h$ for the B run. Since the ratio, $z_i/h$, as can be seen in Table 2, only changes slightly with mesh size, we use the ratio $z_i/\Delta_f$ to express ABL resolution. With $z_i \in \{350 - 399\}$ m across the four simulations we furthermore find that the domain size is large enough compared to the ABL height; the “rule of thumb” says that $L_x/z_i > 5$, $L_y/z_i > 5$ and $L_z/z_i > 2$ needs to be satisfied (reference not known).

The resolved turbulence in high Reynolds number LES should be independent of processes taken place on scales below the filter scale, $\Delta_f$. To state that a given mesh is fine enough and that the simulation has is independent of the SGS viscosity is equivalent to stating that the large-eddy Reynolds number is a function of the effective resolution alone. The effective resolution is here defined as the ratio between the largest and smallest scales resolved in the simulation, $z_i/\Delta_f$. We define the large-eddy Reynolds number

$$Re_\ell = \frac{u_\ell}{v_t} = \frac{u_*z_i}{C_k\Delta_f e^{1/2}}, \quad (9)$$

where in contrast to Moeng and Wyngaard (1988) and Sullivan and Patton (2011) the friction velocity, $u_*$, is the characteristic velocity scale since turbulence in our study is produced by shear.

In eq. 9 we use a definition of SGS viscosity consistent with that used in the LES code. $C_k = 0.1$. Pollard et al. (1972) propose $\ell = c_{cn}u_* (|f|N)^{-1/2}$ from studies with a simple model of the upper ocean. From ABL LES simulations Zilitinkevich et al. (2007) find $c_{cn} = 1.36$ using same definition of $h$ as used in our study. The spin-up time in their LES is, however, different compared to our study, and hence a different numerical value should be expected, due to the inherent lack of
stationarity in the problem. We adopt $z_i = c_{cn'} u_*(|f|N)^{-1/2}$, and find values of $c_{cn'}$ as provided in Table 2; most pronounced is a small dependence on mesh size. Together with the SGS model (Lilly 1967; Moeng and Wyngaard 1988) (here without the stability correction - see next subsection),

$$\varepsilon' = C_\varepsilon e^{3/2}/\Delta f,$$

and the SGS identity of constants ($c_s = C_{s3}^{3/4} c_{cn'}^{-1/4}$ with $c_s = 0.18$) we can also express the large-eddy Reynolds number as

$$Re_\ell = \left( \frac{z_i}{c_s \Delta f} \right)^{4/3} \left( \frac{u^2_2(|f|N)^{1/2}}{c_{cn'} \varepsilon'} \right)^{1/3}.$$  \hspace{1cm} (10)

We thus recover the $(z_i/\Delta f)^{4/3}$ dependence also found in Sullivan and Patton (2011) and in Direct Numerical Simulation (Pope 2000). Since the product of all the other parameters in the second parentheses of eq. 10 are mesh independent ($u^2_2/c_{cn'} = 0.030 \text{m}^2 \text{s}^{-2}$ in all four simulations), $\varepsilon'$ needs to be constant in the inertial sub-range (assuming that $\Delta f$ is in the inertial sub-range).

In Figure 5 we plot $Re_\ell$ multiplied with $(\Delta f/z_i)^{4/3}$ for the three heights $z/z_i = 0.1$, $z/z_i = 0.5$ and $z/z_i = 0.9$. At $z/z_i = 0.9$, we observe mesh independence going from simulation C to D.

Closer near the surface where the dissipation rates, $\varepsilon'$, are much higher, mesh independence is still not achieved. In Sullivan and Patton (2011) mesh independence through a similar analysis was reported from $z_i/\Delta f > 60$ in a convective boundary layer. This correspond to our run C at $512^2 \times 256$. The different mechanisms producing turbulence in convective and conditional neutral boundary layers (Moeng and Sullivan 1994), and the difference in the resulting characteristic turbulence scales, is thus of significant importance when studying mesh influence. Without going into details of all the budget terms in the turbulent kinetic energy equation we show in Figure 6 the ratio between resolved shear production, $SP = -\left( \langle \tilde{u}' \tilde{w}' \rangle \frac{\partial \langle \tilde{u} \rangle}{\partial z} + \langle \tilde{v}' \tilde{w}' \rangle \frac{\partial \langle \tilde{v} \rangle}{\partial z} \right)$ - the only term creating turbulent kinetic energy - and the dissipation, $\langle \varepsilon' \rangle$, derived from the Deardorff (1980)

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SGS model:

\[
\langle \mathcal{E} \rangle = \left( 0.19 + 0.74 \frac{l}{\Delta f} \right) e^{3/2},
\]

(11)

where \( l \) is a stability-limited length scale calculated according to \( l = \min[l^*, \Delta f] \) with \( l^* = 0.67 \sqrt{e/N^2} \). In principle there is also production of turbulent kinetic energy through a sub-filter shear production, \( \langle \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} \rangle \), but since this term is balanced by an equal amount of turbulent kinetic energy transferred from the resolved scales to the sub-filter scales, we do not consider it here. The ratio \( SP/\langle \mathcal{E} \rangle \), show heights at which a local balance between shear production and dissipation is achieved. This height increases with decreasing resolution, and for the coarsest simulation A it is never achieved, and even for the finest resolution runs, C and D is the height interval very narrow. For run C and D it is found at \( z/z_i \sim 0.1 \). We will return to this balance when looking at structure functions later in the paper.

Very small dissipation rates are found near the ABL top \( (z/z_i = 0.9) \) for all four simulations. Strictly speaking, Run D is the only simulation where \( \langle l^* \rangle /\Delta f > 1 \) at \( z/z_i = 0.9 \) (not shown), hence only in Run D is there sufficient resolution to resolve the smallest scales for the problem design. At the larger-scale end of the eddy spectrum, the Dougherty-Ozmidov length scale \( L_o = \sqrt{\langle \mathcal{E} \rangle /\langle N^2 \rangle^{3/2}} \) (Dougherty 1961; Ozmidov 1965) provides a measure of eddy sizes, \( \ell \), for which overturning would be inhibited \( (\ell > L_o) \) by the strong stratification arising from entrainment of warm air from the “free” atmosphere above and turbulent mixing throughout the ABL. At \( z/z_i = 0.9 \) we find \( L_o/\Delta f = \{0.2, 0.5, 1.2, 2.4\} \), which means that only in run C and D are the smallest scales unaffected by the strong stratification. Due to very high values of \( L_o \) as we approach the surface where \( N^2 \) vanishes, for all simulations at \( z/z_i < 0.75 \) we find that \( \ell < L_o \) for all resolved eddies.

Instantaneous horizontal \((x-y)\) slices of stream-wise and vertical velocity \((u_h \text{ and } w, \text{ respectively})\), reveal significant differences in the qualitative patterns between the coarsest and finest
simulations (Figures 7-8). Here, stream-wise velocity is defined $u_h = (\tilde{u}, \tilde{v}, 0) \cdot \hat{k}_h$, where the stream-wise vector (in the direction of the mean wind) is defined $\hat{k}_h = (\langle \tilde{u} \rangle, \langle \tilde{v} \rangle) / |(\langle \tilde{u} \rangle, \langle \tilde{v} \rangle)|$.

Figure 7 presents snapshots at $z/z_i = 0.1$, while height $z/z_i = 0.9$, is presented in Figure 8, respectively.

A comparison of the horizontal and vertical velocity fields from simulations A and D, collected at the same non-dimensional vertical location, shows a dramatic increase in the intensity and number of small-scale eddies with increasing resolution. This is expected given the increase in large eddy Reynolds number in D (e.g., Jiménez 2012). The abundant small-scale eddies in D blur the relatively smooth large-scale velocity patterns readily observed in A. The impact of increased resolution on vertical velocity is noticeably pronounced. At $z/z_i = 0.9$, the inability of run A to resolve the small scales associated with the buoyant destruction of turbulent kinetic energy as previously discussed is evident: the near intermittent velocity patterns observed in run D are qualitatively different from run A. A slight change in the main wind direction is also observed between the two resolutions at all heights and is due to the inability to resolve the turbulent momentum fluxes and shifts in $z_i$, which both influence the wind veer with height (see next subsection).

**b. Profiles of 1st and 2nd order moments**

As previously mentioned, the turbulent momentum fluxes play a significant role in producing turbulence, *viz.* the importance of shear production in the turbulence kinetic energy budget. Figure 9 shows the resolved $\langle \tilde{u}' \tilde{w}' \rangle$, SGS $\langle \tau_{13} \rangle$, and the total momentum fluxes. Except for simulation A, profiles of the total momentum flux in the two horizontal directions (solid lines, Figure 9) do not change substantially with resolution changes for heights $z/z_i > 0.2$. On the other hand, the ratio between the resolved and SGS contributions increases significantly as the resolution increases. The first grid point at which the momentum fluxes are evaluated is at $z = \Delta z$. Whereas the mag-
nitude of the total momentum flux vector at this level only differ by 2% between run A and run D, the angle \( \tan^{-1} \left( \frac{\langle \tilde{v}' \tilde{w}' + \tau_{23} \rangle}{\langle \tilde{u}' \tilde{w}' + \tau_{13} \rangle} \right) \), is more different. One finds a 3 degree difference between run A and D (the angle in run D is 22.9 deg). If we on the other hand only look at the resolved contribution, \( \tan^{-1} \left( \frac{\langle \tilde{v}' \tilde{w}' \rangle}{\langle \tilde{u}' \tilde{w}' \rangle} \right) \), we find a 5 degree difference. I.e. the run D is capable of resolving relatively more of the smaller scale \( \langle \tilde{v}' \tilde{w}' \rangle \) co-variance compared to the coarser run A. Since the momentum flux vector is aligned with the vector of the mean shear, \( (d\langle \tilde{u}\rangle/dz, d\langle \tilde{v}\rangle/dz) \), this has implications for the wind direction (Berg et al. 2013). A change in mean wind direction was observed in Figure 7-8 when comparing run A and run D.

The mean wind \( S \) is shown in Figure 10 (left panel). All simulations produce a super-geostrophic velocity with maximum speed location increasing with increasing resolution (\( z/z_i \sim 0.85 \) for run A to \( z/z_i \sim 0.93 \) for run D). Some discrepancy between simulations can be seen in the near-surface mean wind profiles, but they become more similar after rescaling the profiles with each simulation’s respective \( u_* \), at least up to around \( z/z_i \sim 0.2 \). Visualization of true logarithmic scaling (which should only exist in true shear-driven boundary layers, i.e. in the absence of stratification and Coriolis forces), is best performed by looking at the non-dimensional wind shear, \( \phi_m = \frac{\kappa \frac{\partial S}{\partial z}}{u_*} \) in close proximity to the lower boundary. \( \phi_m \) is plotted in Figure 10 (center panel), where a true near-surface logarithmic layer should appear as a region where \( \phi_m = 1 \). Near-surface departure from \( \phi_m = 1 \) (i.e. the overshoot) is constant in magnitude for all runs but shifts towards the surface with increasing resolution, a result consistent with Brasseur and Wei (2010). The relatively low magnitude of the overshoot (less than 10%) is attributed to application of Sullivan et al.’s (1994) two-part SGS model. Especially for the two highest-resolution simulations (Runs C and D), the influence of the stable stratification appears as a constant increase in \( \phi_m \) from \( z/z_i \sim 0.08 \) and up.

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In Figure 10 (right panel) we show the mean wind direction, $\varphi$, for the four runs. Stronger veering (wind direction change with height) with increased resolution is observed. This is in agreement with the findings just reported on the angle between resolved momentum fluxes.

We now turn to the heat flux profiles in Figure 11 (left panel). For all resolutions a close to linear profile from the surface to the minimum value of heat flux is observed. The minimum value decreases and the height of this minimum increases with increasing resolution. This is in agreement with the Direct Numerical Simulation (DNS) study by Jonker et al. (2013). In their DNS no “overshoot” is observed above $z_i$. Such “overshoot” is present in our coarse resolution runs A and B but diminishes in the fine resolution runs C and D. Looking at the SGS contribution, $\langle \tau_w \theta \rangle$ we see that the minimum value for simulation A occurs at a height below the minimum of the total heat flux compared to run C and D, where it is located above the minimum of the total flux. Since the heat flux is ultimately linked to the gradient of potential temperature we show the profile of $\langle \tilde{\theta} \rangle$ in Figure 11 (right panel). In the inset we observe how the coarse resolution fails to resolve the gradient and how it instead “smears” it out over a larger depth compared to the fine resolution runs. Due to the increased heat flux in the coarse simulations the bulk ABL temperature increases slightly with decreasing resolution (0.1 K).

Figure 12 presents the total turbulent kinetic energy, $TKE = \langle \tilde{u}_i \tilde{u}_i \rangle / 2 + \langle e \rangle$, where summation is implied and $e$ is the SGS turbulent kinetic energy in eq. 4. In the left panel the total TKE converges across simulations throughout much of the ABL except at $z/z_i \sim 1$, where turbulence is produced by shear associated with the the super geostrophic jet and destroyed by buoyancy, which are both highly dependent on the mesh resolution due to the small scales involved: we observe that the smaller jet observed in simulation A (Figure 10 do not give rise to the same amount of turbulence as for the other more resolved runs. Close to the surface, increasing mesh resolution naturally resolves the increasingly smaller scales. Convergence throughout the ABL of total $TKE$ implies...
commensurate altering of the partitioning between resolved and SGS energy with mesh resolution variations. The contribution from SGS energy is increasing with approximately 50% each time the filter, $\Delta f$, is doubled.

The right panel of Figure 12 shows a surrogate for turbulence intensity, i.e. $\sqrt{TKE}/S$. We choose this definition instead of the wind-energy community’s usual definition: $\sigma_{u_h}/|u_h|$, where $\sigma_{u_h}$ denotes the standard deviation of the stream-wise velocity component; however since $\sigma_v \sim 0.8\sigma_u$ and $\sigma_w \sim 0.5\sigma_u$, (Panofsky and Dutton 1984), the difference between the two definitions should only result in magnitude differences of $\sim 3\%$. Again we observe mesh independence throughout the ABL except at $z/z_i \sim 1$ and close to the surface. In wind energy meteorology such a result could potentially be quite useful: even coarse resolution LES can produce sufficiently accurate turbulence intensity predictions to determine appropriate wind turbine classes for siting purposes (e.g., International Electrotechnical Commission 2005), where for this configuration coarse resolution means $\Delta f = 23.3\, m$. Close to the surface the SGS model fails to deliver the part of TKE missing due to unresolved eddies, and hence the somewhat bold statement above also do not apply to turbines operating in the surface layer.

**c. The spectral tensor and inertial range scaling**

Further insight into the second-order statistics can be gained by looking at the spectral properties of the simulations. As a starting point, the spectral tensor in stationary and horizontal homogeneous conditions is:

$$\Phi_{ij}(k_x,k_y,z) = \frac{1}{(2\pi)^2} \int \int R_{ij}(r_x,r_y,z) e^{-i(k_x r_x + k_y r_y)} \, dr_x \, dr_y, \quad (12)$$

with the co-variance function,

$$R_{ij}(r_x,r_y,z) = \langle \tilde{u}_i(x,y,z) \tilde{u}_j(x + r_x, y + r_y, z) \rangle, \quad (13)$$

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and horizontal wave numbers, $\mathbf{k} = (k_x, k_y)$ aligned with the LES coordinate system. The spectral tensor has the properties, $\Phi_{ij}(k, z) = \Phi_{ji}^*(k, z)$ and $k_i \Phi_{ij}(k, z) = 0$, where the * denotes complex conjugation. In order to account for the fact that the wind direction is not aligned with the coordinate axis, the spectral tensor has been rotated at each height, $\Phi_{ij}^{rot} = M_{ik} \Phi_{kl} M_{jl}$, where $M_{ij}$ is the matrix which rotates a wind vector into the mean horizontal wind direction, so that $k_1$ is in the direction of the mean wind at each height.

Figures 13 and 14 show the diagonal terms of the spectral tensor for the $128^2 \times 64$ (A) and $1024^2 \times 512$ (D) simulations at $z/z_i = 0.1$, respectively. The main features in the spectral tensors clearly align with the stream-wise and span-wise wave numbers, $k_1$ and $k_2$ for the two horizontal terms, $\Phi_{11}$ and $\Phi_{22}$, respectively; this result is especially true for the high-resolution simulation D, whereas some misalignment is observed for the coarser simulation A. The mean wind is associated with lowest wave number, i.e. in the center of the plots; the misalignment increases with increasing wave number such that the smallest scales exhibit the largest misalignment. Again, this result is most pronounced in Run A.

The average of $\Phi_{11}$ and $\Phi_{22}$ shows the azimuthal symmetry [and hence follows the incompressibility constraint, $k_i \Phi_{ij}(k) = 0$, Pope (2000, page 220)], for all but the smallest scales in Run D, which makes $(\Phi_{11} + \Phi_{11})/2$ an obvious candidate for azimuthal averaging (also denoted as “ring averaging”). Azimuthal symmetry is also observed in the vertical component $\Phi_{33}$. Run A does not display azimuthal symmetry for either $(\Phi_{11} + \Phi_{22})/2$ or $\Phi_{33}$.

Following Peltier et al. (1996); Kelly and Wyngaard (2006); Wyngaard (2010) we exploit the symmetry observed in $\Phi_{33}$ and $(\Phi_{11} + \Phi_{22})/2$ by calculating two-dimensional ring-averaged horizontal velocity spectra, $E_h(k_h)$, and vertical velocity spectra, $E_w(k_h)$, as a function of horizontal wave number, $k_h = (k_1^2 + k_2^2)^{1/2}$:
\[ E_h(k_h) = \frac{1}{2} \int_0^{2\pi} (\Phi_{11}(k_h, \varphi) + \Phi_{22}(k_h, \varphi)) \, k_h \, d\varphi \]  
\[ E_w(k_h) = \int_0^{2\pi} \Phi_{33}(k_h, \varphi) \, k_h \, d\varphi \]  

In the inertial sub-range, the spectra are suppose to follow the dimensional “−5/3” scaling, with

\[ E_h(k_h) = \alpha_h \delta^{2/3} k_h^{-5/3} \]  
\[ E_w(k_h) = \alpha_w \delta^{2/3} k_h^{-5/3} \]

with constants \( \alpha_h = 0.54(55/18)\alpha_{1d} \), and \( \alpha_w = 0.61(55/18)\alpha_{1d} \) (Wyngaard 2010), and the one-dimensional Kolmogorov constant taken to be \( \alpha_{1d} = 0.5 \) (Sreenivasan 1995). Figure 15 presents ring-averaged two-dimensional spectra, \( E_h(k_h) \) and \( E_w(k_h) \). At \( z/z_i = 0.1 \) the horizontal spectra for run C and D start to show an inertial sub-range. Since the spectra have been multiplied by the inverse constants, \( \alpha_h \) and \( \alpha_w \), collapse between the horizontal and vertical spectra indicate that their mutual relationship is found to follow its theoretical prediction. This is the case at \( z/z_i = 0.1 \) for run C and D. Moving to \( z/z_i = 0.5 \) we see extended range reasonable close to \(-5/3\) scaling for all runs and a collapse of the two spectra. As \( kz_i \) increases and the scales are being affected by the SGS model the slopes decline slightly. At \( z/z_i = 0.9 \) all resolved scales in all the four runs (except the very smallest in run D affected by SGS dissipation) are larger than the Ozmidov scale, \( L_o \). Hence they are influenced by the stable stratification and therefore do not exhibit fully three-dimensional turbulence - together with the small scales present at this height inertial range scaling is inapplicable.

Compared to more typical one-dimensional spectra, \( i.e. \):

\[ F_{ij}(k_1) = \int \Phi_{ij}(k_1, k_2) \, dk_2, \]  

the advantage of interrogating two-dimensional ring-averaged spectra becomes apparent by studying the spectral tensor plots (Figures 13 and 14). Averaging \( F_{ij}(k_1) \) over \( k_2 \) introduces aliasing errors from span-wise motions. Furthermore in situations including the Coriolis force, using a square domain with principle coordinates, \( x \) and \( y \), the integration limits change, since the struc-
ture of $\Phi_{ij}$ aligns along $k_1$ and $k_2$ as opposed to along $k_x$ and $k_y$ - in effect smaller scales, are somewhat effected.

The disadvantage of using two-dimensional spectra lies in the lack of available measurements. Measurements tend to be performed in the temporal domain and after assuming Taylor’s frozen-eddy hypothesis (Taylor 1938) and presented as one-dimensional spectra $F_{ij}(k_1)$ in the stream-wise direction. Figure 16 shows one-dimensional spectra $F_{ii}(k_1)$, where the spectra have been multiplied with the inverse Kolmogorov constant $\alpha_{id}$ at $z/z_i = 0.5$, i.e. at the height which most clearly contained an inertial sub-range in the 2D spectra according to Figure 15. The three curves in each panel do not fully collapse in the inertial sub-range, demonstrating that they are not fully consistent with $(4/3)F_{11} = F_{22} = F_{33}$ as one would expect for isotropic tensors (see Pope 2000, for example). The collapse of the curves improves with increasing resolution, but even at the finest resolution (Run D, right panel of Figure 16), the range over which they collapse, and follow the $-5/3$ scaling law is restricted compared to its two-dimensional counterpart. The $-5/3$ law is thus more difficult to discern in the one-dimensional spectra compared to two-dimensional spectra; a well known result that we attribute to sampling issues connected to $k_x - k_y$ vs $k_1 - k_2$ as described above - an effect which is rarely highlighted in the literature. Recently is has also been documented by Ansorge (2019) how a systematic displacement of structures in the lowest part of the boundary layer dictates the use of two-dimensional filters only.

d. Velocity increments, structure functions and generalized log-law

Finally, structure function analysis allows interrogation of the Gaussianity (or non-Gaussianity) of velocity increment statistics in the stream-wise and in the vertical directions. Stream-wise velocity increments at a distance $r$ in the stream-wise direction are defined as:
\[
\delta u_h(r) \equiv \hat{k}_h \cdot \left[ \tilde{u}'(x + r\hat{k}_h, t) - \tilde{u}'(x, t) \right],
\]

(17)

where \(\hat{k}_h\) is the stream-wise unit vector defined previously, while

\[
\delta w(r) \equiv \tilde{w}'(x + r\hat{k}_h, t) - \tilde{w}'(x, t)
\]

(18)

define vertical velocity increments. Normalized probability density functions (pdf) of the velocity increments (Figures 17 and 18) reveal some striking features. First of all the pdfs become more Gaussian with decreasing distance \(r\), i.e. departure from Gaussian statistics is most pronounced for small scales in the flow, which is in agreement with most previous observations and theory describing turbulent high Reynolds number flow (Frisch 1995). The pdfs of the finest-resolution simulation (Run D) exhibit the broadest tails, while in the coarse simulation (Run A) the pdf tails level-off in a concave shape indicating truncation caused by the SGS model. From the spectral analysis (Section 4.c), the inertial range for this mesh size \((128^2 \times 64)\) is very narrow and hardly follows conventional scaling. Vertical velocity exhibits the largest non-Gaussianity, in agreement with visual inspection of the smallest scales in the instantaneous horizontal slices of vertical velocity in Figures 7 and 8. Finally, the most non-Gaussian velocity increments in Run A occurs at \(z/z_i \sim 0.5\) compared to at \(z/z_i \sim 0.1\) for Run D, which results from higher-resolution supporting a broader inertial range due to the large turbulent scales of motion present at \(z/z_i \sim 0.5\).

Defining the structure function of \(n^{th}\) order as ensemble averages, \(\langle \delta u_h^n(r) \rangle\) and \(\langle \delta w^n(r) \rangle\) for the stream-wise and vertical components, respectively, the third and fourth normalized moment, i.e. skewness \(Sk\) and kurtosis \(K\), are given by: \(Sk \equiv \langle \delta u_h^3 \rangle / \langle \delta u_h^2 \rangle^{3/2}\) and \(K \equiv \langle \delta u_h^4 \rangle / \langle \delta u_h^2 \rangle^{2}\) and similar for the vertical component. Velocity skewness and kurtosis are presented in Figures 19 and 20. For stream-wise velocity, the negative skewness agrees with the exact result in turbulence theory (i.e. the “\(-4/5\)” law Frisch 1995), however the constant (i.e. the 4/5) is not reproduced.
by our LES (not shown). Skewness is more negative for the stream-wise velocity component compared to the vertical component. For all resolutions and at both heights, skewness approaches zero for large values of the horizontal separation distance $r$ for both stream-wise and vertical velocity components. Velocity skewness and kurtosis show subtle mesh dependency for both stream-wise and vertical velocity components at both heights. Vertical velocity reveals the largest kurtosis occurring at $z/z_i \sim 0.5$; where mesh dependence between Runs C and D is again very small at $z/z_i \sim 0.5$. For large $r$, the vertical component is slightly super-Gaussian with a kurtosis just above a value of 3, while the stream-wise component at similar $r$ are below 3, i.e. sub-Gaussian at $z/z_i \sim 0.1$ and closer to Gaussian at $z/z_i \sim 0.5$; Stevens et al. (2014) found similar results. Also evident in the plots are the decreasing distance with increasing resolution at which both skewness and kurtosis depart from their near Gaussian state, i.e. $Sk \sim 0$ and $K \sim 3$.

Davidson et al. (2006) demonstrated that the stream-wise structure functions follow a generalized logarithmic law for scales larger than the inertial range and smaller than some fraction of $z_i$, and showed that this is equivalent to assuming that a hierarchy of eddies exists whose kinetic energy scales as $u_x^2$. Based on scaling arguments for higher order moments of stream-wise velocity fluctuations (Meneveau and Marusic 2013), De Silva et al. (2015) postulated that even-numbered structure functions of stream-wise velocity increments scale as:

$$\langle \delta u_h(r)^{2p} \rangle^{1/p} = E_p' + D_p' \ln \left( \frac{r}{z} \right)$$

(19)

for scales $z < r \ll h_{z_i}$, where $h_{z_i}$ is a fraction of the turbulent boundary layer depth $z_i$. $E_p'$ and $D_p'$ are expected to be universal functions in high Reynolds number turbulence; De Silva et al. (2015) finds that this might indeed be true based on various experimental data sets of very high Reynolds number turbulence.
From proposing a logarithmic region via the second-order structure function, it then immediately follows that the velocity spectra should scale like $k^{-1}$. Davidson et al. (2006) explain the difficulties in observing $k^{-1}$ spectral scaling law in one-dimensional spectra $F_{11}(k_1)$, and the authors list reasons similar to those mentioned in the previous section; two-dimensional ring-averaged spectra should not have the same issues. Figure 21 presents one-dimensional (right panel) and two-dimensional ring-averaged (left panel) spectra for all four simulations at a height of $z/z_i = 0.1$, a height at which it has been previously demonstrated that shear production and dissipation balance (at least for the finest-resolution simulation, Run D). Pan and Chamecki (2016) showed the possibility of a more general scaling law that does not require strict balance between dissipation and production. Following Davidson and Krogstad (2014), Pan and Chamecki (2016), and Chamecki et al. (2017), we define a characteristic length scale $\ell_E = u_{\epsilon}^3/\epsilon$, recognizing the importance of dissipation compared to classical surface layer scaling $\kappa z$ in characterizing the turbulent eddies in the inertial range. A comparison reveals the ratios $\kappa z/\ell_E = \{0.58, 0.73, 0.84, 0.93\}$ for the four simulations (Runs A-D) approach a value of one with increasing resolution; a result similar to that showed in Figure 6 where the balance between shear production and dissipation improves with increasing resolution. In Figure 21, a very distinct plateau at $k\ell_E \sim 1$ can be seen in both the $k_h E_h(k_h)$ and in $k_1 F_{11}(k_1)$ spectra indicating $k^{-1}$ scaling; where, Run D scales the best and the scaling is almost non-existent in Run A. The nearly perfect scaling of $k_1 F_{11}(k_1)$ for very low $k\ell_E$ is likely fortuitous compared to the more narrow range observed in $k_h E_h(k_h)$.

We now look at the higher order structure functions in the stream-wise direction, $\langle \delta u_h(r)^n \rangle$ at $z/z_i \sim 0.1$. Since the moments are formally calculated from:

$$\langle \delta u_h(r)^n \rangle = \int \delta u_h(r)^n \ p(\delta u_h(r)) \ d\delta u_h,$$

(20)
where \( p(\delta u_h(r)) \) is the probability density function of increments, \( \delta u_h(r) \). Figure 22 plots the integrand for \( n = 2, \ldots, 10 \) for the smallest and largest values of \( r \). All integrands for \( n = 2, 4 \) are converged (less than 0.001 on the vertical axis) while \( n = 6 \) is borderline and \( n = 8, 10 \) are not fully converged for the smallest value of \( r \). Though, it is important to remember that the generalized log-law (eq. 19) is only valid for \( r > z \), hence non-convergence for values of \( r \) well within the inertial range is not terribly crucial.

The findings in Davidson and Krogstad (2014), Pan and Chamecki (2016), and Chamecki et al. (2017) leads us to evaluate the following definition in our mesh sensitivity study of the stream-wise structure functions:

\[
\langle \frac{\delta u_h(r)^{2p}}{u_*^2} \rangle^{1/p} = E_p + D_p \ln \left( \frac{r}{\ell_E} \right) \tag{21}
\]

for order \( n = 2p \), i.e. only considering the even-ordered structure functions; the even-ordered structure functions are presented in Figure 23. Notice that changing our length scale choice from \( z \) to \( \ell_E \) implies that \( E_p \neq E'_p \) and \( D_p \neq D'_p \). All structure functions reach an asymptotic state for \( r/\ell_E \sim 30 – 50 \), where this state corresponds to distances which are completely decorrelated. Hence, \( \langle \delta u_h(r)^2 \rangle = 2\sigma_{u_h}^2 \).

The logarithmic region more clearly presents itself when plotting the structure functions as function of \( \ln (r/\ell_E) \); where, Figure 24 presents results for Run D. Using an approach similar to Pan and Chamecki (2016), a least-square fit from \( r = \ell_E \) to \( r = 0.4z_i \) shows a coefficient of determination \( R^2 > 0.99 \) clearly indicating the existence of a logarithmic relationship. Figure 25 shows \( D_p \) and \( E_p \) derived from the fit for each simulation. For \( n \leq 6 \) the mesh dependence for \( D_p \) is small with stronger intermittency effects in the finer-resolution simulation (Run D), in agreement the velocity skewness and kurtosis (Figure 19). For \( n = 8, 10 \) the mesh dependence increases as do the error bar magnitudes. A similar picture arises in the plot of \( E_p \). Both panels in Figure 25 include the data from De Silva et al. (2015) presented as gray dots. \( D_p \) from the current simulations agrees

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nicely with the De Silva et al. (2015) data, while $E_p$ values are low in the LES data compared to the observations, i.e. the higher order moments are suppressed. Since the high moments are mainly associated with fluctuations of the smallest scales of motion, i.e. close to the inertial range the SGS influence is here also the largest, and we would therefore also expect lower values values of $E_p$. Since $E_p$ depends on the chosen characteristic length scale, we also show $E_p$ using $z$ instead of $\ell_G$ for Run D (orange dots). For $n = 2, 4$ data using $z$ as the length scale agree well, while the LES values remain lower for higher values of $n$. Pan and Chamecki (2016) also compared their atmospheric canopy flow LES data against the data from De Silva et al. (2015) and found nice agreement for $n = 2$, but did not look at higher values of $n$. Careful inspection of Pan and Chamecki’s (2016) Figure 7 could indicate some mesh dependence with similar shape to that found here, i.e. decreasing values of $D_p$ and increasing values of $E_p$ with increasing LES Reynolds number $Re_\ell$. In addition, Pan and Chamecki (2016) studied meshes spanning $54 \leq Re_\ell \leq 136$, which are notably lower than those studied here $182 \leq Re_\ell \leq 2012$ (see Table 2).

We can also use the $k^{-1}$ scaling observed in Figure 21 to estimate $D_2$, since

$$S(k) = \gamma u_s^2 k^{-1},$$

with $\gamma = D_2/4$ in the limit where $Re \to \infty$. In eq. 22, the notation $S(k)$ represents any stream-wise velocity spectrum. Using the appropriate proportionality constants predicted from their inertial range behavior, $\gamma = 0.35$ for $F_{11}(k_1)$ and $\gamma = 0.93/(0.54 \times (55/18)) = 0.57$ for $E_h(k_h)$, which correspond to $D_2 = 1.4$ and $D_2 = 2.2$ for the one-dimensional and two-dimensional spectra, respectively. From the second-order structure function, $D_p = 1.93 \pm 0.11$. Thus, ring-averaged two-dimensional spectra perform much better than one-dimensional spectra for such predictions.

The findings thus indicate that non-Gaussian statistics on scales in the $k^{-1}$ regime, i.e. scales larger than the inertial sub range, found in the LES is in both qualitative and quantitative agreement.
with flows at much higher Reynolds number at least up to order $n = 6$. This is despite the existence of a distinct inertial range scaling at $z/z_i \sim 0.1$ where the analysis was carried out. Thus direct impact from the SGS model cannot be ruled out. We however also know from Figure 10 that the range at which the $\phi_m = 1$ is narrow and so then is the heights at which these results can be applied.

5. Concluding remarks

A canonical neutral atmospheric boundary layer is simulated using large-eddy simulation on four different meshes. As is standard practice with LES, the simulations use a mesh dependent subgrid-scale (SGS) parameterization that alters the partitioning between resolved and SGS motions. Hence designing metrics to assess solution convergence is not straightforward. Because of the high computational cost of three-dimensional time-dependent calculations mesh studies are not typically performed when using LES for applications, e.g., within wind energy meteorology. However, our findings for a neutral atmospheric boundary layer suggest that the statistics are not fully converged with horizontal mesh spacing $\Delta \sim 2.5$ m. The mesh dependence is largest in areas of the domain where the spatial scales of turbulence are small, i.e. near the surface and at the top of the ABL in the entrainment zone. Vertical profiles of $\sqrt{TKE}/S$ quantify the solution sensitivity to the mesh resolution. These show that LES indeed provide close-to mesh independent profiles of integrated and non-dimensional quantities from approximately 10% to 90% of the height of the ABL. This means that LES can directly be used even at coarser resolution if only such quantities are desired. We have, however, also shown that the resolved part of the TKE is highly dependent on the mesh resolution throughout the ABL: the contribution from SGS energy is increasing with approximately 50% each time the filter, $\Delta_f$, is doubled. In a wind energy application context this has pros and cons: modern wind turbines are huge machines and often have hub heights in the range 120-170 m, i.e. they are located above the surface layer where we have shown that for
example turbulence intensity is mesh independent. On the other hand, during low ABL heights the turbines might enter the entrainment layer at the top of the ABL, where processes involving buoyancy become important. To properly resolve these processes high resolution is needed - even higher than the mesh sizes utilized in this paper. If we furthermore want to address the dynamical loading through velocity fluctuations on the various parts on a wind turbines, such as blades and tower, accurate prediction of the spectral properties of turbulence is needed.

All of the simulations produce non-Gaussian statistics, but the scale at which the non-Gaussianity becomes significant diminishes with increasing resolution, \textit{i.e.} using data from an LES performed on a coarse mesh in an application where the wind field is low-pass filtered would predict erroneous non-Gaussian statistics. In some ways the averaging of wind turbine rotors can be seen as a low-pass filter, and there are ongoing discussions surrounding whether non-Gaussian statistics affect wind turbine operations (Milan et al. 2013; Berg et al. 2016; Schottler et al. 2017; Meneveau 2019).

The \textit{generalized log-law} for even-ordered structure functions in the $k^{-1}$ regime is found with mesh dependent exponents matching previous studies for orders $n = 2, 4, 6$ where convergence has been obtained. We take this as support for the maturity and size of LES simulations and hence the role LES deserves in applications where high accuracy and low intrinsic uncertainty are required.

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## Table 1. Overview of simulations

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<tr>
<th>Name</th>
<th>Grid points</th>
<th>((L_x, L_y, L_z)) [m]</th>
<th>((\Delta x, \Delta y, \Delta z)) [m]</th>
<th>(\Delta f) [m]</th>
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<td>128(^2) × 64</td>
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<td>(20.0, 20.0, 14.0)</td>
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<td>3.86</td>
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<td>(10.0, 10.0, 7.0)</td>
<td>11.6</td>
<td>1.85</td>
<td>2.3 × 10(^5)</td>
</tr>
<tr>
<td>C</td>
<td>512(^2) × 256</td>
<td>(2560, 2560, 896)</td>
<td>(5.0, 5.0, 3.5)</td>
<td>5.8</td>
<td>0.88</td>
<td>1.1 × 10(^5)</td>
</tr>
<tr>
<td>D</td>
<td>1024(^2) × 512</td>
<td>(2560, 2560, 896)</td>
<td>(2.5, 2.5, 1.75)</td>
<td>2.9</td>
<td>0.43</td>
<td>1.0 × 10(^5)</td>
</tr>
</tbody>
</table>
Table 2. Bulk parameters.

| Name | $h$ [m] | $z_i$ [m] | $z_i/h$ [-] | $u_*$ [m s$^{-1}$] | $z_i/f|N|^{1/2} u_*^{-1}$ [-] | $T_k$ [s] | $z_i/\Delta f$ [-] | $Re_T$ [-] |
|------|--------|----------|-------------|----------------|-----------------------------|--------|----------------|---------|
| A    | 348    | 399      | 1.15        | 0.230         | 1.74                       | 1733   | 17.1           | 182     |
| B    | 353    | 395      | 1.12        | 0.229         | 1.73                       | 1722   | 34.1           | 398     |
| C    | 338    | 372      | 1.10        | 0.225         | 1.65                       | 1648   | 64.1           | 886     |
| D    | 321    | 350      | 1.09        | 0.221         | 1.59                       | 1579   | 120.1          | 2012    |
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\[
\langle (\delta u_h(r))^2 \rangle^{1/p} / u_*^2
\]

\( p = 1 \)

\( p = 2 \)

\( p = 3 \)

\( p = 4 \)

\( p = 5 \)

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