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The Atmospheric Boundary Layer and the "Gray Zone" of Turbulence: A critical review

Rachel Honnert^{1*}, Georgios A. Efstathiou², Robert J. Beare², Junshi Ito³, Adrian Lock⁴, Roel Neggers⁵, Robert S. Plant⁶, Hyeyum Hailey Shin⁷, Lorenzo Tomassini⁴, Bowen Zhou⁸

6	¹ Météo-France, CNRM-CNRS UMR-3589, Toulouse, France
7	² Department of Mathematics, University of Exeter, Exeter, UK
8	³ Department of Geophysics, Graduate School of Science, Tohoku University, Japan
9	⁴ Met Office, Exeter, UK
10	⁵ Institute for Geophysics and Meteorology, University of Cologne, Germany
11	⁶ Department of Meteorology, University of Reading, Reading, UK
12	⁷ National Center for Atmospheric Research, Boulder, Colorado, USA
13	⁸ Key Laboratory for Mesoscale Severe Weather/MOE and School of Atmospheric Sciences, Nanjing
14	University, Nanjing, China

15	Key Points:
16	• The horizontal grid resolution of atmospheric models has become fine enough that
17	models are able to partially resolve turbulent motions in the atmospheric bound-
18	ary layer. This resolution regime comprises the "gray zone" of turbulence.
19	• The traditional parameterization methods for the representation of turbulence are
20	no longer valid in the turbulence "gray zone".
21	• Due to the gray-zone problem, it is no longer the case that increases to the model
22	resolution will necessarily improve the quality and usefulness of simulation results.
23	• We review the current efforts by modelers to overcome the gray-zone problems in
24	order to provide useful simulations at high resolutions.
25	• We conclude that the task is far from being hopeless, and propose that extensions
26	to the approaches being developed for this field may also prove valuable for other
27	geophysical modeling problems.

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^{*}CNRM UMR 3589,Météo-France

^{42,} avenue Gaspard Coriolis

³¹⁰⁵⁷ Toulouse cedex 01, FRANCE

Corresponding author: R. Honnert, rachel.honnert@meteo.fr

28 Abstract

Recent increases in computing power mean that atmospheric models for numerical weather 29 prediction are now able to operate at grid spacings of the order of a few hundred me-30 ters, comparable to the dominant turbulence length scales in the atmospheric bound-31 ary layer. As a result, models are starting to partially resolve the coherent overturning 32 structures in the boundary layer. In this resolution regime, the so-called boundary-layer 33 "gray zone", neither the techniques of high-resolution atmospheric modeling (a few tens 34 of meters resolution) nor those of traditional meteorological models (a few kilometers 35 resolution) are appropriate because fundamental assumptions behind the parameteriza-36 tions are violated. Nonetheless, model simulations in this regime may remain highly use-37 ful. In this paper, a newly-formed gray-zone boundary-layer community lays the basis 38 for parameterizing gray-zone turbulence, identifies the challenges in high-resolution at-30 mospheric modeling and presents different gray-zone boundary-layer models. We discuss 40 both the successful applications and the limitations of current parameterization approaches, 41 and consider various issues in extending promising research approaches into use for nu-42 merical weather prediction. The ultimate goal of the research is the development of uni-43 fied boundary-layer parameterizations valid across all scales. 44

45 1 Introduction

1.1 Boundary-Layer Turbulence

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The atmospheric boundary layer (ABL) occupies the lowest part of the atmosphere, 47 where most human activities take place and where weather phenomena have significant 48 impacts on the anthropogenic and natural environment. The ABL is in direct contact 49 with the surface and responds to surface forcings on a time scale of about an hour (Stull, 50 1988). In contrast to the free troposphere, which is located immediately above, the ABL 51 is readily identified by its highly turbulent nature, which is driven by its constant inter-52 action with the surface. Heat, moisture, momentum and contaminants are transferred 53 and mixed by turbulent eddies having a variety of scales, ranging from a few meters to 54 kilometers. Only under extremely stable conditions, when surface cooling is very strong 55 and winds are very light, does turbulence cease in the ABL. 56

Turbulent eddies dominate the atmospheric micro-scales (cf. Orlanski, 1975). They are associated with various atmospheric phenomena such as strong gusts, pollutant dispersion, frost and fog that have significant social and economical impacts. The largest turbulent structures have scales on the order of the ABL height (about 1-3 km), while the smallest structures are dissipated at a few millimeters.

The convective ABL (CBL) commonly occurs during daytime over continental land, 62 and is characterized by a surface that is warm compared to the air immediately above, 63 resulting in strong surface heat fluxes. Such fluxes give rise to buoyant updraft motions, 64 similar to warm Rayleigh-Bénard structures, called thermals, which are convective ed-65 dies extending from the surface to the top of CBL. They are associated with the peak 66 of the energy containing scales shown in Fig. 1. The thermals are transitory structures 67 that can move as they evolve. They break up to form smaller eddies so that their energy cascades from scale to scale through a continuous spectrum of eddy size called the 69 "inertial sub-range" of turbulence until the Kolmogorov scale is reached and the energy 70 is dissipated (cf. Fig. 1). 71

Supplementing the thermal production of turbulence, mechanical production of turbulence results from the wind shear in the ABL (e.g. due to the fact that wind "vanishes" at the surface), and this can also affect the structure and turbulent transfer in the
ABL. Wind shear affects the boundary layer thermals, tilting them or weakening them.
Under conditions when the wind is strong or the temperature flows are small (for example in the early morning), boundary layer thermals may be organized into convective rolls



Figure 1. A schematic diagram of the turbulent kinetic energy in the CBL, plotted as a log-log graph as a function of scale. The spectral density of turbulent energy (S_e) is shown as a function of wave number k, and of the corresponding length scale $l = 2\pi/k$.

or cloud streets, which are quasi-linear two-dimensional structures (Young et al., 2002).
However, under strong surface heating and light winds a regime of *free convection* occurs in the CBL with thermals dominating the transfers of heat, momentum and moisture from the surface to the overlying ABL and thence to the free troposphere.

The convection inside the CBL is often dry, with no latent heat release within the 82 updrafts. However, if the moisture content is sufficient then shallow clouds (cumulus or 83 stratocumulus) may appear at the top of the ABL where thermals reach their lifting con-84 densation level. Deep moist convection refers to coherent turbulent motions of moist air 85 well into the troposphere and the development of associated deep clouds such as cumu-86 87 lus congestus or cumulonimbus. Although shallow clouds at the top of the ABL will be of interest here, we do not discuss deep clouds in any detail, excepting in so far as we 88 may be concerned with ensuring the appropriate interactions with initiating motions from 89 ABL turbulence. 90

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1.2 Turbulence modeling and the Terra Incognita

Traditionally, global models of the atmosphere use grid lengths on the order of 10 km or more, but limited-area mesoscale forecasting models may use grid lengths as low as 1 km. Thus, turbulent eddies are usually filtered out from meteorological models and the impact of turbulent transfer on the larger scale flow is parameterized through the use of boundary layer or turbulence schemes.

For modeling at relatively coarse grid lengths, which are larger than the scales of the largest eddies, the turbulence is entirely sub-grid (or filtered). The corresponding ABL parameterization schemes are designed to handle 1D vertical turbulent transfers that arise from the effects of the full spectrum of unresolved turbulent eddies. An additional shallow convection scheme may be needed to parameterize associated shallow cumulus clouds (cf. Section 3.4).

Modeling at fine grid lengths of O(10 m) occupies the regime of large-eddy sim-103 ulation (LES), where models are able to resolve explicitly most of the turbulent motions. 104 More specifically, simulations may be considered to be LES when the grid length is sub-105 stantially smaller than the dominant turbulence length scales (i.e. $l_p = 2\pi/k_p$ in Fig. 1). 106 Sub-grid turbulence is considered to be isotropic when the grid scale lies within the in-107 ertial sub-range (Fig. 1) and the dominant turbulence length scales become very well-108 resolved on the numerical grid (see Sullivan and Patton (2011) for example). At these 109 resolutions sub-grid turbulent transfers are therefore 3D and the role of the sub-grid pa-110 rameterization is to take account of the transfer of energy from the smallest resolved scale 111 to the dissipation scales (k_d) across a clearly-defined inertial sub-range. 112

The advance of atmospheric modeling from its infancy in the 1950s to its widespread 113 operational use today has been strongly related to the increase of available computer power. 114 In particular, the development of high performance supercomputers has led to a signif-115 icant increase of the horizontal grid resolution in numerical weather prediction. As res-116 olution becomes finer, models start to resolve deep convective clouds. Weather centers 117 around the world are now using high-resolution regional models for weather prediction 118 or climate purposes. The UK Met Office runs its UK variable resolution model (UKV) 119 with a 1.5 km grid length over the British isles (Lean et al., 2008) while Météo-France 120 uses the AROME-France convective scale model at 1.3 km (Seity et al., 2011) alongside 121 an ensemble system at 2.5 km (Raynaud & Bouttier, 2017). In the convection-allowing 122 regime, deep convective structures become partially resolved and no longer occupy small 123 fractional areas of the grid. Therefore, the use of conventional deep convective param-124 eterizations at these resolutions becomes highly questionable and they are often switched 125 off. 126

Pushing towards higher resolutions with grid lengths of O(100 m), atmospheric mod-127 els become able to partially resolve the largest turbulent structures in the ABL, such as 128 the strong thermals in the CBL. Recent attempts to run such high-resolution atmospheric 129 models for weather prediction applications include the Météo-France 500 m grid-length 130 AROME-airport (Hagelin et al., 2014) run in 2014 for the Single European Sky Air Traf-131 fic Research project and the UK Met Office 333 m "London model" (Boutle et al., 2015) 132 which was operational for the 2012 London Olympics. Environment-Canada simulated 133 the urban climate of Vancouver using a grid length of 250 m during the Vancouver 2010 134 Olympic and Paralympic Games (Leroyer et al., 2011). 135

Wyngaard (2004) first identified that when the size of the largest turbulence struc-136 tures in the ABL is comparable to the model grid spacing, the fundamental assumptions 137 behind conventional turbulence parameterizations are violated. He named this resolu-138 tion regime the Terra Incognita, and the concept broadened to become the gray zone of 139 turbulence in the mesoscale modeling community, focusing on the convective boundary 140 layer. In the CBL gray zone, the turbulence kinetic energy (TKE) is only partially re-141 solved, in contrast to the LES resolution regime where it is mostly resolved and in con-142 trast to the mesoscale regime where it is fully parameterized. 143

This paper is organized as follows. Section 2 describes the different facets of the gray zone of turbulence and the related modeling problems. In Section 3 we present the possible solutions that have been proposed in the literature so far, followed by a discussion in Section 4. Conclusions are provided in Section 5.

- ¹⁴⁸ 2 Characteristics and challenges of the gray zone of turbulence
- 149 2

2.1 Definition of the gray zone of turbulence

Wyngaard (2004) first studied the terra incognita using near-surface observational
 data from the Horizontal Array Turbulence Study (HATS) program. The purpose of the
 HATS field program was to study the interaction between two scales of turbulence (re-

solved/filtered and sub-grid/sub-filtered), with the ultimate goal being the improvement
of LES parameterizations. The experimental setting consisted of two horizontal crosswind lines of sonic anemometers at two different levels. The filter operation was a filter in time, with Taylor's frozen-turbulence hypothesis being applied to convert to an
equivalent spatial filter.

¹⁵⁸ Wyngaard (2004) defined the "terra incognita" at $l \approx \Delta$, where l represents the ¹⁵⁹ dominant turbulence length scale and Δ represents the filter length scale. When con-¹⁶⁰ sidered in terms of a numerical model, the filter length must be interpreted as an effec-¹⁶¹ tive resolution rather than the grid length directly (e.g. Ricard et al., 2013; Skamarock, ¹⁶² 2004). The effective resolution depends on the internal diffusion of the model. For in-¹⁶³ stance, a very diffusive atmospheric model may fail to resolve ABL turbulence even at ¹⁶⁴ hectometric grid size Δx , if its effective resolution Δ exceeds l.

Inspired by the pioneering work of Wyngaard (2004), Honnert et al. (2011) stud-165 ied the characteristics of the CBL gray zone by averaging (coarse-graining) LES data from 166 a number of well-documented case studies: the International H₂O project (Couvreux et 167 al., 2005), the Wangara campaign (Clarke et al., 1971), the African Monsoon Multidis-168 ciplinary Analysis field campaign (Redelsperger et al., 2006), the Barbados Oceanographic 169 and Meteorological Experiment (P. Siebesma et al., 2004), and the ARMCu case (Brown 170 et al., 2002) (cf. Fig. 2). The use of HATS data constrained Wyngaard's 2004 analyses 171 to the surface layer, but the use of LES allows the gray zone of turbulence to be stud-172 ied at higher levels throughout the ABL. The disadvantage is that results may become 173 sensitive to the quality of the LES. Honnert et al. (2011) used LES data as a reference 174 to document the transition of TKE and turbulent fluxes from the LES regime through 175 the CBL gray zone and into the mesoscale regime. Coarse graining of the turbulent struc-176 tures in the LES data produces smoother fields at hectometric scales in the CBL gray 177 zone until the turbulent variability becomes completely sub-grid scale at the mesoscale. 178

Figure 2 presents horizontal cross-sections of vertical velocity at 500 m altitude (in 179 the middle of the ABL) at different horizontal scales ranging from 62.5 m (the LES data) 180 up to 8 km. This example was produced by coarse graining an LES dataset based on the 181 International H_2O observational campaign (Weckwerth et al., 2004) using the Méso-NH 182 model (Lac et al., 2018; Lafore et al., 1998). In this example, the transition between the 183 CBL gray zone and the mesoscale occurs at around the 2 km scale, at which some weak 184 turbulent structure can be seen. Honnert et al. (2011) demonstrate that the transition 185 depends on the quantity under consideration: turbulent structures in the water vapor 186 mixing ratio field occur on larger scales than those associated with the vertical veloc-187 ity, in agreement with De Roode et al. (2004). 188

Honnert et al. (2011) considered the largest turbulence length scales l in the CBL to be represented by the sum of the ABL height z_i and the depth of the shallow cloud layer z_c . The basic idea is that the horizontal size of the largest structures is closely linked to their vertical extent. According to this scaling, Honnert et al. (2011) found the CBL gray zone to extend between filter scales of $0.2(z_i + z_c)$ to $2(z_i + z_c)$.

¹⁹⁴ A complementary perspective is provided by Beare (2014), who defines an effec-¹⁹⁵tive length scale for numerical models which accounts for the modeled energy dissipa-¹⁹⁶tion emerging from both the discretised advection and the sub-grid schemes. Specifically ¹⁹⁷the effective dissipation length scale $l_{d,\text{eff}}$ is given by $l_{d,\text{eff}} = 2\pi/k_{d,\text{eff}}$, where:

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$$k_{d,\text{eff}}^2 = \frac{\int_{k_0}^{k_1} k^2 S_e(k) dk}{\int_{k_0}^{k_1} S_e(k) dk}$$
(1)

k is the wave number and S_e is the TKE power spectrum. Beare (2014) considers a CBL gray-zone simulation to be one in which there is no clear separation between the production length scales and the model dissipation scale. In other words, there is no iner-

tial sub-range in the model: recall Fig. 1. A similarity relationship as a function of $z_i/l_{d,eff}$



Figure 2. Horizontal cross-section of LES vertical velocity data at 500 m altitude (top left) and coarse graining of that data onto a range of scales up to 8 km. The units are ms^{-1} . Adapted from Honnert et al. (2011).

expresses the relative impact of the modeled dissipation scales on the physical production and can be used as a definition for the CBL gray zone. Beare (2014) identifies the transition between the CBL gray zone and the mesoscale regime as occurring at $z_i/l_{d,eff} =$ 0.7.

Figure 3 summarizes the different resolution regimes in atmospheric simulations 207 based on the above and other related studies. The CBL grav-zone transition is deter-208 mined by the dissipation length scale analysis of Eq. 1 from Beare (2014), while the LES 209 transition is identified based on the findings of Sullivan and Patton (2011). Between the 210 mesoscale and LES limits, we identify both a gray zone and a near gray zone (see Ef-211 stathiou et al., 2018). In the latter regime, most of the TKE is resolved $(e_{\rm res}/e_{\rm tot} \gg 0.5)$ 212 but the simulations should not be considered as LES converging because the grid length 213 is not fine enough to present a clear inertial sub-range (see also Sullivan & Patton, 2011). 214 The regime might also be thought of as a coarse LES simulation and most practical ap-215 plications treat the regime similarly to a standard LES. However, such a treatment can 216 have significant implications, especially in cases where the turbulence length scales are 217 evolving (Efstathiou et al., 2018). Taking $l \approx z_i$ and $z_i \approx 1000$ m, we find that LES 218 converging simulations can be achieved at $\Delta x \sim 20$ m while the CBL gray zone is roughly 219 at 2 km > Δx > 200 m. 220

2.2 Where is the 'truth'?

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Turbulent motions are chaotic by definition. Turbulence modeling does not attempt to describe them in full detail but introduces a statistical description of the turbulence. Traditionally numerical weather prediction models simulate the Navier-Stokes equations subject to an averaging or filtering operation. The mean quantities after filtering (\overline{f}) are often interpreted as representing the most probable state of the atmosphere assuming that the distribution of possible sub-filter states is reasonably regular. Turbulence pa-

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Figure 3. Schematic description of simulation regimes as a function of Δ/l , where Δ is the filter scale and l is the scale of the energy containing structures. Also shown is an estimate of typical model grid spacings. The horizontal cross-sections are taken from Fig. 2.

rameterizations for such models are often based on an ensemble average (Mellor & Yamada, 1982): i.e., an average over an infinite number of possible independent realizations of the flow. More generally, the averaging operator is assumed to fulfill Reynolds assumption (Stull, 1988, e.g., $\overline{gf} = \overline{gf}$, where f and g are functions and \overline{f} denotes the average of f).

An alternative to ensemble averaging is to consider the filtering to be a time or space 233 average. This approach is taken, for instance, when researchers average LES output data 234 in order to characterize turbulent statistics (Couvreux et al., 2010; A. P. Siebesma & Cui-235 ipers, 1995, see also Sections 2.1 and 2.4) and to develop mesoscale parameterizations 236 (e.g. Rio et al., 2010). If a spatial averaging scale is sufficiently large as to sample many 237 eddies then there is often no practical difference between ensemble and spatial averag-238 ing. However, for a grid scale that is hectometric the form of the assumed averaging op-239 erator becomes crucial. 240

Using a space-time filter at scales of the gray zone of turbulence, model output fields should become turbulent, and partially-resolved turbulent structures appear (cf. Fig. 2). Such outputs represent one possible state of the atmosphere on the filtered scales. Realscale experimental data represent only one possible state of the atmosphere also, and this would likely differ from the model state even if one were to have a perfect model.

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2.3 Transition from sub-grid to resolved turbulence

As discussed above, turbulence in the CBL gray zone is partially resolved. Using 247 LES data, the partitioning of turbulent energy into that which is sub-filter and that which 248 is resolved can be computed for a given filter. The partition will depend upon the fil-249 ter scale and the size of the turbulent structures. Honnert et al. (2011) considered such 250 partitions for TKE and turbulent fluxes across the transition from the LES converging 251 regime to the mesoscale limit in cases of free dry and cloudy CBLs. The partition func-252 tion was scaled using the similarity parameter $\Delta x/(z_i+z_c)$ with Δx being the coarse-253 graining filter scale. Figure 4 shows such a transition curve for the TKE. The approach 254 has also been extended to other types of ABL (Shin & Hong, 2013). 255

The transition curve for the partitioning of turbulent quantities across scales has become widely used as a reference tool and a test-bed for the development and testing of parameterizations for the CBL gray zone (Boutle et al., 2014; Efstathiou & Beare, 2015; Ito et al., 2015; Malavelle et al., 2014; Shin & Hong, 2015; Shin & Dudhia, 2016).



Figure 4. Functions showing the partition of the total TKE e_{total} into resolved (e_{res}) and sub-grid (e_{sbg}) parts, as a function of $\Delta x/(z_i + z_c)$ (from Honnert et al., 2011): $e_{\text{res}}/e_{\text{total}}$ is in warm colors and $e_{\text{sbg}}/e_{\text{total}}$ is in cold colors. A similarity relation was found to hold in the CBL at altitudes z between $0.05z_i$ and $0.85z_i$.

Honnert et al. (2011) evaluated the behavior of a state-of-the-art mesoscale model 260 (Méso-NH) in the CBL by comparing simulations at different scales against the refer-261 ence curve of Fig. 4. Within the CBL gray zone, the resolved turbulence was found to 262 be too large when the model's turbulence scheme was used without its mass-flux part. 263 The scheme did not mix the boundary layer efficiently enough, regardless of the mixing 264 length scale parameter that was used within the scheme to calculate the diffusivity. In 265 contrast, Honnert et al. (2011) found the resolved turbulence to be too weak when the 266 mass-flux scheme component of the scheme was activated. This effect strongly depends 267 on the mass-flux scheme (Shin & Dudhia, 2016). One of the mass-flux-type ABL schemes 268 tested in Shin and Dudhia (2016) showed a strong resolved turbulence even though the 269 mass-flux component was activated, because the mass-flux part was not large enough to 270 estimate the vertical transport by strong updrafts. 271

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2.4 Traditional assumptions in models of the atmospheric boundary layer challenged by the gray zone of turbulence

The results discussed in Sect 2.3 illustrate that in the transition between sub-grid and resolved turbulence, traditional assumptions made in models of the atmospheric boundary layer, either at coarse or at very fine resolutions, are no longer valid in the gray zone of turbulence.

Large-scale models assume that the filter length scale (and also the related grid length 278 of the model) is much larger than the important turbulent length scales in the bound-279 ary layer, and that therefore the representation of turbulence in the boundary layer does 280 not strongly depend on the resolution of the model. They additionally assume, as men-281 tioned in Section 2.2, that turbulent transfer is represented by an ensemble average of 282 all possible flow realizations inside each grid box and as a result only the mean effects 283 of turbulent motion are considered. On the opposite end of the spectrum, LES models 284 require that the inertial sub-range is well resolved and so that the sub-grid turbulence 285 scheme depends on model resolution in straightforward ways that can be deduced from 286 scaling arguments. In neither case, however, is there any guarantee of an appropriate scale-287 awareness of the sub-grid turbulence within the gray zone of turbulence. 288

Another important issue is that large-scale models assume that sub-grid turbulent transport is dominated by the vertical component, and are therefore one-dimensional. However, neither is the sub-grid turbulence isotropic in three dimensions as commonly assumed by LES models. Thus, the gray zone of turbulence raises issues around the extent of anisotropy.

Wyngaard (2004) rigorously analyzed the turbulent momentum fluxes in the sur-294 face ABL with data from an anemometer array. The arrangement is illustrated in Fig. 5. 295 He showed that some production terms for turbulent fluxes that may be negligible in the 296 LES and mesoscale limits can nonetheless be significant in the gray zone of turbulence. 297 Such terms are associated with anisotropy of the flow. It is important to bear in mind 298 however, that the buoyancy-driven turbulence which dominates in the middle of the CBL 299 is more strongly uni-directional than the shear-driven turbulence which plays an impor-300 tant role in the surface layer. 301

Honnert and Masson (2014) use LES coarse-graining of idealised CBL simulations 302 to assess the scale dependence of turbulence production terms for TKE in the CBL above 303 the surface layer. They show that 3D dynamical production terms become non-negligible 304 over flat terrain at resolutions finer than $0.5(z_i+z_c)$, a result which implies that for such 305 scales then 1D parameterizations do not provide an adequate representation of the TKE. According to Honnert and Masson (2014) the turbulence is anisotropic at about 0.02 <307 $\Delta x/(z_i+z_c) \leq 0.5$. This range is consistent with the analysis of Beare (2014) for defin-308 ing the CBL grav-zone onset from a different perspective (Section 2.1). Interestingly, Efstathiou 309 and Beare (2015) also related the gray-zone onset to the need for different treatments 310 of vertical and horizontal diffusion in their sub-grid model when simulating a quasi-steady 311 state CBL. 312

Moreover, in both large-scale models as well as LES models, sub-grid turbulence 313 314 schemes are usually assumed to be deterministic. Transport in the CBL is characterised by a population of turbulent eddies that cover a range of scales. With increasing model 315 resolution the largest eddies are resolved first. Assuming that a space-time filtering ap-316 proach is being taken, as in most traditional large-scale models of the ABL, then the part 317 of the eddy size distribution that remains sub-grid will become increasingly under-sampled. 318 with few of the largest unresolved eddies being present on the scale of a grid cell. Thus, 319 one expects to find stochastic behavior near the grid scale in the gray zone of turbulence. 320 and the traditional assumption that the number of eddies or updrafts in each grid cell 321



Figure 5. Arrangement of sonic anemometers in the HATS experiments. Single and double arrays are located at heights z_s and z_d above the surface, and the crosswind separation between individual sonic anemometers at each height is L_s and L_d respectively. Two reference sonic anemometers (circled) are used to monitor the possibility of flow interference among the anemometers in the s and d arrays. Adapted from Sullivan et al. (2003)

is large enough to fulfill the "law of large numbers" underlying deterministic parame-terizations is no longer valid.

Other important assumptions concern the representation of non-local expressions 324 in turbulence parameterizations. These are often formulated using mass flux approaches 325 (Section 3.4). As resolution increases, the large non-local motions will be partially re-326 solved within the CBL gray zone. Mass-flux schemes used in meso-scale models assume 327 that the non-local part of the flux is attributable to these CBL thermals, that the re-328 sulting flux is stationary and that the thermals occupy a relatively small area compared 329 to their more quiescent environment. Each model grid cell is supposed to contain both 330 a meaningful number of such thermals and their associated compensatory subsidence. 331 The assumption that the vertical velocity in the grid cell is zero or that the thermal frac-332 tion is negligible breaks down by definition in the CBL gray zone where the thermal length 333 scale is on the order of the grid spacing. 334

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2.5 Gray zone in an evolving convective boundary layer

Atmospheric models have a fixed grid length but the turbulence characteristics may 336 change in the course of a simulation. A pertinent example is the development of a CBL 337 that is strongly forced by surface heating, as often occurs over cloud-free land during the 338 morning. Figure 6 shows the evolution of such a developing CBL in a case study using 339 the Met Office Large Eddy Model (LEM) with $\Delta x = 200, 400$ and 800 m (Efstathiou 340 et al., 2016). Shaded in gray are the times and heights where the flow is considered to 341 be in the CBL gray zone, according to the analysis of Beare (2014). In the 800 m run 342 the CBL remains in the gray zone throughout the simulation. In contrast, the 200 and 343 400 m simulations lie in the CBL gray zone only during the early CBL development, al-344 beit with the 400 m run taking somewhat longer to transition to the coarse LES regime. 345 Moreover, near the surface and the top of the ABL the CBL gray zone persists for longer 346 since the turbulent length scales are affected by the presence of these boundaries to the 347 turbulent part of the flow. Thus, we see that a simulated evolving CBL can be in dif-348

- ³⁴⁹ ferent resolution regimes that can vary both in time and space depending on the scale
- ³⁵⁰ of the convective structures.



Figure 6. The time evolution of the CBL depth (black line) in a case study simulation of an evolving CBL (Efstathiou et al., 2016) using three different horizontal grid spacings. Shaded in gray color are the parts of the CBL that are considered to be in the gray zone of turbulence according to the analysis of Beare (2014).

A particular problem in gray-zone simulations of an evolving CBL concerns the spinup of realistic levels of resolved TKE from the initial state. Efstathiou et al. (2016); Zhou

et al. (2014) and Kealy et al. (2019) have shown that spin-up is significantly delayed with 353 coarsening resolution within the CBL gray zone. Shin and Hong (2015) also pointed out 354 that their gray-zone CBL parameterization delayed the spin-up of resolved motions. The 355 consequence of delayed spin-up is that temperature profiles can become super-adiabatic 356 in response to the lack of non-local mixing that the resolved TKE would otherwise pro-357 vide. Such a delay can also have significant implications when simulating the full diur-358 nal cycle of convection, including the transition from shallow to deep moist convection 359 (e.g. Petch et al., 2002). 360

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2.6 From shallow to deep moist convection to synoptic-scale systems

Various properties of convective clouds and mesoscale systems in sub-kilometric mod-362 els have been demonstrated to be rather sensitive to the choices made in the formula-363 tion of turbulent mixing within the gray zone of turbulence. Some good examples can 364 be seen in the idealized modeling studies of Bryan and Morrison (2012); Craig and Dorn-365 brack (2008); Fiori et al. (2010); Verrelle et al. (2015). Similar case studies in realistic 366 conditions can be found in Bengtsson et al. (2012); Duffourg et al. (2016); Martinet et 367 al. (2017); Ricard et al. (2013), while a rich statistical perspective is provided by Stein 368 et al. (2015). The studies of Tomassini et al. (2016); Sakradzija et al. (2016) focus par-369 ticularly on the interplay between boundary-layer turbulence and shallow convective clouds. 370

The representation of boundary-layer turbulence in numerical weather prediction 371 models does not only interact with (shallow and deep) convective cloud, but is also closely 372 interrelated with the representation of the land surface, the atmospheric dynamics, and 373 microphysics (Field et al., 2017). Boundary-layer processes are important even for syn-374 optic scale weather systems. In the mid-latitudes, boundary-layer friction provides a damp-375 ing mechanism for barotropic vortices through Ekman pumping (Boutle et al., 2015). Baro-376 clinic developments are also dampened by changes to low-level stability which can be un-377 derstood in terms of tendencies of potential vorticity that are produced by turbulent mix-378 ing processes (Adamson et al., 2006; Stoelinga, 1996). By contrast, in the tropics, boundary-379 layer dynamics may often act to enhance synoptic-scale systems. This is well illustrated 380 by African easterly waves, for which potential vorticity generation by boundary-layer pro-381 cesses can feed into the dynamics and contribute to wave growth (Tomassini et al., 2017). 382 Moreover, boundary-layer turbulence is important in the establishment of summer time 383 low-level jets over land which may transport high moist static energy air and feed deep 384 convective development (Chen & Tomassini, 2015). This mechanism is particularly rel-385 evant in monsoon regions and at continental-scale precipitation margins. 386

3 Modeling the atmospheric boundary layer in the gray zone of tur bulence

As explained in Section 2, the gray zone of turbulence is not a physical phenomenon, but rather it describes interrelated problems that arise due to the assumptions behind our current turbulence and shallow convection schemes. In this section, we consider some possible solutions that have been proposed to those problems, and their limits.

393 **3.1** Full transport model approach

Wyngaard (2004) suggested using the full transport equations for representing the sub-grid scalar transport of a conserved scalar field c at gray-zone resolutions in the boundary layer. Without imposing the usual assumptions in mesoscale modeling he introduced a tensor form for the parameterization of the turbulent flux (f_i) of c (see Appendix A for an outline of the derivation):

$$f_i = -K_{ij} \frac{\partial \overline{c}}{\partial x_j} \tag{2}$$

where K_{ij} is a tensor form of the eddy diffusivity which is a function of a turbulent time 400 scale, the shear tensor and the Reynolds stress. Thus, Wyngaard's 2004 model can be 401 viewed as a generalized form of the usual diffusion approach which can account for anisotropy 402 of the turbulence. As implied by the arguments of Section 2.4, this extension is an at-403 tractive possibility for modeling sub-grid fluxes from the LES to the mesoscale limit. The 404 eddy diffusivity is a function of the flow and should be treated as a tensor and not as 405 a scalar. Other elements of the full tensor may become important in the gray zone of turbulence (such as the tilting terms) since the heterogeneity of the convective structures 407 might impose strong horizontal gradients. 408

Hatlee and Wyngaard (2007) first implemented the approach to study HATS data 409 close to the surface. Kelly et al. (2009) extended the approach to the ocean surface layer 410 by analyzing data from the OHATS (Ocean Horizontal Array Turbulence Study) obser-411 vations and developed a simple parameterization for pressure fluctuation induced by mov-412 ing surface waves. The full transport equations have been implemented by Ramachandran 413 and Wyngaard (2011) and Ramachandran et al. (2013) in simulations of a convective 414 case in the ocean. They showed that the anisotropic terms in the sub-filter flux equa-415 tions can indeed become important when the grid length approaches the dominant pro-416 duction scales, in accordance with the HATS analyses of Hatlee and Wyngaard (2007). 417 Therefore their model produced much better estimations of the momentum and heat fluxes 418 compared to the standard eddy-diffusivity approach. 419

The full transport model apears to be a promising first approach to modeling in the gray zone of turbulence. Such an approach is expected to behave analogously to a higher-order closure scheme in the mesoscale limit with the appropriate choice of length scales (Wyngaard, 2004). However, the shortage of validation studies, and in particular the absence of a full implementation of the method accross the complete range of modelling scales, does not allow firm conclusions to be drawn on the performance or the practical applicability of the scheme.

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3.2 TKE turbulence modeling

TKE-based turbulence models determine eddy diffusivities based on the magnitude of sub-grid TKE, *e*, specifically:

$$K_c = C_c l_m \sqrt{e} \tag{3}$$

where C_c is a constant which may depend on the variable c of interest, while l_m is the mixing length. l_m may be set using the CBL height in mesoscale models, but is based on the grid spacing in LES applications of the approach. The sub-grid TKE itself is obtained by solving its prognostic equation:

 $\frac{\partial \overline{e}}{\partial t} = -\left(\overline{u_i}\frac{\partial \overline{e}}{\partial x_i} + \frac{\partial \overline{u_i'e}}{\partial x_i} + \frac{1}{\rho_0}\overline{u_i'\frac{\partial p'}{\partial x_i}} - \nu\frac{\partial^2 \overline{e}}{\partial x_i^2}\right) - \overline{u_i'u_j'\frac{\partial \overline{u_j}}{\partial x_i}} + \beta\overline{u_3'\theta'} - 2\nu\overline{\left(\frac{\partial u_j'}{\partial x_i}\right)^2}$ (4)

where θ is the potential temperature, p is the pressure, ν is the molecular diffusivity and β is the buoyancy parameter. Other symbols have been already introduced. The first (in parentheses) term on the right hand side describes the tendency of e due to large scale advection, turbulence, pressure gradient correlations and molecular diffusion, the second and third terms represent the production of turbulence by wind shear and buoyancy respectively and the last right-hand side term is the dissipation of e.

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3.2.1 Pragmatic approaches over complex terrain

Turbulence parameterizations for atmospheric models have been developed based on assumptions that are, strictly speaking, only valid for horizontally homogeneous and flat terrain, and may not be suitable for complex terrain. For example, Monin-Obukhov similarity theory is commonly used to compute surface fluxes and assumes horizontally homogeneous fluxes from the surface into the boundary layer. In complex terrain, Arnold
et al. (2012) recommends as a first approach the use of fully prognostic three-dimensional
TKE schemes for grid spacings between 100 and 300 m.

Beljaars et al. (2004) proposed a parameterization of turbulent orographic form drag 450 that takes into account the model resolution and is used at ECMWF. However, while 451 there are studies of the behavior of orographic drag in the gray zone of deep convection 452 (5 km resolution), (Sandu, ECMWF Newsletter 150) there are none as yet at the hec-453 tometric scales. At hectometric scales, it is not well understood which part of the drag 454 should be taken into account through an explicit parameterization of orographic drag 455 and which part by the turbulence scheme. We note that the model of the Met Office does 456 not include an orographic drag contribution at such scales. Moreover, the theoretical back-457 ground of the processes involved is not well understood even at mesoscales (see Sandu, 458 ECMWF Newsletter 150). Hence, analysis of the problems in representing orographic 459 drag in the grav zone of turbulence is more difficult than an analysis based on the dy-460 namic production of TKE in the turbulence scheme. 461

Over complex terrain in the CBL gray zone, the full three-dimensional effects have
been found to be important in the shear production term for TKE (Arnold et al., 2014;
Goger et al., 2018). Goger et al. (2018) therefore propose an extension of the 1D prognostic TKE equation used in the COSMO (COnsortium for Small-Scale Modeling) model
turbulence scheme because that scheme otherwise underestimates the TKE. The 1D form
considers only the contributions to shear production from vertical gradients of horizontal winds, but Goger et al. (2018) supplement this with a further contribution of

$$\frac{\partial \overline{e}}{\partial t}\Big|_{\text{shear}} = (C_s \Delta x)^2 \left[\left(\frac{\partial \overline{u}}{\partial x}\right)^2 + \left(\frac{\partial \overline{v}}{\partial y}\right)^2 + \frac{1}{2} \left(\frac{\partial \overline{u}}{\partial y} + \frac{\partial \overline{v}}{\partial x}\right)^2 \right]^{\frac{3}{2}}$$
(5)

where C_s is chosen to be the Smagorinsky constant (see Section 3.3). This extension was tested in simulations over the Alps for a grid length of 1.1 km and had beneficial effects. The verification indicated improvement in the TKE on the slopes, which suggests that the addition of 3D effects is particularly suitable for inclined surfaces.

474 3.2.2 Adaptive length scales

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In order to incorporate scale-awareness (Section 2.4), various authors have attempted 475 to develop approaches for the gray-zone of turbulence that are based on rethinking the 476 mixing length that is used in TKE-based approaches (Eq. 3) or other semi-empirical length 477 scales used in higher-order turbulence models. Ito et al. (2015) for example, has proposed 478 an extension of Mellor-Yamada-Nakanishi-Niino (MYNN) model for the gray zone of tur-479 bulence. The MYNN model is a higher-order turbulence closure designed for 1D mesoscale 480 applications (Nakanishi & Nino, 2009). The sub-grid TKE is predicted using an empir-481 ical length scale to parameterize various terms. In the extension the length scale is mod-482 ified in order to hold the TKE dissipation invariant to the grid resolution. To partition the TKE into appropriate resolved and sub-grid contributions the extension also con-484 siders the partition function proposed by Honnert et al. (2011) (as discussed in Section 2.3). 485 Horizontal diffusion based on Ito et al. (2014) is also included in order to take account 486 of anisotropy (Section 2.4). Ito et al. (2015) showed that a CBL gray-zone simulation 487 employing this extension was able to realize reasonable vertical transports. 488

Kitamura (2015) used a coarse-graining approach on LES data from a CBL simulation in order to estimate the length scale dependence on grid spacing, assuming the form of a TKE-based Deardorff (1980) model for the turbulent fluxes. Notably the estimated length scale was found to depend upon both the horizontal and vertical grid spacings. Kitamura (2016) implemented the resulting mixing length formulations in a modified Deardorff (1980) model, which improved the representation of the vertical heat flux and the magnitude of the resolved convection in the CBL gray zone. Zhang et al. (2018) blended between the sub-grid turbulent mixing length scales
that are appropriate for the LES and mesoscale limits to create a grid-scale-dependent
3D TKE scheme. The scheme includes a non-local component in the vertical buoyancy
which is also down-weighted by a blending function (cf. Boutle et al., 2014) depending
on the resolution regime. The blended approach was implemented in WRF and exhibited improved behaviour in comparison with a conventional TKE scheme.

Kurowski and Teixeira (2018) also proposed to pragmatically merge the mixing lengths from LES and NWP formulations to obtain a mixing length for intermediate scales:

$$\left(\frac{1}{l_{BL}}\right)^2 = \left(\frac{1}{l_{1D}}\right)^2 + \left(\frac{1}{l_{3D}}\right)^2 + \left(\frac{1}{l_s}\right)^2 \tag{6}$$

where l_{3D} is Deardorff LES mixing length (Deardorff, 1980), l_s is a surface mixing length (see Kurowski & Teixeira, 2018) and l_{1D} is the large scale NWP mixing length from Teixeira and Cheinet (2004). In their formulation, the mixing length is smaller than the smallest of the three components. Their merged mixing length does not explicitly depend on resolution, but in practice it increases with increasing grid size until the mesoscales.

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3.2.3 Two turbulence kinetic energies

A related approach has been proposed by Bhattacharya and Stevens (2016) who 508 introduce two turbulent kinetic energies in order to distinguish between the energy con-509 tained in large eddies spanning the CBL and that within eddies that are sub-grid with 510 respect to the vertical grid spacing. The two energies are conceptually linked via the tur-511 bulent energy cascade. Bhattacharya and Stevens (2016) formulated distinct length scales 512 to describe mixing and dissipation associated with each energy. However, the problem 513 remains of how to divide the energy due to the boundary-layer-scale eddies into resolved 514 and unresolved parts. The approach is yet to be tested in a weather or climate model. 515

3.3 Extending the Smagorinsky-Lilly scheme into the gray zone of tur ⁵¹⁷ bulence

The Smagorinsky-Lilly (Lilly, 1967; Smagorinsky, 1967) scheme is a widely-used standard for large-eddy simulations of many and various engineering and geophysical flows. Scalar fluxes are represented by:

$$f_i = -K_c \frac{\partial \overline{c}}{\partial x_i},\tag{7}$$

as described in Appendix A ppendix A (Eq. A3). The eddy diffusivity is expressed as

$$K_c = l_t^2 \mid \overline{S} \mid / \Pr \tag{8}$$

where Pr is known as the Prandtl number, $|\overline{S}|$ is the modulus of the shear tensor $\overline{S}_{ij} = (\partial \overline{u_i}/\partial x_j) + (\partial \overline{u_j}/\partial x_i)$, and l_t is the turbulence mixing length. The specification is completed by choosing the mixing length to be $l_t = C_s \Delta$ where C_s is known as the Smagorinsky constant. Following the analysis of Lilly (1967) it is often set to 0.17 although different values up to 0.23 have been suggested and used in atmospheric models. The Smagorinsky scheme acts in all three directions with the same eddy diffusivity. Comparing to Eq. 2, the scheme is an approximate form of the full turbulent stress tensor model, valid when the full turbulent stress tensor is assumed isotropic, such that $K_{ij} = K_c \delta_{ij}$.

526 3.3.1 Bounding approach

Efstathiou and Beare (2015) showed that the standard Smagorinsky scheme becomes too diffusive in the CBL gray zone. Therefore, in order to reduce the over-damping effect arising from the increase in mixing length l_t with horizontal resolution Δx , a modification was made in an attempt to conserve the effective diffusivity of the flow across different grid lengths. As a first approximation, the vertical Smagorinsky diffusivity profile was bounded so that values could not exceed those produced by a 1D mesoscale approach. The horizontal diffusion was handled by a 2D closure and allowed to vary in order to account for anisotropy of the flow at CBL gray-zone resolutions. This bounding approach was able to match the energetics of the coarse-grained fields across the transition from the LES to the mesoscale regime in a quasi-steady state CBL.

537 3.3.2 Dynamic Smagorinsky

The standard Smagorinsky approach is designed for the LES regime and assumes 538 a clear scale separation with the presence of a clear inertial sub-range (Section 2.4). The 539 idea behind a dynamic model is to treat C_s as a flow-dependent variable, which can be 540 estimated by comparing the resolved flow against the same flow filtered onto a coarser 541 "test" scale. The idea can also be extended through comparison of the resolved flow against 542 that at two different filtered scales in order to estimate a flow-dependent and scale-dependent 543 C_s . The aim of such a scale-dependent dynamic model is to respect the characteristics 544 of the turbulence spectrum without necessarily requiring the resolved flow to lie within 545 the inertial sub-range. Hence, it is a promising extension of Smagorinsky that is well suited 546 to coarse LES resolutions (e.g. Kleissl et al., 2006; Mirocha et al., 2013) and perhaps even 547 to CBL gray-zone resolutions. 548

Efstathiou et al. (2018) modified and implemented a scale-dependent, Lagrangianaveraged dynamic Smagorinsky sub-grid scheme based on Bou-Zeid et al. (2005) into the Met Office Large Eddy Model. Extending an earlier study by Basu et al. (2008), they found the approach to perform well for an evolving CBL in capturing the resolved turbulence profiles in comparison with coarse-grained LES fields, especially in the *near grayzone* regime (Fig. 3). However, such a dynamic approach reaches a limit of applicability if the test filter is required to sample the flow at a scale for which the turbulence is not adequately represented by the model.

One way around this issue could be the use of the Dynamic Reconstruction Model of Chow et al. (2005) which attempts to reconstruct the smallest resolved scales and uses those to dynamically derive the sub-grid mixing length. Simon et al. (2019) tested this approach to simulate a quasi-steady CBL at gray-zone resolutions and found significant improvement over conventional schemes and especially compared to the standard Smagorinsky scheme.

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3.4 Modifying boundary layer 1D non-local parameterizations

CBL thermals (cf. Section 2.4) are manifestations of non-local turbulence, and are responsible for the development of a zone of counter-gradient fluxes at the top of the CBL which is ill-represented by an eddy diffusivity form (Eq. 3).

⁵⁶⁷ In mesoscale models, the turbulent transport from the surface to the top of the ABL ⁵⁶⁸ by convective thermals can be parameterized by the use of an additional counter-gradient ⁵⁶⁹ term (Deardorff, 1972) so that,

$$f_c = -K_c \left(\frac{\partial \overline{c}}{\partial z} - \gamma\right) \tag{9}$$

where f_c is the turbulent flux of c and γ is the counter-gradient term. More complex parameterizations have been based on the transilient matrix (Stull, 1984)) or the mass-flux scheme (Cheinet, 2003; Hourdin et al., 2002; Pergaud et al., 2009; Rio et al., 2010; A. P. Siebesma et al., 2007; Tan et al., 2018). In a mass-flux scheme the turbulent flux is expressed as

$$f_c = -K_c \frac{\partial \overline{c}}{\partial z} + M_u (c_u - \overline{c}) \tag{10}$$

- where M_u is the mass-flux associated with the ABL thermals, and c_u is the mean value
- c_{177} of c inside the thermals. The second term on the right-hand side represents the trans-
- ports by coherent thermal plumes whereas the first term is expressed in eddy diffusiv-
- ⁵⁷⁹ ity form and represents the contributions from smaller-scale more-localized eddies (Fig. 7).
- ⁵⁸⁰ This mass flux approach also lends itself naturally to extensions that treat shallow boundary-
- ⁵⁸¹ layer clouds.



Figure 7. Schematic diagram of small local eddies (red dashed circles), contrasted against a non-local thermal (blue tube) which extends from the surface (green) to the cloud layer (in gray).

Representations of the form of Eqs. 9 and 10 are designed for mesoscale models but the split provides an interesting starting point for possible gray zone treatments of turbulence. As resolution increases the large non-local motions will be partially resolved within the CBL gray zone for $\Delta \sim z_i$ but the small eddies might remain purely sub-grid. With this point in mind, the adaptation of mesoscale models to the CBL gray zone could be achieved by revisiting traditional non-local ABL schemes.

A mass-flux scheme used at the mesoscales assumes that a non-local flux is created 588 by the CBL thermals. This flux is assumed to be stationary and is created by several 589 thermals which occupy small areas compared to their more quiescent environment. Each 590 model grid cell is supposed to contain both a meaningful number of updrafts and their 591 associated compensatory subsidence. Such assumptions break down by definition in the 592 CBL gray zone where the thermal length scale l is of the order of the grid spacing Δx 593 (Section 2.4). Related issues have been studied in the context of the mass-flux represen-594 tation of deep convective clouds and are discussed by Arakawa et al. (2011); Arakawa 595 and Wu (2013) for example. 596

Honnert et al. (2016) modified a mass-flux scheme for the CBL gray zone (Pergaud et al., 2009), by generalizing the mass flux equations without the need for assumptions that the vertical velocity in the grid cell is zero or that the thermal fraction is negligible. In this framework, the velocity of the parameterized updraft is reduced when the resolution increases, which then permits the model dynamics to produce resolved structures. The study also incorporates a dependency on the normalized resolution $\Delta x/(z_i + z_c)$ in the surface closure conditions, as discussed further by Lancz et al. (2017).

Shin and Hong (2015) have proposed a one-dimensional parameterization for the 604 CBL grav zone based on Eq. 9, but which gradually reduces the parameterized vertical 605 transport as model resolution increases. The local transports from small-scale eddies and the sub-grid non-local transports are computed separately and reduced at different rates. 607 The non-local transport is formulated from three linear profiles which capture its three 608 most important roles: surface-layer cooling, mixed-layer heating, and entrainment at the 609 CBL top of air from aloft. Each of these profiles is constructed as a function of stabil-610 ity parameters in the surface- and/or entrainment layers. The method is designed to re-611 produce the total non-local turbulent transport, and the required sub-grid portion is com-612 puted by multiplying an explicit grid-size dependent function which can also vary ac-613 cording to the transported variable, the height (Honnert et al., 2011), and the stability 614 (Shin & Hong, 2013). The local transport is formulated as an eddy diffusivity, and is mul-615 tiplied by a different grid-size dependent function (Shin & Hong, 2015). Both idealized 616 and real-case simulation results with the CBL gray-zone parameterization showed im-617 provements over the use of the conventional unmodified parameterization at CBL gray-618 zone resolutions. 619

Such changes, however, do not solve all the problems of the gray zone of turbulence. The modified mass-flux, for example, remains based on horizontal homogeneity assumptions. Thus, it should be coupled with a local turbulence scheme that is itself adapted to the CBL gray zone, especially over mountains where it does not produce enough turbulent transports and can lead to unrealistic vertical velocities.

As noted in Section 1.2, the UK Met Office runs operational forecasts at gray zone 625 scales of 1.5 km and 333 m. Particularly in the latter case some of the large eddies re-626 sponsible for much of the transport are resolved, but other turbulent motions are par-627 tially or completely unresolved and continue to require some non-local parameterization. 628 The approach has been to devise a pragmatic blending between mesoscale and LES pa-629 rameterizations (Boutle et al., 2014). The former is provided by the Met Office bound-630 ary layer scheme (Lock et al., 2000) (which is similar to Eq. 9 for a CBL) and the lat-631 ter by a 3D Smagorinsky (Eq. 7) scheme. The blending is scale-dependent, being based 632 on the ratio of the grid scale to a diagnosed length scale characterising the turbulence. 633 The benefits of this blended parameterization in the UM are well illustrated by Boutle 634 et al. (2014), where a realistic stratocumulus case was simulated using horizontal grid 635 lengths from 100 m to 1 km, the turbulence changing from largely resolved to largely un-636 resolved. However, the diffusive nature of the Smagorinsky scheme can result in the de-637 layed spin up of non-local motions especially during the handover from the non-local mesoscale 638 to the Smagorinsky scheme in deepening CBLs, as shown in Efstathiou et al. (2016). Efstathiou 639 and Plant (2019) extended the blending approach by incorporating a scale-dependent 640 dynamic Smagorinsky scheme instead of the standard static Smagorinsky scheme. They 641 found some promising results in idealized simulations of an evolving CBL, particularly 642 in relation to the spin-up of resolved turbulence (cf. Section 3.3.2). 643

644 645

3.5 The gray zone of turbulence as a Rayleigh-Bénard convection problem

⁶⁴⁶ Zhou et al. (2014) examined the grid-dependent nature of gray-zone CBL simulations using a mesoscale parameterization of turbulence. The analysis is based on the Rayleigh-⁶⁴⁸ Bénard (RB) thermal instability framework, with the Rayleigh number (Ra) redefined ⁶⁴⁹ by its turbulent counterpart

$$Ra = -P_{rT} \frac{N^2 H^4}{\nu_T^2},$$
(11)

where P_{rT} is the turbulent Prandtl number, N (s⁻¹) is the buoyancy frequency, ν_T (m²s⁻¹) 650 is the eddy viscosity, and H (m) is a length scale over which N is computed. H scales 651 with the boundary layer depth z_i (m). It is set to the surface layer depth (about 0.1 z_i) 652 in Ching et al. (2014), and to z_i in Zhou et al. (2014). In extending the RB analysis to 653 the CBL, the effects of wind shear, which are mostly concentrated in the surface layer 654 and the entrainment zone, are ignored. Turbulent mixing terms are also linearized by 655 assuming an eddy-diffusion representation. Despite its simplicity, the RB framework is 656 useful for understanding model behaviors associated with conventional ABL schemes act-657 ing on CBL gray zone grids. For example, the onset of convection in the resolved flow 658 was explained based on the RB framework. The onset depends on a critical value of Ra659 which is itself a function of grid spacing in the CBL gray zone. Sufficient instability in 660 the surface layer eventually leads to strong grid-scale convection after Ra has reached 661 its critical value. 662

The turbulent nature of grid-scale convection can mask mesoscale circulations, such as a well-defined sea breeze. Ching et al. (2014) drew on the Rayleigh-Bénard framework to develop a scheme based on the Rayleigh number which aims to suppress any convective motions in CBL gray zone simulations. Specifically the thermal diffusivity was modified in order to keep Ra below its critical value and so convective overturning remained as a sub-filter process even at very fine grid lengths. This stands in contrast to the other methods discussed in this paper.

670

3.6 Stochastic approach

As discussed in Section 2.4, scale adaptive modeling of transport in the boundary-671 layer gray zone is intrinsically linked with representing stochastic behavior. Stochastic 672 backscatter techniques have a well-established value in improving LES simulations close 673 to the earth's surface. The length scale of the dominant eddies close to the surface is con-674 strained by the presence of the surface, so that $l \sim z$. It follows that the near-surface 675 flow may lie within the turbulence gray zone of $l \sim \Delta$ even for situations in which the 676 turbulence in the interior of the flow is well resolved (Mason & Thomson, 1992; Wein-677 brecht & Mason, 2008). The backscatter of energy from unresolved scales onto the grid 678 can improve turbulent statistics in such cases and has also proved helpful in the near gray 679 zone. A recent extension by O'Neill et al. (2015) allows for grid-independent spatial vari-680 ations in the backscatter rate. 681

An important issue in the performance of gray-zone turbulence parameterizations, 682 as alluded to several times above, is a mechanism to initiate resolved-scale turbulent struc-683 tures in an evolving flow. In reality turbulent length scales might be growing from subgrid to resolved scales but as the simulated growth may be overly slow, the explicit in-685 clusion of some local near-grid-scale variability can prove useful. Backscatter, and other 686 stochastic methods, can provide such mechanisms. (An alternative may be to make the 687 low-level temperature profile unrealistically unstable by, for example, suppressing the nonlocal flux, as shown in Efstathiou and Beare (2015).) The issue is most often discussed 689 in terms of the spin-up of resolved turbulence in time from an initial smooth field. How-690 ever, similar issues also arise in transitioning to resolved turbulence downstream of the 691 smooth lateral boundary conditions that are usually imposed in numerical weather pre-692 diction. Lateral boundary spin-up has received less attention in the literature to date, 693 but we note that some methods addressing the problem have been developed in the en-694 gineering community, involving the injection of synthetic turbulence (e.g. Xie & Castro, 695 2008) and these ideas may provide a suitable remedy. 696

Various stochastic parameterization approaches have been developed for climate models and ensemble-based numerical weather prediction as modifications to mesoscale parameterization methods. To date, these have often been focused on the parameterization of diabatic processes, especially deep convection, and reviews of such techniques

are provided by Khouider et al. (2010); Palmer (2012) and Plant et al. (2015). Some of 701 these ideas may also be applied in the CBL gray zone. Simple methods have included 702 rescaling the parameterization tendencies by a random multiplicative factor or making 703 random choices for some of the scheme parameters (Palmer, 2001). Alternatives have 704 attempted to embed stochastic variability at a deeper level, within the sub-grid process 705 description. A suitable starting point is to partition the total turbulent flux into con-706 tributions from multiple transporting elements, which may include information about 707 size. Grid-scale adaptivity can then be achieved by size-filtering the population (Brast 708 et al., 2018), while stochasticity can be represented in the element properties. A natu-709 ral choice is to consider that a random number of elements may be found within a grid 710 area (Leoncini et al., 2010; Plant & Craig, 2008) while others allow LES-informed ran-711 dom switching between distinct modes of turbulent heating (Dorrestijn et al., 2013) or 712 random variability in the element/environment mixing rate (Suselj et al., 2014). The vari-713 ables for which suitable spectra of elements have been constructed include the local ther-714 modynamic state (Cheinet, 2003; Neggers et al., 2002, 2009), the mass flux carried by 715 the elements (Plant & Craig, 2008; Sakradzija et al., 2014, 2016), or even size itself (Neggers 716 et al., 2019; Park, 2014; T. M. Wagner & Graf, 2010). 717

A simple stochastic method has been implemented operationally in the Met Of-718 fice UM turbulence-gray-zone configurations which draws on some of the above ideas. 719 It can be considered as a simplified stochastic backscatter scheme where random boundary-720 layer temperature and humidity perturbations are applied to the smallest resolvable scale 721 (taken to be 8 grid-lengths). The magnitude of the perturbations are designed to rep-722 resent realistic boundary layer variability that would arise from a variety of poorly re-723 solved processes at km-scale (not just boundary layer thermals but also surface hetero-724 geneities and convection). The scheme also includes a time correlation of the perturba-725 tions on an approximate large-eddy turnover time scale. At present no attempt has been 726 made to make these perturbations scale in a physically appropriate way, e.g. with the 727 relative scale of the boundary-layer eddies to model resolution. Overall the scheme gives 728 significant improvements to the initiation of small diurnally triggered convective show-729 ers over the UK and also improves spin-up of convective scale motions from the bound-730 aries. Some other related approaches for introducing physically-based boundary-layer 731 fluctuations are described by Muñoz-Esparza et al. (2014); Kober and Craig (2016); Leoncini 732 et al. (2010). 733

Kealy et al. (2019) examined in more detail the impact of random boundary layer
temperature perturbations on the spin-up of resolved turbulence at gray-zone resolutions.
They found that the combination of imposed perturbations along with a scale-dependent
sub-grid turbulence scheme has the most pronounced effect on the spin-up of resolved
motion.

739

3.7 Grid refinement approach

Zhou et al. (2017) have proposed a rather different modeling methodology for CBL 740 gray-zone simulations, based on refining the horizontal grid spacing in the surface layer 741 (the bottom 10-15%). They adopt a two-way nesting technique to couple the simulation 742 of the surface layer with that in the rest of the CBL. Since thermals in the CBL orig-743 inate from the surface layer, the idea is that an improved representation of the surface 744 layer should induce a good representation of the thermal population throughout the CBL. 745 An LES turbulence closure is used in the surface layer and a mesoscale form of param-746 eterization is adopted aloft. Zhou et al. (2018) demonstrate results which show substan-747 tial improvement of first and second order turbulent statistics, especially when horizon-748 tal resolution is refined up to half of the CBL depth (Zhou et al., 2017). 749

The grid refinement approach should be considered as a numerical method rather than a parameterization. In the high-resolution surface nest, assumptions behind ABL



Figure 8. Schematic summarizing the relations between the various approaches that have been introduced and discussed. To simulate the turbulence in the gray zone, each method has a starting point in LES or mesoscale model and to a certain extent gets rid of the initial hypotheses. The dotted line shows where a parameterization family has no theoretical limit, but no application yet.

schemes are completely replaced by traditional LES assumptions (i.e. inertial sub-range 752 grid spacing and isotropic sub-grid turbulence). The grid refinement method does not 753 really differentiate grid spacings aloft, and can be applied as a general nesting method. 754 The method is of limited use to LES because the turbulent flows are already well resolved 755 in the CBL, although Sullivan et al. (1996) and Hug et al. (2014) did apply a similar method 756 with LES as an improved wall model to better resolve fine-scale surface-layer turbulence. 757 The method is also unnecessary for mesoscale models, because however well resolved the 758 thermals are in the nested high-resolution surface grids, they are not expected to have 759 any impact on the coarse mesoscale grids where they are entirely subgrid-scale. 760

3.8 Summary and critical review

761

Section 2 discusses the major challenges of modeling in the CBL gray zone. In the 762 LES regime, the subgrid-scale turbulence is small, homogeneous and isotropic. At the 763 near gray-zone, turbulence starts to become anisotropic (Section 2.4) and the possibil-764 ity of some resolved-scale turbulence (Section 2.1) is a challenge, not least in producing 765 spin-up problems. In the gray-zone regime, the horizontal homogeneity hypothesis, usu-766 ally used at mesoscales, is no longer valid (Section 2.4) and CBL thermals that are en-767 tirely subgrid at the mesoscale (Section 2.2) are partly resolved. Figure 8 summarizes 768 the different regimes and the validity domains of the different parameterizations. 769

The experiences of performing CBL gray-zone simulations with conventional (LES or mesoscale) parameterizations show that models are likely to fail to capture a correct

resolved turbulence or else to produce unrealistic over-energetic turbulent structures (Honnert 772 et al., 2011). The behavior of models in the gray zone of turbulence depends on various 773 physical factors (surface characteristics, topography, and time of day, among others) and 774 also on the model specifications (such as the grid spacing, the diffusion, numerical damp-775 ing, etc). Moreover, the model grid spacing itself can be a poor proxy of the actual model 776 resolution (Ricard et al., 2013; Skamarock, 2004). In particular, the grav zone of turbu-777 lence cannot be limited to the hectometric scales: gray-zone issues can impact on mod-778 eling at both larger (Goger et al., 2018) and finer scales (Wyngaard, 2004). 779

780 Nonetheless, there does seem to be a critical core of new ideas emerging that is well worth pursuing in sub-kilometer simulations. No parameterization is created ex nihilo. 781 Historically, LES and mesoscale schemes have drawn upon assumptions and simplifica-782 tions that are informed by our understandings of the atmospheric boundary layer. For 783 instance, most mesoscale schemes assume that turbulent fluxes are horizontally homo-784 geneous so that only the vertical flux needs to be parameterized. On the other hand, most 785 LES schemes assume that sub-grid turbulence is isotropic. The subgrid flux is charac-786 terized by a single mixing length when an eddy viscosity model is employed. 787

Figure 8 shows two categories of scheme. One category treats the gray zone of tur-788 bulence by starting from mesoscale approaches and attempt to adapt and extend them 789 for higher resolution applications (mass-flux modifications and Shin and Hong (2015), 790 RB representation and most of the stochastic parameterizations). These schemes typ-791 ically aim to reduce the non-local subgrid turbulence, but remain focused on a vertical 792 1D representation of the CBL. Some of these schemes operate by blending LES and mesoscale 793 formulations, including the two turbulence kinetic energy approach (Bhattacharva & Stevens, 794 2016) and the blended model of (Boutle et al., 2014). The blended approaches seem able 795 to produce scale-adapted subgrid CBL thermals, as well as LES isotropic turbulence when 796 necessary. However, there is as yet no good evidence that they can capture the anisotropic 797 character of the turbulence in the near gray zone regime. The incorporation of additional 798 wind shear terms in a TKE scheme, as in (Goger et al., 2018), may compensate for the 799 lack of 3D turbulence in the gray zone, but it does not produce the limiting forms of be-800 havior of 1D CBL thermals at the mesoscale or a 3D isotropic scheme in LES. The other 801 major category attempts to treat the gray zone of turbulence as essentially "coarse LES" 802 by adapting and extending LES turbulence models into the gray-zone regime (full trans-803 port model, all adaptations of the mixing length, bounding model and dynamical Smagorin-804 sky). Such schemes have had some successes, especially in extending from the LES, isotropic, 805 mainly-resolved turbulence regime into the near gray-zone anisotropic-turbulence region, 806 but they cannot represent non-local turbulence typical of the CBL at the mesoscale. 807

Although most of the parameterizations that have been developed so far cannot 808 be seamlessly used from LES to the mesoscales, they do provide some interesting clues 809 towards solving practical problems in the gray zone of turbulence. Some promising re-810 sults have emerged from both major categories. Some simple blending/hybrid schemes 811 using non-local turbulence (Boutle et al., 2014; Efstathiou & Plant, 2019; Shin & Hong, 812 2015), TKE (Ito et al., 2015; Zhang et al., 2018) or mass-flux approaches (Honnert et 813 al., 2016) may significantly improve the representation of first-order quantities and tur-814 bulence statistics in the CBL gray zone. 815

⁸¹⁶ 4 Discussions

Modeling within the CBL gray zone is increasingly becoming seen as necessary for near future operational use because there is a growing demand for higher resolution forecasting, especially for the prediction of high-impact weather events. A wide range of novel approaches have been presented (Section 3) in this article incorporating various new parameterization ideas to address the challenges of the CBL gray zone. Moreover, an increasing number of researchers are actively working on the topic. Thus, the turbulence gray zone has clearly become a hot topic in atmospheric modeling. However, key questions remain.

825 826

4.1 Is the gray zone of turbulence stalling the improvement of atmospheric modeling?

Our review has shown that most of the gray-zone turbulence studies to date have 827 been based on idealized or real but relatively simple well-known cases over homogeneous 828 surfaces (e.g. the Wangara case study). Some caution is therefore needed. In order to 829 develop atmospheric modeling we require not just that there is an appropriate treatment 830 of turbulent motions in the gray zone but also that their treatment should enable the 831 correct interactions with other atmospheric processes. These points are discussed in Sec-832 tion 2.6 and are highlighted by LeMone et al. (2010) or J. S. Wagner et al. (2014) for 833 example. However, there are also well-documented cases that clearly benefit from im-834 proving resolution into the gray zone of turbulence, despite potential issues with sub-835 grid scale turbulence parameterization. This can be seen in the simulations of Warren 836 et al. (2014) for a slow-moving organized convective system over a complex terrain area 837 in southwest England. 838

Most scale-aware gray-zone schemes for the CBL have been developed with a fo-839 cus on cloud-free conditions or with shallow cumulus clouds. It is much less clear how 840 many of the schemes would perform in deep moist convection environments, including 841 organized systems or tropical cyclones. It is also less clear how they might couple to synoptic-842 scale motions (Section 2.6). A useful study from this perspective is that of Green and 843 Zhang (2015) who investigated the partition between resolved and sub-grid turbulent fluxes in turbulence gray-zone simulations of hurricane Katrina. In their simulations, the par-845 titioning and the character of the resolved turbulent structures varied significant with 846 the resolution, but the system's intensity was not affected because the total turbulent 847 fluxes remained almost the same. Other case studies of other phenomena with other ap-848 proaches to the gray zone of turbulence would clearly be valuable. 849

The complexity of partially-resolved structures in the gray-zone boundary layer and 850 the feedbacks between resolved and sub-grid dynamics during deep convective cloud de-851 velopment are not yet understood. Pronounced sensitivity to turbulent mixing in sub-852 kilometer simulations of deep convection has been identified in a number of recent stud-853 ies. Verrelle et al. (2015) showed that insufficient mixing led to strong undiluted ther-854 mals and unrealistic resolved TKE in a super-cell simulation. In Hanley et al. (2014), 855 simulated deep clouds were found to exhibit small features compared to radar observa-856 tions, although their representation could be somewhat improved by increasing the sub-857 grid turbulence mixing length. Moreover, Verrelle et al. (2017) identified the presence 858 of non-local structures in deep clouds that can pose significant challenges to conventional 859 mixing schemes. Ito et al. (2017) examined a number of heavy rainfall cases and found 860 that the rate of improvement in the skill of the forecasts became progressively smaller 861 for further increases of horizontal resolution into the sub-kilometric regime. Although 862 their simulations seemed to be relatively insensitive to the CBL representation, the re-863 sults do indicate that interactions of the near-grid scale with the larger scale environ-864 ment, and with other processes, might still be important in the gray zone of turbulence. 865

An important context for these findings is the resolution required for the represen-866 tation of deep convective clouds. There is a convective gray zone associated with such 867 clouds at grid spacings of around 1-10 km. So called "convection permitting" simu-868 lations with the convection parameterization switched off have been shown to yield some 869 significant benefits for $\Delta x < 5$ km (Roberts & Lean, 2008). However one would not ex-870 pect the deep clouds to be well represented on a numerical grid unless one can adequately 871 resolve the turbulent mixing processes at the cloud edges. These have a scale of ~ 100 m 872 (Craig & Dornbrack, 2008), so improvements in modeling explicit deep convection might 873

prove modest until those grid lengh scales are reached, *unless* a better parameterization of turbulent mixing processes can be introduced.

As illustrated by Stirling and Petch (2004) and Kealy et al. (2019), the impact of small-scale boundary-layer variability is important for an accurate representation of the diurnal cycle of convection in the turbulence gray zone, not least for the timing of deep cloud initiation. This point encourages further development of stochastic approaches and improvement can reasonably be anticipated from imposing appropriate small-scale variability in the CBL.

882 883

4.2 Should resolved convective motion be allowed in the turbulence gray zone?

Ching et al. (2014) argue that any partly-resolved turbulent motions in gray-zone 884 ABL simulations are not realistic and should be damped. Since the simulations are not 885 in the LES converging regime and the results depend heavily on the imposed dissipation, 886 they should not be trusted. Hence, these authors pursue an ensemble-average approach 887 to the model filter operation, in which their gray-zone ABL simulations are valued for 888 producing improved numerical accuracy for a mesoscale modeling approach (cf. Mason 889 & Brown, 1999). The authors showed an example of noisy resolved motions that masked 890 the lake-breeze field. However, they do recognize the importance of resolved convective structures in the CBL for the triggering of deep convection, as discussed in the previ-892 ous subsection. 893

The initiation of resolved motion in gray-zone ABL simulations is generally considered to be a valued aspect for the majority of gray-zone ABL studies and for operational atmospheric models. By allowing some partially-resolved convective overturning motion, most modelers are (conceptually at least) following a spatially-filtered approach in which an *appropriate* level of variability near to the filter scale is considered to be desirable. It should be stressed that this is also the view taken by coarse-graining studies and in simulation strategies developed from those.

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4.3 Testing models in a realistic set-up - The Gray Zone Project

The Gray Zone Project promotes international collaborations and community activities in the development of scale-aware deep and shallow convection and boundarylayer parameterizations and focuses on grid lengths of about 200 m to 10 km. It has been initiated by WGNE (Working Group on Numerical Experimentation) and the GEWEX (Global Energy and Water Exchanges) Global Atmosphere System Studies.

A first phase of the Grav Zone Project examined the simulation of a maritime cold 907 air outbreak that was observed during a field campaign (Field et al., 2014). Model in-908 tercomparisons have been reported for simulations with global models (Tomassini et al., 909 2016), limited-area models Field et al. (2017) and large-eddy simulations (de Roode et 910 al., 2019). Model resolutions were systematically varied in order to explore their behav-911 iors across a range of spatial scales, and results were compared to the observations. A 912 second phase of the project is now being planned and will investigate shallow cumulus 913 914 clouds at turbulence gray-zone resolutions as part of the EUREC4A project in 2020 (Elucidating the role of clouds-circulation coupling in climate, Bony et al., 2017) and also the tran-915 sition from shallow to deep convective clouds over the eastern tropical Atlantic based on 916 the GATE field campaign (Global Atmospheric Research Program's Atlantic Tropical 917 Experiment, Kuettner, 1974). 918

4.4 Prognostic adaptive schemes the way forward?

Most proposed methodologies in the boundary-layer gray zone have either LES or 920 mesoscale parameterizations as their starting point. However, various mesoscale param-921 eterizations based on prognostic equations do exist (e.g. Lappen & Randall, 2001; Tan 922 et al., 2018), and since these tend to be more adaptive to the resolved flow, they may 923 be worth more attention in terms of developing extensions for the gray zone of turbu-924 lence. Such mesoscale parameterizations are often designed with an assumption that the 925 thermal fraction is assumed small, which is a defect in the gray zone of turbulence. Mod-926 ifications such as those in Honnert et al. (2016) to introduce a scale-aware thermal area 927 fraction may therefore be necessary in extending their use. A related starting point could 928 also be that of Thuburn et al. (2018), who recently proposed a two-fluid theoretical frame-929 work for the representation of convection in models, using coupled prognostic primitive 930 equations for both the coherent eddy structures (convective plumes) and their environ-931 ment. 932

An approach that seems to be able to bridge the gap between the LES and the mesoscale 933 limits, is the full transport model of Wyngaard (2004). Nevertheless, solving several prog-934 nostic higher-order equations, involving several terms that require further closure assump-935 tions and parameters, can be computationally expensive. Linear algebra closure mod-936 els such as Lazeroms et al. (2016) could offer a potential route forwards to reducing com-937 putational costs while retaining the tensor representation of the fluxes that is at the core 938 of the approach. In either case, the dynamic modeling technique of filtering at multiple 939 scales (Bou-Zeid et al., 2005; Chow et al., 2005) can be used to determine the necessary 940 length scales and tuning parameters, thereby making such schemes not only scale-aware 941 but also flow-dependent. Dynamic calculation of length scales in an evolving CBL has 942 been shown to be beneficial for the CBL gray zone (Efstathiou et al., 2018; Efstathiou 943 & Plant, 2019). 944

It is clear that special care needs to be taken in the gray zone of turbulence for the representation of horizontal fluxes (Zhou et al., 2017). The conventional 2D Smagorinsky adaptation for horizontal mixing has been shown to be inappropriate in the representation of CBL mixing (Ito et al., 2014; Zhou et al., 2017). A recent scale-aware representation of horizontal diffusion from Zhang et al. (2018), based on Honnert et al. (2011) and using the blending approach of Boutle et al. (2014), has shown promising results.

951 5 Conclusions

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We have reviewed the current state of a newly-emerged research area in the numer-952 ical modeling of geophysical flows and discussed the significant challenges that arise for 953 the atmospheric modeling community. Numerical models are now moving towards sub-954 kilometer grid spacings at which they produce partially-resolved turbulent structures. 955 As a result in the "gray zone" of turbulence, the fundamental assumptions underpinning 956 our conventional treatments of sub-grid scale variability are no longer valid. Furthermore, 957 at CBL gray-zone resolutions the resolved scale variability becomes highly dependent on 958 the representation of sub-grid motion that in turn can compromise the accuracy and value 959 of the numerical model simulations. 960

A model's horizontal grid spacing cannot by itself determine the onset of the CBL 961 gray zone or explain the transition of the TKE and heat and moisture fluxes from the 962 LES to the mesoscale limit. The key to describing the transition is to consider the rel-963 ative extent of the dominant turbulence length scales compared to the effective grid spac-964 ing. This means that different structures, whether these are CBL thermals or clouds at 965 the top of the ABL, might be in different resolution regimes especially as they evolve over 966 time (similar to Fig. 6). It also means that one should take into account the imposed 967 dissipation from the numerical methods in use, which can damp or smooth the resolved 968

field. The interplay of numerical and "physical" diffusion (from the turbulence parameterization) will determine the effective resolution of an atmospheric model; i.e. its ability to partially resolve features at the limits of its grid resolution (Skamarock, 2004).

The proposed grav-zone CBL parameterization schemes in the literature, as pre-972 sented here, are largely based on two approaches: treating the gray zone of turbulence 973 as either a coarse LES or a high-resolution mesoscale model depending on the starting 974 point of each parameterization. However, there are some approaches that attempt to avoid 975 the bulk of the gray zone of turbulence, either by increasing the horizontal resolution in 976 certain parts of the CBL or by filtering out any turbulent motions. The latter approach 977 considers the simulation to belong the mesoscale resolution regime where all of the tur-978 bulent transfer is parameterized in an ensemble-average sense. Even though many of the 979 schemes considered show certain merits and benefits in the gray zone of turbulence, most 980 of them have been tested in idealized settings. As a next step more comprehensive stud-981 ies are needed using realistic case studies to identify the interactions of partially-resolved 982 turbulent mixing with deep convective clouds and with the larger scale circulations. 983

The full turbulent transfer equations should, at least in principle, be able to handle the transition of turbulent transfer from well resolved to fully parameterized. However, solving the full turbulent transport equations would be computationally expensive and suitable closure assumptions would be needed, perhaps depending on the level of information that is available from the resolved motions. As this approach may not be practical, even with the available computing power, the anisotropic production terms in the transport equations might be usefully retained in various simplified ways.

It is very clear that the existence of the turbulence gray zone has important im-991 plications and consequences for atmospheric modeling and for the future of numerical 992 weather prediction in particular. Recent studies, such as those discussed in Section 4, 993 have demonstrated that at sub-kilometer grid spacings increasing convergence with in-994 creasing grid resolution is not guaranteed, especially in simulations with deep convec-995 tion. However, the full extent of the impact of partially resolved turbulent flow on the 996 actual performance of weather forecasting needs to be further investigated. This is partly 997 due to the fact that some of the feedbacks between the turbulent mixing in the CBL and 998 synoptic-scale systems are not yet well understood. Nevertheless, the refined resolution 999 can still prove to be beneficial, especially when it is combined with better representa-1000 tion of topography and surface heterogeneity and especially in cases with strong large-1001 scale forcing. 1002

Although this article has been focused on the CBL gray zone and atmospheric sim-1003 ulations, other aspects of geophysical fluid flow modeling experience their own gray zone. 1004 The representation of any important physical phenomenon with a length scale of the same 1005 order as the grid spacing is liable to be problematic in numerical simulations. Such a sit-1006 uation is clearly undesirable but sometimes cannot be avoided, due to finite computa-1007 tional limitations or else because the phenomenon itself covers a range of scales. The CBL 1008 gray zone is *relatively* simple in various respects, the dominant turbulent structures be-1009 ing well understood and having a well-defined length scale dictated by the CBL depth. 1010 Thus, it provides a good base case for the study of possible methods for treating gray 1011 zone motions in geophysical flows more generally. Promising approaches to gray zones 1012 may be more easily identified in this setting, and conversely, it seems difficult to imag-1013 ine that approaches performing poorly for the CBL gray zone would somehow work well 1014 in other, more complex settings. 1015

Appendix A The full transport equations

In Section 3.1 a tensor form of the eddy diffusivity was presented. Following Wyngaard (2004), this may be derived from the scalar-flux transport equation. The sub-grid flux

of a conserved scalar field c in the i direction is denoted $f_i = \overline{cu_i} - \overline{c} \ \overline{u}_i$ where the overbar is a spatial filter, and it evolves as (Wyngaard, 2004):

$$\frac{\partial f_i}{\partial t} + \overline{u}_j \frac{\partial f_i}{\partial x_j} = -f_j \frac{\partial \overline{u}_i}{\partial x_j} - \tau_{ij} \frac{\partial \overline{c}}{\partial x_j} + \text{PT} + \text{FLXDIV}, \tag{A1}$$

The first two terms on the right hand side are production terms, the first (tilting term) 1017 representing the stretching and "tilting" of turbulent eddies and the second represent-1018 ing the interaction of turbulent fluxes (Reynolds stresses, τ_{ij}) with the scalar gradient 1019 (gradient term). Other terms express the pressure – scalar interactions (PT) and the di-1020 vergence of the sub-grid flux of f_i (FLXDIV). The flux divergence terms contain higher 1021 order contributions that express the sub-grid turbulent transport of f_i . PT acts as a prin-1022 cipal sink for the scalar flux and can be parameterized as $-f_i/T$ in its simplest linear 1023 form, with T representing a characteristic time scale of the sub-grid turbulence. 1024

Wyngaard (2004) proposed a model for the sub-grid scalar fluxes that is obtained by retaining the first two production terms in Eq. A1, assuming a steady state, and balancing the production with the pressure terms. The model is given by:

$$f_i = -T\left(f_j \frac{\partial \overline{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial \overline{c}}{\partial x_j}\right). \tag{A2}$$

Although Eq. A2 expresses an algebraic model, it would be entirely straightforward to retain a prognostic form based on Eq. A1.

Dropping the tilting terms and retaining only the gradient production terms in the direction of the flux (isotropic gradient production), Eq. A2 reduces to:

$$f_i = -T\tau_{ii}\frac{\partial \overline{c}}{\partial x_i} = -K_c\frac{\partial \overline{c}}{\partial x_i}.$$
(A3)

This corresponds to the down-gradient diffusion model that is commonly used as a basis for turbulence parameterization in both LES closures and mesoscale ABL schemes. $K_c = T\tau_{ii}$ is the eddy diffusivity. Without these additional assumptions, the formal solution of Eq. A2 is given by Eq. 2 (Wyngaard, 2004):

$$f_i = -K_{ij} \frac{\partial \bar{c}}{\partial x_i} \tag{A4}$$

where K_{ij} is a tensor form of the eddy diffusivity which is a function of T, the shear tensor $\partial \overline{u}_i / \partial x_j$ and τ_{ij} .

1041 Glossary

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- Atmospheric Boundary layer The bottom layer of the atmosphere that is in contact with the surface of the earth.
- Free Troposphere The part of the Earth's troposphere which excludes the boundary
 layer. Turbulence in the boundary layer is ubiquitous but in the free troposphere
 is produced only sporadically, by mechanical forcing in regions of pronounced wind
 shear or thermally inside convective clouds.
- Backscatter Energy transfers in turbulent three-dimensional fluid motions occur to both
 larger and smaller spatial scales. The net transfer within the inertial subrange is
 downscale but the backscatter refers to the upscale component of energy trans fer, from subgrid-scale to resolved motions.
- Baroclinic waves Synoptic-scale disturbances that grow in the mid-latitudes due to
 baroclinic instability and which are responsible for the development of weather
 systems.
- Deep Clouds Clouds with predominantly vertical development that form as a result
 of deep convection in the troposphere. They may extend from the top of the bound ary layer towards the upper troposphere (cumulus congestus) or as far as the tropopause

1058	(cumulonimbus). Such clouds may be associated with thunderstorms, heavy rain-
1059	fall and hail.
1060	Large-Eddy Simulation A three-dimensional numerical simulation of turbulence, in
1061	which the largest eddies are explicitly resolved, while the effects of subgrid-scale
1062	eddies in the inertial subrange are parameterized.
1063	Large/synoptic-scale The scales of the general atmospheric circulation related to the
1064	high-tropospheric long-wave patterns.
1065	Low-level jet A jet of wind that appears in the boundary layer.
1066	Mesoscale Refers to atmospheric phenomena having horizontal scales ranging from a
1067	few to several tens of kilometers, including thunderstorms, squall lines and topographically
1068	induced circulations such as mountain waves, mountain and valley breezes as well
1069	as sea and land breezes.
1070	Parameterization The representation, in a dynamic model, of physical effects in terms
1071	of admittedly oversimplified parameters, rather than realistically requiring such
1072	effects to be consequences of the dynamics of the system (from American Mete-
1073	orological Society Glossary).
1074	Shallow Clouds Low-level, usually non-precipitating, clouds which may be considered
1075	to form part of the ABL. Cumulus and stratocumulus are forms of shallow con-
1076	vective clouds.
1077	Troposphere That portion of the atmosphere where most weather occurs and which
1078	extends from the Earth's surface to a sharp temperature inversion at the tropopause,
1079	between 10 and 20 km aloft.
1080	Surface Layer The lowest $10-15\%$ of the atmospheric boundary layer where first or-
1081	der quantities such as wind and temperature follow an approximately logarithmic
1082	profile and turbulent fluxes may be considered almost constant.
1083	Non-local turbulence A term used in the context of 1D mesoscale parameterizations
1084	to refer to coherent turbulent structures that typically extend to the full depth
1085	of the turbulent layer. In the CBL, non-local turbulence is associated with buoy-
1086	ant thermals.

1087 Acronyms

- 1088 ABL Atmospheric Boundary Layer
- 1089 **CBL** Convective (Atmospheric) Boundary Layer
- 1090 **COSMO** COnsortium for Small-Scale Modeling
- 1091 **GEWEX** Global Energy and Water Exchanges Global
- 1092 LEM Met Office Large Eddy Model
- 1093 **LES** Large Eddy Simulation
- 1094 MYNN Mellor-Yamada-Nakanishi-Niino model
- 1095 **NWP** Numerical Weather Prediction
- 1096 **RB** Rayleigh-Bénard
- 1097 **TKE** Turbulent Kinetic Energy
- 1098 **VLES** Very Large-Eddy Simulation
- 1099 WGNE Working Group on Numerical Experimentation
- 1100 **WRF** Weather Research and Forecasting

1101 Notation

- $_{1102}$ c a conserved scalar.
- c_u value of c inside the mass-flux thermal plume
- 1104 \overline{c} mean value of c
- $_{^{1105}}$ C_c a constant value for a given scalar c

- C_s Smagorinsky coefficient 1106 Δ grid spacing, model resolution 1107 Δx model horizontal grid spacing 1108 Δz model vertical spacing 1109 e TKE 1110 e_{sgs} subgrid-scale TKE 1111 $e_{\rm res}$ resolved TKE 1112 e_{tot} total (resolved plus subgrid-scale) TKE 1113 1114 f_i sub-grid scalar flux γ counter-gradient term 1115 H a length scale over which N is computed 1116 \boldsymbol{k} wave number 1117 $k_{d,eff}$ dissipation wave-number in Beare (2014) 1118 k_d dissipation wave-number 1119 k_0, k_1 wave-number limits in Beare (2014) 1120 K_c the eddy diffusivity associated with the conserved variable c1121 K_{ii} a tensor form of the eddy diffusivity 1122 *l* length scale of the dominant energy containing structures 1123 l_m mixing length used in a TKE based parameterization 1124 l_t Smagorinsky mixing length scale 1125 l_d dissipation length scale 1126 ν_T the eddy viscosity 1127 M_u mass-flux of ABL thermals 1128 **Pr** Prandtl number 1129 P_{rT} turbulent Prandtl number 1130 **Ra** Rayleigh number 1131 τ_{ij} Reynolds stress 1132 S_e TKE power spectrum 1133 T time scale for sub-grid turbulence 1134 $\boldsymbol{\theta}$ potential temperature 1135 \boldsymbol{u} a wind component 1136 w vertical velocity 1137
 - z_c depth of the cloud layer
 - 1139 z_i CBL height
 - 1140 z altitude
 - 1141 Acknowledgments
 - ¹¹⁴² This article is a review paper : Data were not used, nor created for this research

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