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The Challenge of Small-Scale Turbulence in Planetary Boundary Layers

Juan Pedro Mellado

Max Planck Institute for Meteorology, Bundesstr. 53, 20146 Hamburg, Germany
E-mail: juan-pedro.mellado@mpimet.mpg.de

Turbulence is key for the evolution of planetary boundary layers. There are important regimes, however, in which the effect of turbulence is unclear, particularly near the surface and at the boundary-layer top, where metre and submetre scales become important. Characterising the interaction of turbulence and density stratification, radiative transfer and cloud physics at those small scales remains challenging for measurements and for numerical models that parametrise turbulence. Direct numerical simulations – whereby the Navier-Stokes equations describing the fluid motion are solved directly, without a turbulence parametrisation – are providing further insight into those interactions. In this paper, we summarise recent results that illustrate this approach, and we indicate remaining challenges that could be solved in the near future.

1 Introduction

The planetary boundary layer (PBL) is the lower layer of the atmosphere, the layer that directly feels surface effects on time scales smaller than a day. Planetary boundary layers are important in climatology – modulating the fluxes between atmosphere, land and ocean –, and in meteorology – influencing weather conditions. As fluid mechanical systems, PBLs are fascinating because their multi-scale, complex nature lead to a very rich behaviour, sometimes visible to the naked eye. The range of scales is large, extending from millimetres or less to scales commensurate with the PBL depth, which varies between a few hundred metres and a couple of kilometres. The complexity stems from the interaction between turbulence, which already constitutes a research field in itself, and other challenging phenomena such as density stratification, radiative transfer and cloud physics[1,2]. However, our understanding of this interaction remains limited in crucial aspects, particularly at metre and submetre scales – this motivates our work.

Our aim is to advance our understanding of the interaction between small-scale turbulence and density stratification, radiative transfer and cloud physics in those PBL regimes and PBL regions that are particularly important for climate research and weather prediction. Besides theory, we use direct numerical simulation (DNS), whereby the Navier-Stokes equations describing the fluid motion are solved directly, without a turbulence parametrisation[3,4]. Previous research on PBLs has often been based on numerical models that rely on turbulence parametrisations, but these parametrisations introduce sometimes too large uncertainties. Obtaining accurate data at metre and submetre scales is also challenging for measurements. The use of DNS to complement measurements and more conventional numerical models opens a new avenue, which is now possible due to the strong development of high-performance computing.

We illustrate this approach by summarising recent results obtained with simulations performed in the IBM Blue Gene/Q supercomputer (JUQUEEN) at the Jülich Supercomputing Centre. After reviewing the general formulation of the problem (Sec. 2), we organise the presentation into two topics: cloud-free convective boundary layers (Sec. 3 and Sec. 4), and the stratocumulus-topped boundary layer (Sec. 5).

2 Formulation

The flow dynamics is described in terms of the velocity field $\mathbf{v}(\mathbf{x}, t)$ and the buoyancy field $b(\mathbf{x}, t)$ acting in the vertical direction Oz. The small magnitude of the velocities found in the PBL and the small size of the domains considered in these studies compared to the scale height of the atmosphere justifies an incompressible approach. Density variations smaller than 5% allow using the Boussinesq limit. The governing equations are

$$
\begin{aligned}
&\partial_t \mathbf{v} + \nabla\cdot(\mathbf{v}\otimes\mathbf{v}) + 2\Omega\mathbf{k}\times(\mathbf{v} - G\mathbf{i}) = -\nabla p + \nu\nabla^2\mathbf{v} + b\mathbf{k} \\
&\qquad \nabla\cdot\mathbf{v} = 0 \\
&\partial_t \chi_i + \nabla\cdot(\mathbf{v}\chi_i) = \nabla\cdot(\kappa_i\nabla\chi_i - \mathbf{j}_i) + s_i \;, \qquad i = 1, \dots, n \\
&\qquad b = b^e(\chi_i)
\end{aligned}
\tag{1}
$$

The kinematic viscosity is ν, κ_i is a scalar diffusivity, p is a modified kinematic pressure, Ω is the angular velocity of the rotating frame of reference (e.g., $\Omega_0 \sin\phi$ where Ω_0 is Earth's angular velocity and ϕ is the latitude), G the corresponding geostrophic wind, and $\mathbf{i}$ and $\mathbf{k}$ are the unit vectors along Ox and Oz, respectively. The fields χ_i represent prognostic scalars (e.g., the enthalpy, the total water content or some combination thereof), $\mathbf{j}_i$ are specific transport fluxes (e.g., gravitational settling in cloud mixtures), and s_i are specific source terms (e.g., condensation rate in cloud mixtures). The buoyancy function $b^e(\chi_i)$ needs to be specified depending on the problem. In the simplest case, $i = 1$, $s = 0$ and $b^e(\chi) = \chi$, but more complex thermodynamics can be prescribed[5,6], including an anelastic formulation.

The geometry consists of a horizontal layer of fluid, and the system is statistically homogeneous inside horizontal planes. Periodicity is used as lateral boundary conditions, which is acceptable as long as the domain size is large compared to the auto-correlation lengths of the turbulent fields. Dirichlet or Neumann conditions are used at the top and bottom boundaries, depending on the problem.

The evolution equations are solved using finite-difference approximations based on spectral-like sixth-order compact Padé schemes[7]. Biased formulas are employed at the top and bottom boundaries[8]. Time advancement is performed with low-storage Runge-Kutta schemes. The algorithm to solve the pressure-Poisson equation is based on a Fourier decomposition in the horizontal planes, which leads to a set of difference equations along the vertical direction Oz. A factorisation thereof is used to satisfy the solenoidal constraint down to machine accuracy[9].

The code is written in Fortran90 and uses hybrid parallelisation: MPI for the domain decomposition in the two horizontal directions (pencils), and OpenMP to further parallelise within each node the loops where the linear systems are solved and where the different terms are added to the right-hand-side of Eqs. 1. The size of the domain decomposition can be tuned to get the best scaling.

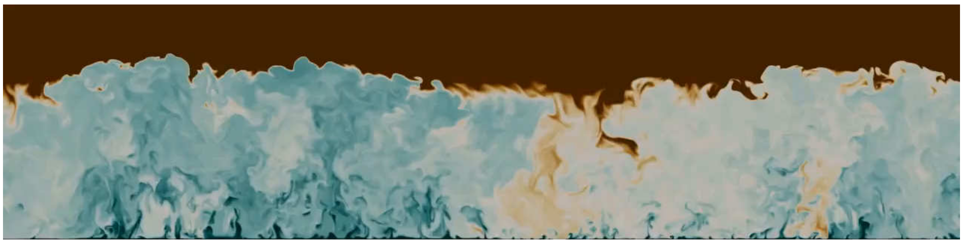

Figure 1. Vertical cross-section of the specific humidity in a convective boundary layer that grows into a dry, linearly stratified atmosphere. Green colours indicate moist regions and brown colours indicate dry regions. Small plumes near the surface converge into large-scale updrafts, whereas entrained air at the boundary-layer top converge into large-scale downdrafts, creating large-scale convection cells. The grid size is $5120 \times 5120 \times 1024$, although this figure shows only one fourth of the horizontal extent.

3 The Plume Merging Layer in Convective Boundary Layers

During daytime, the land warms the overlying atmosphere and a convective boundary layer (CBL) forms. A similar configuration can be set in the laboratory by filling a water tank with layers of increasingly lighter fluid and heating the bottom surface. Atmospheric and laboratory measurements of temperature properties near the surface show deviations from the predictions made according to the classical similarity theory[10,11]. These deviations are attributed to the formation of large-scale circulations that strongly interact with the flow inside the near-surface region (cf. Fig. 1), which invalidates the basic assumption made in the classical similarity theory, namely, that near-surface properties are independent of outer-layer variables. This prompts the following question: how do near-surface properties depend on outer-layer features that modify the large-scale circulations?

We have addressed this question by investigating the influence on near-surface properties of the buoyancy stratification above the CBL[12]. The CBL is forced by a constant surface buoyancy flux, B_0, and grows into a fluid with a constant buoyancy gradient, N^2. We have compared two cases: a neutral stratification case, $N^2 = 0$, which is representative of a CBL that grows into a residual layer during the early morning, and a strong stratification case, $N^2 > 0$, which is representative of a quasi-steady CBL during the midday. The two cases differ in the large-scale organisation of the flow, so that, by comparing them, we can ascertain what is the influence of that large-scale organisation inside the near-surface region.

We have found that, near the surface, the vertical profiles of mean buoyancy and buoyancy variance are approximately independent of N^2. As observed in atmospheric measurements and Rayleigh-Bénard convection, these profiles show deviations from the scaling laws derived according to classical similarity theory: whereas the mean buoyancy gradient varies as $z^{-4/3}$ with respect to the distance from the surface, z, the variance of the buoyancy fluctuation varies as $z^{-0.9}$ instead of $z^{-2/3}$. Although the forms of these scaling laws are independent of N^2, their vertical extent do depend on N^2. This result can be interpreted as a dependence of the inner-layer depth on N^2: in the stably stratified case, the inner-layer depth is $\simeq 25\%$ of the CBL depth, which is more than three times the value found in the neutrally stratified case.

We have used spectral analysis to better understand this behaviour. According to this

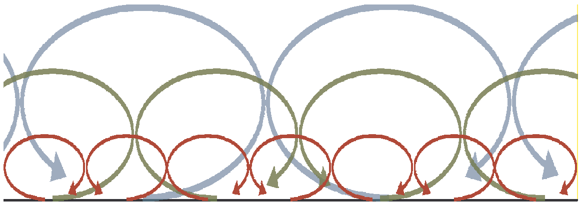

Figure 2. Sketch illustrating the hierarchy of circulations that defines the plume-merging layer near the surface[12]. The hierarchy is established by the merging of smaller plumes into larger ones, starting at the surface scales and ending at the large-scale circulations. In this sketch, only three hierarchy levels are shown.

analysis, the flow structure near the surface can be understood as a hierarchy of oblate circulations that have an aspect ratio 5:2 and that remain attached to the surface (cf. Fig. 2). The hierarchy is established by smaller plumes merging into larger ones, starting at the surface scales and ending at the large-scale circulations. This flow structure has been used to define a new near-surface layer in free convection, the plume-merging layer. Such an attached-eddy flow structure near the surface, with different features, is also characteristic of wall-bounded shear flows[13,14]. The structure of the plume-merging layer is independent of the stratification regime, but its depth strongly increases with stratification. This result partly explains the aforementioned behaviour of buoyancy properties when varying N. In particular, the spectra show that buoyancy properties near the surface are characterised by small and intermediate scales, and that is why the dependence on N^2 is relatively small, even though the width of the large-scale circulations increase more than threefold between the cases $N^2 = 0$ and the cases $N^2 > 0$.

4 Moisture Statistics in Convective Boundary Layers

Another important aspect of the CBL is moisture, since surface processes and cloud formation critically depend on it. Previous work has shown that moisture statistics strongly depend on the entrainment flux, i.e., the rate at which dry, tropospheric air is incorporated into the CBL by turbulence (cf. Fig. 1). However, that previous work is mainly based on a few single-case studies, and extrapolation to different meteorological conditions remained difficult. Besides, the entrainment flux is *a priori* unknown in important CBL regimes, such as when the CBL grows into a linearly stratified atmosphere.

We have addressed those two issues[15]. Based on dimensional analysis and a formulation of the problem in terms of the buoyancy and the water-vapour content – instead of the temperature and the water-vapour content –, we have shown that the moisture statistics depend solely on one nondimensional parameter, in addition to the ratio h/L_0 and the reference Reynolds number that characterise the CBL dynamics; h is the CBL depth and $L_0 = (B_0/N^3)^{1/2}$ is a reference Ozmidov length scale characterising the transition layer between the shear-free CBL and the free troposphere[16]. We have chosen the flux-ratio parameter $\varphi \equiv (2F_{q,0})/(F_{q,0} + F_{q,1})$, where $F_{q,0}$ is the surface moisture flux, an external parameter in this study, and $F_{q,1} \equiv (\gamma_q L_0)(N L_0)$ is a reference scale for the entrainment moisture flux. This reference scale can be interpreted as the product of a moisture variation $\gamma_q L_0$ in the entrainment zone and a velocity scale $N L_0$, γ_q being the hydro-lapse rate in the free troposphere.

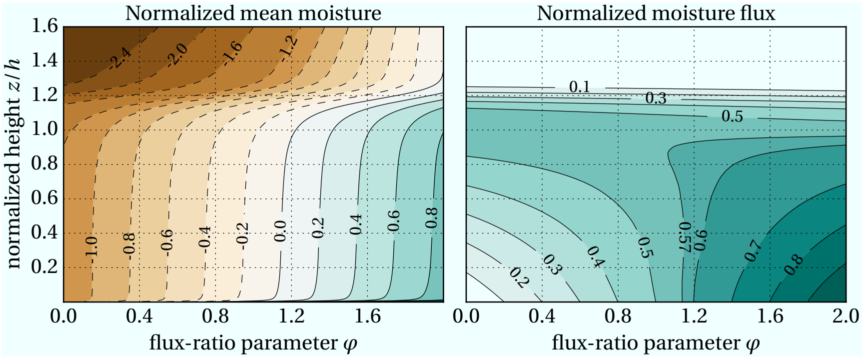

Figure 3. Contour plots of the normalised mean specific humidity and its mean vertical flux as a function of the normalised distance from the surface and the flux-ratio parameter φ: $\varphi = 0$ corresponds to pure drying conditions (the surface flux is zero) and $\varphi = 2$ to pure moistening conditions (the hydro-lapse rate is zero).

Fig. 3 confirms that $F_{q,1}$ and φ are physically meaningful parameters for the description of moisture statistics in a CBL. The flux-ratio parameter, by definition, varies between 0 and 2. For $\varphi \approx 0$ we are close to the pure drying regime: the CBL dries because the flux of moisture out of the CBL (entrainment drying) dominates over the surface flux into the CBL (surface moistening) – the flux increases from approximately 0 near the surface to a maximum $\approx 0.56\,F_{q,1}$ near the CBL top. As φ increases, the CBL dries less rapidly because surface moistening increasingly compensates entrainment drying. For values of φ slightly greater than 1, the surface moistening starts to dominate over entrainment drying and the CBL starts to moisten. We found that the cross-over value $\varphi_{\rm crit} \approx 1.16$ marks this transition between drying and moistening regimes. For $\varphi \approx 2$ we approach the pure moistening regime: $F_{q,1}$ is negligible compared to the surface moisture flux $F_{q,0}$, and $F_{q,0}$ fully characterises the mean vertical flux, which decreases from $F_{q,0}$ to $\approx F_{q,0}/2$ across the mixed layer.

A broader implication of this result is that one single simulation for a given Reynolds number is sufficient to study moisture properties for arbitrary combinations of surface fluxes and free-troposphere lapse rates of temperature and moisture. This simplification has allowed us to better characterise the moisture variance and skewness near the surface and in the entrainment zone at the CBL top[15].

5 Stratocumulus-Topped Boundary Layers

The last example considers a cloudy PBL regime, in particular, stratocumulus-topped boundary layers. Because of their large coverage and high albedo compared to the underlying surface, stratocumulus clouds in maritime PBLs affect significantly the Earth's radiative balance. Predicting the evolution of this cloud type remains a long-standing challenge for weather-prediction and climate models[17,18]. One reason is the incomplete understanding of cloud-top mixing at metre and submetre scales, which leads to large intra-model discrepancies in the mixing rates between the cloud and the environmental air, and thereby in the resulting cloud-cover evolution[19,20]. DNS constitutes one way to advance

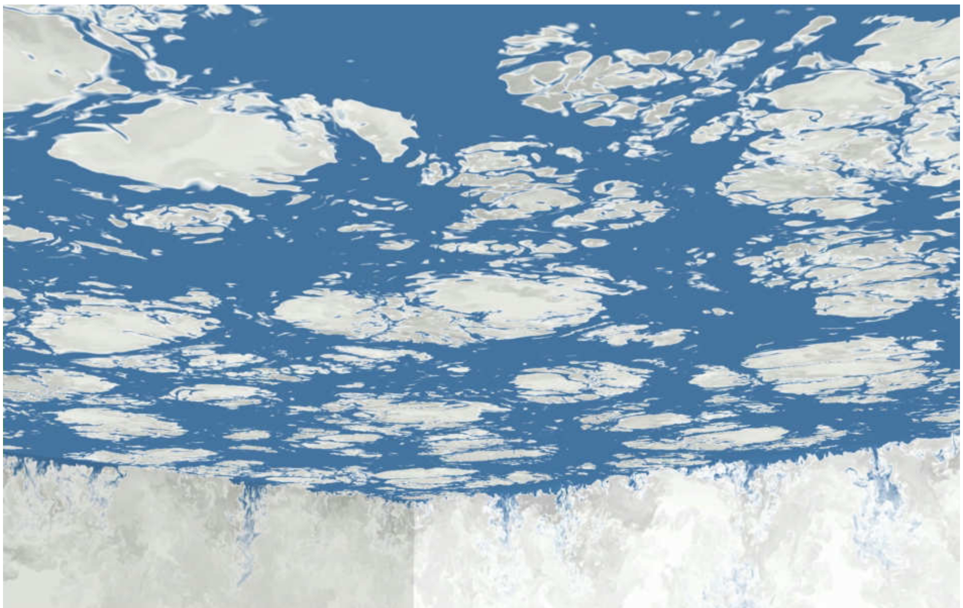

Figure 4. Composite of two vertical cross-sections and a horizontal one at the top showing the liquid mass fraction in a stratocumulus cloud. The white colon represents liquid, gray colon indicating the higher liquid water content induced by radiative cooling. The blue colon represents cloud free regions. In the vertical planes, we can observe cloud holes penetrating 50 m to 100 m into the cloud bulk. Inside the horizontal plane, we can see the penetration of cloudy updrafts into the upper clear sky; those white patches form the bases of the cloud domes that are often observed from the airplane when flying above such a stratiform cloud regime.

this understanding, since it provides accurate data at those metre and submetre scales.

The two major phenomena driving the turbulence in this type of PBLs are cloud-top radiative cooling and evaporative cooling, which promote turbulence as the cold, heavy air that forms near the cloud top falls through the cloud. (A distinct property of stratocumulus clouds is that turbulence is mainly driven from the cloud top instead of the surface.) However, these two major sources of turbulence generation can be modified by local processes at the cloud top. We have addressed the role of gravitational settling of cloud droplets.

To study the role of gravitational settling in cloud-top mixing, we need to retain the transport flux of enthalpy and water substance, i.e., the vector $\mathbf{j}_i$ in Eqs. 1. We have followed previous work and assumed a log-normal droplet size distribution with a constant number density[21,22]. The difference with that previous work is that we have resolved motions down to 10 cm instead of 5 m. Have we observed any difference?

We have found that the reduction of entrainment velocity by droplet sedimentation in stratocumulus can be 2 to 3 times larger than previously conjectured[23]. The integral analysis of Eqs. 1 shows that the reason is twofold. First, there is a non-negligible direct contribution from mass loading, as falling droplets leave behind more buoyant air in the inversion. Second, the reduction of evaporative cooling as droplets fall out of the inversion is stronger than previously observed in large-eddy simulations, where excessive mixing by turbulence parametrisations and numerical artifacts may have partially masked this effect of sedimentation on entrainment.

Such a strong effect of gravitational settling emphasises the importance of characterising better the droplet-size distribution to understand better the effect of mixing on cloud lifetime. This is a challenge, because the transport flux $\mathbf{j}_i$ depends on the fifth moment of the droplet-size distribution, and it is difficult to obtain accurately such a high-order moment.

6 Concluding Remarks

We have provided a few examples of how DNS is helping us to better understand small-scale turbulence in PBLs, namely, the plume merging layer near the surface, moisture statistics in free convection, and the role of droplet sedimentation in stratocumulus clouds. But there remain numerous long-standing problems. For instance, characterising near-surface properties of temperature and moisture in strongly unstable conditions, towards the limit of free convection reviewed in this paper, can help us to improve surface models currently used in climate research and weather prediction. Although not addressed in this paper, understanding how surface heterogeneity affects those properties is equally important and challenging. How those properties behave in the opposite regime, namely, in strongly stable conditions, remains also obscure, and DNS has recently shown its potential to shed light into this problem. Another challenge is the entrainment zone at the PBL top, where characteristic scales for the variance of thermodynamic properties remain unclear, even without clouds – with clouds, we also need to characterise the droplet-size distribution, which possibly needs a Lagrangian description of the droplets instead of an Eulerian description. High-performance computing is providing the tools to rise to these challenges.

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