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Large-Eddy Simulation
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Synopsis

Large-eddy simulation (LES) is a numerical technique for integrating spatially filtered equations of motion that describe high-Reynolds number time-evolving, three-dimensional turbulence. The spatial filtering cuts off the high frequency or small-scale part of the turbulence spectrum. Virtual turbulence generated by LES has been shown to be a surrogate for measurements of turbulent flow fields. LES is widely used for turbulence research and for applications. This article describes the LES technique, and reviews its contributions to and use in atmospheric sciences.

Introduction

Turbulence consists of a three-dimensional chaotic motion that spans a wide range of scales of motion, which increases with the Reynolds number (see Turbulence and Mixing: Overview). A numerical integration of the full (unfiltered) equations (i.e., the Navier–Stokes equations) that explicitly calculates all scales of turbulent motion is known as direct numerical simulation (DNS). However, DNS can simulate only low-to-medium Reynolds-number turbulence (where the range of scales is not very broad) with today’s computer power. Low-to-medium Reynolds number flows are typical of wind tunnel laboratory experiments. The largest DNS performed today uses \( \sim 10^{10} \) grid points, which is still insufficient to simulate turbulence with a very wide range of scales. As an example, consider the atmospheric planetary boundary layer (PBL). The largest turbulent eddies in the PBL are on the order of kilometers and the smallest on the order of millimeters; the entire scale range spans more than six orders of magnitude. To numerically integrate the full Navier–Stokes equations for a turbulent PBL requires at least \( 10^{18} \) numerical grid points (i.e., \( 10^6 \) in all three directions). This is far beyond today’s computing capacity or that in the foreseeable future.

Given this limitation, only a portion of the scale range can be explicitly resolved. The obvious choice is to resolve just the most important scales of the flow of interest and approximate the other scales. This is the philosophy behind large-eddy simulation (LES). For PBL turbulence, as an example, the most important scales (for most meteorological applications) are large eddies which contain most of the turbulent kinetic energy (TKE) (thus called energy-containing eddies) and are responsible for the majority of the turbulent transport. A simulation that explicitly calculates (or resolves) large eddies while approximately representing the effects of smaller ones is LES (Wyngaard, 1984, 2010). As the grid resolution of LES becomes finer, a wider range of turbulent eddies is resolved, less are parameterized, and LES-generated flows become more representative of the entire flow field. LES is a compromise between DNS (in which all turbulent fluctuations are resolved) and traditional Reynolds-averaging approach (in which all turbulent fluctuations are parameterized and only ensemble-averaged statistics are calculated).

The LES technique was developed by Jim Deardorff at the National Center for Atmospheric Research in the late 1960s. His first LES calculation was performed using a computer that allowed for only \( 32 \times 32 \times 32 \) (32 768) grid points. On today’s machines, calculations with \( 10^5 \sim 10^7 \) grid points are a common practice and \( 10^9 \sim 10^{10} \) computations are possible on massively parallel machines. As computer power increases, the LES numerical technique will have a much broader application and more accurate solutions. LES has been developed and used extensively also by the engineering fluid dynamics community, but in this article we restrict our description to LESs of atmospheric flows, with an emphasis on the PBL. Most LES research by the PBL community focuses on applications that include buoyancy, rotation, rough surface, ocean waves, canopy, entrainment, radiation, and/or condensation.

The LES Technique

Governing Equations and Filtering Procedures

The Navier–Stokes equations for an incompressible fluid are

\[
\frac{\partial u_i}{\partial t} = - \frac{\partial u_j u_i}{\partial x_j} + X_i - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \tag{1}
\]

where the velocity field \( u_i \) satisfies the continuity equations

\[
\frac{\partial u_i}{\partial x_i} = 0. \tag{2}
\]

In eqns [1] and [2], \( u_i \) are flow velocities in the three spatial directions, i.e., \( i = 1 \) and \( 2 \) for the horizontal directions and \( i = 3 \) for the vertical direction, \( X_i \) are the ith-component of body forces, \( \rho \) is the air density, \( p \) is the pressure fluctuation, \( \nu \) is the kinematic viscosity of the fluid, \( t \) is time, and \( x_i \) are the spatial coordinates. For PBL applications, the major body forces are gravity and Coriolis forces (see Dynamical Meteorology: Coriolis Force) and hence \( X_i = g \delta / T_0 - f v_j \delta u_j \), where the gravitational acceleration \( g \) is nonzero only in the \( x_3 \) (or \( z \)) direction, \( \theta \) is the virtual potential temperature, \( T_0 \) is the temperature of some reference state, and \( f \) is the Coriolis parameter. The body force \( X_i \) is obtained by expanding eqn [1] over a reference state of hydrostatic equilibrium and also using the Boussinesq approximation (see Dynamical Meteorology: Primitive Equations). A numerical integration of eqns [1] and [2] is called DNS. For LES the governing eqns [1] and [2] need to be spatially filtered.
Spatially filtered Navier–Stokes equations are derived by decomposing all dependent variables, for example the velocity field \( u_i \) into \( u_i = \tilde{u}_i + u_i'' \), where \( \tilde{u}_i \) is the filter-scale component and \( u_i'' \) is the subgrid scale (SGS) (or subfilter). The filter-scale or resolved-scale variable is defined as

\[
\tilde{u}_i(x_i) = \iiint_{\text{volume}} u_i(x'_i) G(x_i - x'_i) \, dx'_i
\]  

where \( G \) is a three-dimensional (low-pass) filter function (typically, a Gaussian, top-hat, or sharp-wave-cutoff filter). A turbulent flow field obtained from a point sensor illustrates the filtering and decomposition process. In Figure 1, the red curve denotes the time varying total flow field. Application of the filter operator shown in eqn [3] to the total flow field yields a smoother field called the filter scale (or resolved scale) as indicated by the blue curve. The difference between the total and resolved-scale components is the subfilter scale or SGS, shown by the green curve. The SGS component is much smaller in magnitude and is of much higher frequency, compared to the resolved-scale component.

Applying the filtering procedure, term-by-term, to eqn [1] leads to the equations that govern large (resolved-scale) eddies:

\[
\frac{\partial \tilde{u}_i}{\partial t} = -\frac{\partial \tilde{u}_i}{\partial x_j} \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_j}{\partial x_i} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{g_i}{T_0} - f \epsilon_{ij3} \tilde{u}_j - \frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + v \frac{\partial^2 \tilde{u}_i}{\partial x^2_i},
\]

where the SGS stress is defined as \( \tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j \). For geophysical turbulence, the last term (molecular viscosity) is negligibly small compared to the other terms and hence can be ignored.

So far in deriving eqn [4] for LES calculations, no approximations have been made. However, to solve eqn [4] we need an SGS model to describe the SGS stress \( \tau_{ij} \).

### Subgrid-Scale (SGS) Models

An SGS model relates the SGS stress (or SGS fluxes) to resolved-scale variables, allowing eqn [4] to be integrated. This is a closure problem. The closure assumption made in an SGS model creates the only uncertainty – other than numerical errors – to LES-generated turbulent flows. This uncertainty may become severe in regions where small eddies are dominant (or play an important role), for example near a rough-wall boundary and perhaps in the entrainment zone of the PBL. Nevertheless, in regions where large turbulent eddies play the major role, LES-generated flows (and their derived statistics such as variances and fluxes) have been shown to be insensitive to the SGS model. This is true in the bulk of the PBL where small turbulent eddies act mainly as passive motions, passing energy downscales toward dissipation. This is a turbulence transport process known as the energy cascade. Thus, a simple SGS model that dissipates energy properly is usually sufficient to represent the net effect of small eddies – for most meteorological applications – if the LES grid resolution is properly chosen.

The most widely used SGS models for the PBL are the Smagorinsky–Lilly (S–L) and Deardorff’s TKE models. They are similar in that both are based on SGS TKE budgets and both relate SGS stresses to resolved-scale strain tensors as

\[
\tau_{ij} = -2K_M S_{ij}
\]

where the strain tensor is \( S_{ij} = (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) / 2 \). SGS heat fluxes are similarly related to local gradients of the resolved temperature field as

\[
\tau_{ij} = -K_H \frac{\partial \theta}{\partial x_i}
\]

### The S–L model

Without the buoyancy effect the SGS eddy viscosity \( K_M \) and diffusivity \( K_H \) are expressed as

\[
K_M = (c_S \Delta_S)^2 S
\]

and

\[
K_H = \frac{K_M}{P_f}
\]

where \( c_S \) is the Smagorinsky constant, \( \Delta_S \) is a filtered length scale often taken to be proportional to the grid size, \( S \) is the magnitude of the strain tensor, \( S = (2 S_{ij} S_{ij})^{1/2} \), and \( P_f \) is the SGS Prandtl number. One of the most important features of the S–L model is that the SGS fluxes are nonlinear functions of the resolved strain rate, a crucial difference from the viscous (molecular) stress–strain relationship. For PBL applications, the Smagorinsky constant \( c_S \) is often set to 0.18–0.25 and the SGS Prandtl number to \( \sim 1/3 \) to satisfy Kolmogorov inertial-subrange theory.

To include the buoyancy effect, the \( K_M \) expression in the original Smagorinsky model is modified to depend on local Richardson number \( R_i \) (the ratio of buoyancy to shear production terms of the TKE budget)

\[
K_M = (c_S \Delta_S)^2 S \left( \frac{R_i}{R_{ec}} \right)^n
\]

where \( R_{ec} \) is the critical Richardson number.
where $R_c$ is the critical Richardson number often set between 0.2 and 0.4, and $n = 1/2$ is often used. When the local Richardson number reaches the critical value, turbulence within that grid cell vanishes and the eddy viscosity is shut off.

**The Deardorff TKE model**

Deardorff extended the S–L eddy viscosity model to include the full SGS TKE $e$:

$$\frac{\partial e}{\partial t} = -\frac{\partial \bar{u}^i \bar{e}}{\partial x_j} - \frac{\partial (\bar{u}^i \bar{e} + \bar{u}^j \bar{p}^{ij})}{\partial x_j} - u^i u^j \frac{\partial \bar{u}^j}{\partial x_j} + \frac{\varepsilon}{T_0} u^i \bar{o}^{ij} - e \quad [10]$$

and then relates $K_M$ and $K_{HI}$ to SGS TKE as

$$K_M = c_K \sqrt[3]{e} \quad [11]$$

and

$$K_{HI} = \left[ 1 + (2l/\Delta_S) \right] K_M \quad [12]$$

where $c_K$ is a diffusion coefficient to be determined and $\ell$ is another SGS length scale, taken as the minimum of the stability-corrected scale and the grid scale:

$$l = \min \left[ 0.76 \sqrt{e/N^2; \Delta_S} \right] \quad [13]$$

where $N = \sqrt{(g/T_0) \partial \theta/\partial z}$ is the Brunt–Vaisala frequency.

The terms on the right-hand side of eqn [10] represent, in order, advection of SGS TKE by the resolved-scale motion, turbulence and pressure transports, local shear production (i.e., nonlinear scrambling), local buoyancy production or consumption, and molecular dissipation. In solving eqn [10], the transport term is usually approximated as

$$\bar{u}^i e + u^j \bar{p}^{ij} = -2K_M \frac{\partial e}{\partial x_j} \quad [14]$$

and the molecular dissipation rate as

$$\varepsilon = c_e e^{3/2} / l \quad [15]$$

where $c_e$ is a dissipation coefficient.

Under the assumption that all SGS motions lie within the inertial subrange, the SGS parameters $c_K$ and $c_e$ can be derived assuming that the SGS motions are isotropic and the energy spectrum has a $-5/3$ spectral slope (Moeng and Wyngaard, 1988). Commonly used values for PBL applications are $c_K \approx 0.10$, and $c_e \approx 0.19 + 0.74 l/\Delta_S$. With these model parameters, LESs are, in a way, forced – in an ensemble-mean sense – to drain energy at a rate sufficient to produce a $-5/3$ spectral slope near the filter cutoff scale.

These two SGS models are closely related. The S–L model can be derived by keeping just the last three terms on the right-hand side in eqn [10]. The SGS constants of the two models are related as $c_s^4 = c_K^4/c_e$ (if the stability correction of the SGS length scale is neglected).

**Deficiency of the eddy-viscosity SGS models**

The above SGS models are based on ensemble average concepts but are used inside of LES on an instantaneous basis, i.e., to represent SGS effects at every grid point and at every time step. Laboratory studies and DNS provide evidence that small-scale turbulent motions are anisotropic and intermittent and that locally the energy transfer can either be forward scatter (from large to small scales) or backscatter (from small to large scales), which causes deviations from the equilibrium $-5/3$ law. Eddy-viscosity SGS models also assume that SGS stresses and strains are perfectly aligned (eqn [5]), and hence the local dissipation rate $\varepsilon = -\tau_0 \bar{e}$ is always positive thus preventing backscatter of energy. These deficiencies of eddy-viscosity models have motivated continued development of new SGS models, including (1) stochastic models where a random field is imposed at the SGS level thus permitting a backscatter of energy, (2) dynamic models where the Smagorinsky coefficient is dynamically predicted using a resolved field filtered at two different scales, and (3) velocity estimation models that attempt to model the SGS velocity fluctuations $u_i^f$ instead of SGS stresses $\tau_{fi}$.

The deficiency of the S–L and Deardorff SGS models is most evident in the surface layer of the PBL. Based on a large body of measurements and scaling arguments, the vertical gradients of the mean fields usually obey Monin–Obukhov (M–O) similarity theory (see Boundary Layer (Atmospheric) and Air Pollution: Surface Layer). However, LESs using the S–L or Deardorff SGS model fail to reproduce the vertical profiles of the mean fields predicted by M–O theory, particularly for shear-driven and stable PBLs. One reason for this shortcoming is that near the surface, small eddies dominate so that almost all of the turbulent eddies are SGS in LES; few motions are actually resolved. This deficiency has been improved somewhat using SGS models that include either a backscatter effect or a contribution from the mean shear near the surface (Sullivan et al., 1994).

**Numerical Setup, Methods, and Boundary Conditions**

The choice of LES grid and domain size depends on the physical flow of interest and the computer capability. LES differs from other meteorological models in that its resolved-scale (or grid-scale) turbulent motion has about the same characteristic scale in all three directions, and hence requires a grid mesh that is close to isotropic. Most computers today can easily perform an LES of about $100 \times 100 \times 100$ grid points. From these grid points, an LES domain is then chosen to resolve several largest (dominant) turbulent eddies and at the same time resolve eddies as small as possible into the inertial-subrange scales. For example, for a convective PBL with 1 km depth, a $5 \times 5 \times 2 \text{ km}^3$ domain of LES with $100 \times 100 \times 100$ grid points would cover 3–5 large dominant eddies in each horizontal direction and at the same time resolve small eddies down to about 100 m $\times 100$ m $\times 40$ m in size assuming model resolution is twice the grid size. For the stable PBL where dominant eddies are smaller, a smaller domain (and consequently a finer grid) is preferred.

Numerical truncation errors and specification of boundary conditions add uncertainties to all numerical models including LES. Most PBL-LES codes use finite difference methods in all three directions to compute derivatives, although some LESs employ a spectral (Fourier) representation in $x$–$y$ planes taking advantage of the horizontally homogeneous nature of the PBL and computational efficiency of using fast fourier transformation. Sharp gradients in flow variables can exist at the top of the PBL because of the presence of a strong, stably stratified overlying layer, which leads to oscillations (dispersion errors)
when finite differencing methods are used. To overcome this flaw, sign preserving (monotone) schemes are often used for scalar transport to maintain physical realizability — at the expense of introducing more numerical diffusion (see **Numerical Models: Methods**).

The surface boundary condition in LES uses M–O similarity theory to relate surface fluxes to resolved-scale variables at the first grid level — at every grid point. Note that for PBL applications, LES cannot possibly resolve the viscous layer, which is less than a centimeter above the surface. The lowest grid level of a PBL-LES lies in the inertial sublayer, which is referred to as the surface layer. The primary empirical input parameter in M–O theory is the surface roughness height, which varies from less than 0.0001 m for a smooth sea to more than 0.1 m for heavily wooded terrain. This rough-wall boundary condition is different from the smooth-wall condition in engineering flows. Caution should be used, however, because M–O theory describes ensemble-mean flux-gradient relationships in the surface layer (see **Boundary Layer (Atmospheric) and Air Pollution: Surface Layer**) and may not apply well at the local LES grid scale. This problem becomes more acute when the LES horizontal grid size is comparable to or smaller than the height of the first grid level.

The upper boundary of a typical LES domain is usually set to be well above the PBL top to avoid influences of boundary conditions on simulated PBL flows. At the top of the domain, turbulence is negligible and a no-stress condition is applied. Because turbulent motions in the PBL may excite gravity waves in the stably stratified inversion layer, a mechanism for allowing gravity waves to escape at the top of the domain is often applied. This includes applying a radiation condition or adding a wave-absorbing sponge layer at the top of the model domain.

For lateral boundary conditions, almost all PBL LESs use periodic boundary conditions because there is no adequate theory to define chaotic flow fields at an open boundary. However, periodic boundary conditions are clearly inappropriate for horizontally inhomogeneous cases, particularly for PBLs over complex terrain or under severe weather conditions. Recently, researchers have been using the nesting technique to avoid the use of periodic boundary conditions. We will get back to this issue later in **Weather Model Nesting**.

**Visualization of LES-Generated Flows**

The solution of eqn [4] consists of three-dimensional, time-evolving, chaotic flow fields. An example of such a flow field is shown in Figure 2 where the vertical velocity of an LES solution of a free convective PBL (using \(512 \times 512 \times 512\) grid points) is presented. The total domain of the LES is 5 km \(\times\) 5 km in horizontal and 2 km in the vertical. The horizontal view shows a spokelike, irregular polygonal structure near the surface, similar to those observed in Rayleigh–Bernard convection experiments. This spokelike feature is most evident in the free convective PBL where there is no mean wind. Intersections between polygons are local horizontal convergence regions and hence are sites to form strong updrafts (purple colors).

Strong updrafts can be seen from the two vertical plan views. These updrafts carry warm surface air and that is how turbulence can effectively transport heat (and other species coming from the surface) upward. Updrafts are more intense and occupy a narrower area than downdrafts; this is known as a positively skewed vertical-velocity field, a unique feature of buoyancy-driven turbulence. Strong updrafts penetrate into the capping inversion and in the process engulf wisps of warm inversion air into the PBL. These wisps of air are subsequently entrained and mixed into the PBL. This penetration-leads-to-entrainment is a phenomenon that has been documented with radar and lidar observations and convection tank experiments (see **Boundary Layer (Atmospheric) and Air Pollution: Convective Boundary Layer**).

Turbulent structures are quite different in a stably stratified (or night-time) PBL. Figure 3 shows the vertical-velocity field from an LES of a stable PBL. In the stable PBL, buoyancy consumes TKE that leads to much weaker turbulence compared
to the convective PBL. There is no spokelike structure and no strong updrafts. There are numerous small-scale interacting turbulent patches. (Field measurements show that the dominant turbulent eddy size in a typical stable PBL is on the order of several tens of meters. So for this simulation, the total domain is set to 400 m in all three directions using 200 × 200 × 200 grid points.)

Statistics Derived from LES Flows

Instantaneous flow fields from LESs are chaotic, so it is their collective effects (or statistics) like variances or fluxes that are useful for applications. Moment statistics can be readily calculated from 3D LES data by correlating the local fluctuations among variables and averaging them over space and/or time. Then the vertical profiles or distributions of these statistics can be systematically documented for various PBL regimes generated under various large-scale conditions. For example, the TKE budgets calculated from LESs (Moeng and Sullivan, 1994) show differences between the shear and buoyancy-driven PBL regimes (Figure 4). In a shear-driven PBL, shear production nearly balances molecular dissipation with all other terms remaining small, while in the convective PBL, the TKE budget is dominated not only by the buoyancy production and molecular dissipation but also by the turbulent and pressure transports; these features are consistent with field observations and laboratory experiments.

A unique feature of LES is the ability to obtain pressure statistics. Pressure fluctuations are difficult, if not impossible, to measure in the field, yet they play an important role in determining moment statistics, such as pressure transport in the TKE budget and the return-to-isotropy behavior for velocity variances. The LES-generated pressure field, which remains to be verified from observation when available, provides a unique tool to estimate important pressure-related statistics.

One should be cautious in using statistics constructed from LES flows, however. Some statistics, especially higher moments, may be sensitive to the LES grid resolution, domain size, and SGS models. A necessary but not sufficient rule of thumb is to accept or consider only the statistics that are insensitive to the LES grid resolution or SGS modeling.

Applications to Atmospheric Turbulence

Significant Accomplishments

LES has become a prominent research tool in advancing our understanding of the structure and physics of PBL turbulence. Before Deardorff’s first LES calculations in the early 1970s, researchers believed that the proper velocity and length scales for PBL statistics were the friction velocity $u_*$ and the length scale $L/Q$, where $Q$ is the Coriolis parameter. Based on his LES calculations, Deardorff discovered that turbulence statistics in the convective PBL are better described by the convective velocity scale $w^* = (g/\gamma_0)z_0 \bar{\omega}^0 1/3$ and the PBL depth $z_i$, where $\bar{\omega}^0$ is the surface buoyancy flux (Deardorff, 1972). (Note that the overbar here denotes ensemble averages, which can be calculated as spatial and time averages from LES-generated flows.) This new finding, now known as mixed-layer scaling, makes it possible to collapse observed data collected from convective PBLs under various environments to form universal vertical profiles. For example, measurements of vertical flux of TKE $wE$ and vertical-velocity variance $\overline{w^2}$ from research aircrafts at various heights, for various surface heat fluxes, form universal profiles only when these statistics are normalized by $w^3$ and $w^2$, respectively, and also when they are shown as functions of the normalized height $z/z_i$ (Figure 5, from Lenschow et al., 1980) (see Boundary Layer (Atmospheric) and Air Pollution: Convective Boundary Layer).

LES also has provided a revolutionary discovery about plume dispersion in the convective PBL. The release of a tracer from an elevated source within an LES-generated convective PBL shows that the maximum mean concentration in the plume at first descends until the plume intercepts the ground before it rises (Figure 6). The descent of the elevated plume maximum is due to the greater aerical coverage of downdrafts, i.e., the positively skewed vertical-velocity field (Lamb, 1978). This finding, also observed at about the same time in the Willis and Deardorff tank experiments, has an important application to air pollution; the result can be used to predict the location and magnitude of the maximum surface concentration of emissions downstream. It provided the basis for the revision of short-range dispersion models in the 1980s (see Turbulence and Mixing: Turbulent Diffusion).

Another breakthrough from LES is the discovery of the asymmetry of turbulent diffusion from area sources at the surface and top of the convective PBL. Any passive, conservative scalar can be linearly decomposed into two conceptual scalar fields: top-down (which is emitted at the PBL top and has 0 flux at the surface) and bottom-up (which is emitted at the surface and has 0 flux at the PBL top). Under quasi-steady state, the fluxes of the top-down and bottom-up scalars are both linear in height and hence, after normalization by their respective boundary flux, are symmetric about the mid-PBL. LES shows that the mean gradients of the top-down and bottom-up concentrations, after normalization by $u^*, z_i$ and the appropriate boundary flux, are not symmetric about the mid-PBL (Wyngaard and Brotz, 1984). While the top-down gradient function remains positive throughout the whole PBL, the
have been evaluated or verified. PBL parameterizations have been proposed but few of them (Atmospheric) and Air Pollution: Modeling and Parameterization) for climate and weather forecasting models. Various PBL parameterizations have been proposed but few of them have been evaluated or verified. Field observations are often incomplete for this application. LES solutions have been used as valuable datasets to examine many closure assumptions in existing PBL schemes. This includes assumptions made in second-order closure modeling: mass flux and entrainment/detrainment closures for mass flux modeling; entrainment-rate closure assumptions in mixed-layer modeling; and counter-gradient effects in eddy-diffusivity models. Recently, LES has been extended to study not just parameterizations of PBL turbulence but all SGS motions in cloud-resolving (cloud-system-resolving) models.

**Recent LES Research for Atmospheric Science**

Earlier LES work focused mainly on idealized cloud-free, flat-terrain convective PBL. This flow regime is most suited to LES because of the presence of large thermal plumes with no other complicated physical processes (like radiation and latent heating) involved. In recent years, however, LES has been expanded to study more complicated and difficult PBL regimes that are relevant to climate and severe weather predictions, or more recently wind-energy applications. We list several topics below.

**Stratocumulus-Topped PBLs**

One climatologically important PBL regime is the stratocumulus-topped PBL where its extensive cloud cover can significantly alter the solar radiation input to the Earth’s surface. For this PBL regime, LES needs to include effects of latent heating (i.e., phase change of water substance) and radiation processes, which unfortunately introduce more uncertainties into LES. In particular, the entrainment process of this PBL regime is very difficult to simulate because it depends sensitively on the SGS model and numerical schemes (Stevens et al., 2005). Many LES practitioners working on this topic have been involved in GCSS (GEWEX Cloud-System Study) Boundary Layer Cloud Working Group, with the goal of using LES as database to improve representations of stratocumulus clouds in climate and weather prediction models.

**Weather model nesting**

Limited by computer power, traditional atmospheric models have been used to perform single-scale simulations. For example, weather models simulate only weather-scale motions of several tens of kilometers in size, while LES resolves just large turbulent eddies of several hundreds of meters in size. The nonresolved part of motions in traditional weather models are either prescribed or roughly parameterized. This is clearly not suitable for applications where weather and turbulent motions strongly overlap or interact. One way to deal with this problem is the development of multiple-scale modeling that nests a turbulence-resolving model (i.e., LES) inside a weather prediction model. The outer domains with coarser grid resolutions resolve weather-scale systems, while the inner domains consist of a fine-grid LES to resolve turbulent motion. With two-way nesting, scale interactions of weather and turbulence motions are allowed.

The nesting technique may also solve the periodic-boundary-condition problem. With nesting, the lateral boundary conditions of LES are provided by their adjacent outer-domain flow fields. Thus no periodic boundary condition is imposed; such LES can be applied to horizontally...
inhomogeneous, nonperiodic conditions. Built on community weather models, notably the Weather Research and Forecasting (WRF) model, this type of multiple-scale modeling has shown promising results when applied to idealized or uniform-surface cases (Zhu et al., 2010). It remains a challenge when applied to complex terrain or severe weather situations (see Boundary Layer (Atmospheric) and Air Pollution: Complex Terrain). (For further reading see the WRF website at http://www.wrf-model.org/index.php.)

Deep cloud systems
With massive parallel computing, LES is no longer limited to idealized PBL applications. For example, as part of the research funded by the NSF Center for Multiscale Modeling for Atmospheric Processes, a very large-domain LES, covering an area of about 205 km × 205 km in the horizontal and about 27 km in the vertical, was performed to simulate a tropical deep convective system (Khairoutdinov et al., 2009). It used 2048 × 2048 × 256 (about 109) grid points and ran on thousands of processors. This LES resolves a broad range of scales that includes mesoscale organization, gravity waves, deep and shallow clouds, all the way down to energy-containing turbulence eddies. This is another kind of multiple-scale modeling but it does not use the nesting approach, and therefore is more accurate. However, it is done at the expense of huge computer resources; a 24-h simulation of this LES took about 400,000 h on IBM’s BlueGene/L supercomputer.

A satellite view of the simulated cloud field shown in Figure 7 (adopted from Khairoutdinov et al., 2009) reveals a detailed structure of the deep convective system. It shows mesoscale organization, deep and shallow clouds (bright white color), thin cirrus clouds (light blue), and random turbulent motions. This computationally expensive LES is now used as a benchmark to study how large clouds interact with small clouds and turbulence. It is also used to develop SGS parameterizations for cloud-resolving models (Moeng et al., 2010). (For this LES see www.cmmap.org.)

Large-domain LES is also used to simulate hurricane and midlatitude squall line systems.

Marine boundary layers with resolved waves
There is a clear impetus for using LES to attack increasingly complex flows for a variety of applications. Air–sea interaction and the coupling between winds and currents with surface gravity (water) waves is an example where LES has provided new information about turbulent flow dynamics and has also guided the interpretation of data collected in field campaigns.

To simulate atmospheric turbulence above a three-dimensional time-dependent surface wave field, the LES governing equations are written in a transformed wave-following coordinate system (Sullivan and McWilliams, 2010). The new complexity introduced here is that the gridlines of the mesh translate vertically adapting to the surface movement. The LES system of equations is augmented by an additional equation governing the grid movement. LES of the atmospheric marine boundary layer with varying stratification illustrate the importance of wind-wave directionality and so-called ‘wave age,’ i.e., the ratio of a reference wind speed and a characteristic wave speed in a surface wave height spectrum. Depending on wave age, the winds are slowed or accelerated by the action of the waves. The mean wind profile, turbulence variances, and vertical momentum flux are thus dependent on the nature of the wave field; the LES predicted dependence of vertical momentum flux on wave age is also found in observations. LES results with moving waves show important differences compared with rough-wall boundary layers and flow over stationary bumps. LES of upper ocean boundary (or mixed) layers also incorporates surface wave effects by including the Stokes drift associated with the wave field. The latter appears as a new forcing term in LES, a so-called vortex force, which is responsible for the generation of Langmuir circulations. Langmuir circulations are potent coherent structures that interact with background ocean turbulence to produce enhanced mixing and entrainment in the ocean boundary layer.

Observations of SGS variables
The basic assumptions used to derive SGS closure models and constants for LES, discussed previously, are often violated in actual LES implementations. Flow near rough boundaries, regions with stable stratification, and the addition of new dynamical processes, e.g., vegetation, hills, and clouds, modulate the background turbulence and introduce new time and length scales that are not accounted for in conventional SGS closures.
Recently, novel observations have been carried out in the atmospheric surface layer with the objective of measuring and quantifying the structures and statistics of SGS variables. The basic principle of the Horizontal Array Turbulence Studies (HATS) is to sample turbulent fields by orienting an array of point sensors, usually sonic anemometers, perpendicular to the main flow direction. Then by adopting Taylor’s hypothesis in the streamwise direction, a ‘horizontal plane of turbulence’ can be constructed. A two-dimensional filter (in horizontal directions) is applied to the wind and temperature fields that mimic the filtering in LES codes. If a sufficient number of sensors are employed, then the fields can be double filtered to yield additional information about the coupling between resolved and SGS correlations. Further, if a vertically stacked array of sensors is used in the field (Figure 8) vertical derivatives of resolved and SGS variables can be acquired. HATS field campaigns have been carried out over flat rough surfaces, moving ocean waves, in a canopy of trees, and over snow. In these studies, the atmospheric stratification varies from unstable to neutral to stable. (For these field data, see http://data.eol.ucar.edu/codiac/projs/SGS00.)

The statistics of SGS variables, from the HATS experiments, are studied similar to their conventional ensemble average counterparts for means and Reynolds-averaged fluxes and variances. Analysis of SGS momentum and scalar fluxes from HATS (Sullivan et al., 2003) shows that the scale separation between the largest energy-containing eddies Δ and the filter scale Δ is a fundamental critical parameter. The variation of the SGS fluxes and variances for different filter widths, height above the surface, and atmospheric stratification collapse when plotted as a function of Δ/Δ. When the ratio Δ/Δ is large (>10) then the SGS variables are more isotropic and can be modeled using expressions described previously. In an intermediate range of scale separation (1 < Δ/Δ < 10), the SGS fluxes become increasingly anisotropic, and more complex closures are required (Wyngaard, 2004). When Δ/Δ < 1 then the resolved motions are small compared to the SGS and second-order closure modeling is appropriate. HATS datasets can be used to estimate the transfer of energy between the resolved and SGS field and viscous dissipation in eqn [10] as well as closure constants. The observations show that the Smagorinsky constant cS in eqn [7], (or cK in eqn [11]) is dramatically reduced near rough boundaries.

**Future Challenges**

In reality, the PBL is much more complicated than what has been simulated by LES so far. Much of the complication arises from the heterogeneous nature of the underlying surface. The earth’s land surface is characterized by spatially varying patches, undulating terrain, and urban development, which can induce circulations that interact with, and hence change turbulence dynamics. Complex surface conditions in particular affect the very stable PBL where turbulence is no longer continuous but becomes intermittent in space and time (see Boundary Layer (Atmospheric) and Air Pollution: Stably Stratified Boundary Layer). The ability to simulate turbulence transition becomes crucial. Wave-current couplings and wave breaking also lead to complex air–sea interactions. All these complex surface conditions can significantly influence turbulent transport in many meteorological applications, such as air pollution, vegetation growth, cloud formation, and hurricane development.

LES is now being adapted to realistic PBL regimes embedded in multiscale meteorological flows. Including complexities, however, introduces additional uncertainties in LES solutions. It is important to examine and validate the fidelity of LES of complicated flows against observations. LES has also been used to study interactions of turbulence with cloud microphysics, biochemistry, and aerosols. Caution should be exercised in these applications since the interactions may depend critically on small-scale turbulent motions, which are SGS in LES.

**See also:** Agricultural Meteorology and Climatology, Boundary Layer (Atmospheric) and Air Pollution: Complex Terrain; Convective Boundary Layer; Modeling and Parameterization; Stably Stratified Boundary Layer; Surface Layer. Dynamical Meteorology: Coriolis Force; Primitive Equations. Numerical Models: Methods. Turbulence and Mixing: Overview; Turbulent Diffusion.
References


Relevant Websites

http://cmmap.colorado.edu/.
http://data.eol.ucar.edu/codiac/projs?SGS00.