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Marcel Lesieur, Olivier Metais and Pierre Comte
Excerpt
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1 Introduction to LES

1.1 Book's scope

Large-eddy simulations (LESs) of turbulent flows are extremely powerful techniques consisting in the elimination of scales smaller than some scale Δx by a proper low-pass filtering to enable suitable evolution equations for the large scales to be written. The latter maintain an intense spatio-temporal variability. Large-eddy simulation (LES) poses a very difficult theoretical problem of subgrid-scale modeling, that is, how to account for small-scale dynamics in the large-scale motion equations. LES is an invaluable tool for deciphering the vortical structure of turbulence, since it allows us to capture deterministically the formation and ulterior evolution of coherent vortices and structures. It also permits the prediction of numerous statistics associated with turbulence and induced mixing. LES applies to extremely general turbulent flows (isotropic, free-shear, wall-bounded, separated, rotating, stratified, compressible, chemically reacting, multiphase, magnetohydrodynamic, etc.). LES has contributed to a blooming industrial development in the aerodynamics of cars, trains, and planes; propulsion, turbo-machinery; thermal hydraulics; acoustics; and combustion. An important application lies in the possibility of simulating systems that allow turbulence control, which will be a major source of energy savings in the future. LES also has many applications in meteorology at various scales (small scales in the turbulent boundary layer, mesoscales, and synoptic planetary scales). Use of LES will soon enable us to predict the transport and mixing of pollution. LES is used in the ocean for understanding mixing due to vertical convection and stratification and also for understanding horizontal mesoscale eddies. LES should be very useful for understanding the generation of Earth's magnetic field in the turbulent outer mantle and as a tool for studying planetary and stellar dynamics.

It is clear that the study of *large-eddy simulations of turbulence* has become a discipline by itself. This book will try to present a global and complete account of this discipline and its vigorous developments since the early 1960s and the pioneering work of Smagorinsky [269]. We will also provide various industrial and environmental applications.

Although we do not expect the reader to be an expert in fluid dynamics and turbulence, it is not the aim of the present book to give a complete account of these aspects. We will try, however, to recall in simple terms some of them while referring to the companion textbook of Lesieur [170] for the more advanced aspects or detailed derivations on these topics.

The objective of the book is twofold. The first is to present the details of many models developed in large-eddy simulations of turbulence. The second is, through examples of application, to give the reader a thorough understanding of turbulence dynamics in isotropy, mixing layers, boundary layers, and separated flows and how such a dynamics may be deeply modified by rotation, stratification, heating, and compressibility. The book contains numerous computer-generated graphics as well as a CD-ROM with movies of some flows computed with LES (isotropic turbulence, mixing layers and jets, backward-facing steps, boundary layers and channel flows, cavities at various Mach numbers, heated-channel flows, frontal cyclogenesis in the atmosphere, etc.). This interdisciplinary textbook addresses a very wide population of graduate students, researchers, and industrial engineers in the domains of mechanical, aerospace, civil, chemical, and nuclear engineering; geophysical and astrophysical fluid dynamics; physics; and applied mathematics.

In the present chapter, we recall the basis of fluid-dynamics and turbulence theory that will be used for LES. We show the limitations of direct numerical simulations in terms of practical applications at high Reynolds numbers owing to the excessive number of degrees of freedom of the system. We recall the history of LES and finish with an analysis of unpredictability effects in the framework of LES analyses.

In Chapter 2, we are mainly concerned with coherent-vortex recognition in terms of pressure and vorticity fields as well as quantities related to the velocity-gradient tensor, such as the very efficient Q and λ_2 criteria. Applications to isotropic turbulence and backward-facing steps are provided, and animations of coherent vortices are observed in both cases.

Chapter 3 presents the LES formalism in physical space with the introduction of the famous Smagorinsky model, for which we will show how the constant may be determined. We will also study the model's wall behavior, which poses serious problems. We also present a thorough description of its more recent so-called dynamic version with a dynamic recalculation of the constant by a double filtering in space.

Chapter 4 presents spectral models for LES applied to three-dimensional isotropic turbulence with the plateau-peak eddy viscosity and eddy diffusivity and the spectral-dynamic model. The chapter shows new EDQNM[1] calculations at very high Reynolds numbers with an analysis of the well-known phenomenon of kinetic energy cascade pileup before the dissipative range (the so-called bump). The chapter contains a complete infrared study of kinetic-energy and pressure spectra done both with EDQNM and LES using the spectral models. It also discusses other types of spectral eddy viscosities such as Heisenberg's and RNG-based.

Chapter 5 shows how the plateau-peak eddy-viscosity model may be applied to inhomogeneous turbulence in flows of uniform density in the particular cases of a temporal mixing layer, where it is able to reproduce a vortex structure of quasi–two-dimensional Kelvin–Helmholtz vortices stretching thin longitudinal hairpins, or dislocated Kelvin–Helmholtz vortices undergoing helical pairing, according to the quasi–two-dimensional or three-dimensional nature of the initial forcing. A thorough LES study of the plane channel using the spectral-dynamic model is carried out at various Reynolds numbers. The study is complemented by direct numerical simulation (DNS) focusing on probability density functions of various quantities, which are discussed with respect to the vortical dynamics.

Chapter 6 presents new subgrid models, such as the structure-function model and its "selective" and "filtered" versions. These models are compared with Smagorinsky's in the framework of a temporal mixing layer. They are applied to a spatially growing mixing layer, where the influences of upstream forcing and the extent of the spanwise domain are discussed. A round jet is also looked at with alternate pairings of vortex rings qualitatively similar to helical pairing in mixing layers. The jet control by upstream perturbations of varicose, helical, or flapping types is studied, with possibilities of strongly enhancing the spreading. The backstep is reconsidered statistically. Afterward a dynamic version of the structure-function model is presented. We discuss hyperviscosities as well as a mixed structure-function/hyperviscous model that parallels in physical space the spectral plateau-peak model. We also present scale-similarity and mixed models as well as some new, recent models.

Chapter 7 is devoted to LES of compressible ideal gases (neglecting gravity effects). We work in the context of density-weighted Favre filters analogous to Favre density-weighted ensemble averages. We introduce a new thermodynamic quantity, the macrotemperature, which may be related by an equation of state to a macropressure. This greatly simplifies the LES formalism for compressible flows. Afterward we discuss the compressible mixing layer both in the temporal and spatial cases. The compressible round jet is

[1] The eddy-damped quasi-normal Markovian theory (EDQNM) is a very efficient statistical model of isotropic turbulence based on two-point closures, which will be presented in more detail in Chapter 4. It also serves to determine subgrid models for spectral large-eddy simulations.

also studied both in the subsonic and supersonic cases. Jet contol by varico-flapping excitations is studied. Then various LESs of low-Mach boundary layers developing spatially upon a flat plate are presented both in the transitional and developed stages. Animations of various vortices and structures are provided. A weakly compressible channel (one side of which contains two small spanwise grooves) is also presented with animations of quasi-longitudinal vortices traveling on both sides. We recall the main features and role of longitudinal riblets equipping boats, planes, and swimming costumes and discuss the influence of compressibility. Turbulence over a square cavity and over a transonic rectangular cavity is studied. Then the structure of turbulence in the neighborhood of the European *Hermès* space shuttle at a local Mach number of 2.5 will be examined with evidence for the presence of Görtler vortices. Finally, DNS and LES of a heated square duct will be looked at. This duct may contain riblets, which increase heat transfer significantly. A curved duct with one wall heated is also studied, and Görtler vortices are recovered.

Chapter 8 is devoted to geophysical fluid dynamics with some DNS and LES of relevance for this topic. We first present a review of geophysical flows at various scales mainly for Earth's atmosphere and oceans. We determine the associated Rossby numbers. Climate issues such as global warming, the ozone hole, El Niño, and the oceanic conveyor belt are briefly discussed. Afterward we study shear flows (free and wall-bounded) of uniform density rotating about a spanwise axis. They are looked at mainly from the point of view of DNS and LES, and we show a wide universality in the dynamics of these flows. Then we present DNS and LES studies of the instability of a baroclinic jet, showing that LES permits us to capture secondary instabilities that are dissipated in DNS. We discuss possible analogies with severe storms.

1.2 Basic principles of fluid dynamics

We work within the assumption of a continuous medium whose characteristic scales of motion are several orders of magnitude larger (by a factor of 10^4 to 10^6) than the mean free path of molecules characterizing the molecular scales. Equations of fluid motion are obtained in the following way (see Batchelor [17] and Lesieur [170]). We work in a frame that may be Galilean, or in solid-body rotation of rotation vector $\vec{\Omega}$, and consider a fluid parcel (of volume δV) of size smaller than the characteristic scales in the flow. Let ρ be the density, and let $\vec{u}$ be the velocity of the parcel gravity center. One introduces the operator D/Dt, the derivative following the fluid motion, which is equal to $\partial/\partial t + \vec{u} \cdot \vec{\nabla}$ if the flow quantities are expressed in terms of a given space point $\vec{x}$ and time t (Eulerian notations). Notice that we have, respectively, for any scalar $A(\vec{x}, t)$ and vector $\vec{a}(\vec{x}, t)$

$$\frac{DA}{Dt} = \frac{\partial A}{\partial t} + \vec{u} \cdot \vec{\nabla} A, \tag{1.1}$$

$$\frac{D\vec{a}}{Dt} = \frac{\partial \vec{a}}{\partial t} + (\vec{u} \cdot \vec{\nabla})\vec{a} = \frac{\partial \vec{a}}{\partial t} + \vec{\nabla}\vec{a} \otimes \vec{u}, \tag{1.2}$$

where $\otimes$ stands for a tensorial product. The three following principles are applied to the parcel in its motion:

- conservation of mass ($\delta m = \rho\, \delta V$),
- balance of forces (Newton's first and third principles stated in 1687), and
- first principle of thermodynamics.

1.2.1 Continuity equation

The conservation of mass yields the continuity equation

$$\frac{1}{\delta m} \frac{D\,(\delta m)}{Dt} = \frac{1}{\rho} \frac{D\rho}{Dt} + \frac{1}{\delta V} \frac{D\,(\delta V)}{Dt},$$

which yields

$$\frac{1}{\rho} \frac{D\rho}{Dt} + \vec{\nabla} \cdot \vec{u} = 0. \tag{1.3}$$

The particular case of incompressibility (conservation of volumes following the fluid motion) reduces to $\vec{\nabla} \cdot \vec{u} = 0$.

1.2.2 Balance of forces

The balance of forces corresponds to the so-called Navier–Stokes equation. It is obtained by equating the "acceleration quantity" $\delta m D\vec{u}/Dt$ to the body forces plus the surface forces acting upon the external surface of the parcel. The body forces applied are gravity, $\delta m\ \vec{g}$, the Coriolis force (if any), $-2\ \delta m\ \vec{\Omega} \times \vec{u}$, and other possible forces. The gravity $\vec{g}$ is irrotational and includes both the Newtonian gravity and the centrifugal force implied by the frame rotation. One assumes the existence of a stress tensor $\overline{\overline{\sigma}}$ such that the force exerted by the fluid on one side of a small surface $d\Sigma$ oriented by a normal unit vector $\vec{n}$ is given by $d\vec{f} = \overline{\overline{\sigma}} \otimes \vec{n}\ d\Sigma$. A Newtonian fluid corresponds to a stress tensor of the form

$$\sigma_{ij} = -p\ \delta_{ij} + \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \vec{\nabla} \cdot \vec{u}\ \delta_{ij} \right], \tag{1.4}$$

where the pressure is defined by $p = -(1/3)\sigma_{ii}$, and μ is the dynamic viscosity coefficient. Such a definition of pressure avoids the introduction of a second viscosity coefficient. After integration of the surface forces over the surface of the fluid particle, we have

$$\frac{Du_i}{Dt} = (\vec{g} - 2\vec{\Omega} \times \vec{u})_i + \frac{1}{\rho}\frac{\partial \sigma_{ij}}{\partial x_j} \tag{1.5}$$

or, equivalently,

$$\frac{Du_i}{Dt} = (\vec{g} - 2\vec{\Omega} \times \vec{u})_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}\mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\vec{\nabla}\cdot\vec{u}\,\delta_{ij}\right]. \tag{1.6}$$

Introducing the geopotential Φ such that $\vec{g} = -\vec{\nabla}\Phi$, we can write the Navier–Stokes equation as

$$\frac{\partial \vec{u}}{\partial t} + (\vec{\omega} + 2\vec{\Omega}) \times \vec{u} = -\frac{1}{\rho}\vec{\nabla} p - \vec{\nabla}\left(\Phi + \frac{\vec{u}^2}{2}\right) + \text{vicous dissipation}, \tag{1.7}$$

where $\vec{\omega} = \vec{\nabla} \times \vec{u}$ is the relative vorticity of the fluid (in the rotating frame) and $\vec{\omega}_a = \vec{\omega} + 2\,\vec{\Omega}$ is the absolute vorticity in the absolute frame. In Eq. (1.7), the viscous contribution has not been explicitly specified.

1.2.3 Thermodynamic equation

A third equation is obtained by applying the first principle of thermodynamics to the fluid parcel: The derivative of the total energy (internal, potential, and kinetic) is equal to a possible heating (or cooling) rate by some source (e.g., radiation, combustion, condensation, or evaporation of water in the atmosphere), plus the power of surface forces, plus the rate of heat exchange by molecular diffusion across the parcel surface. The latter is expressed with the aid of Fourier's law. More specifically, let e_i be the internal energy per unit mass. Then

$$\frac{De_i}{Dt} = \dot{Q} + \frac{1}{\rho}\vec{\nabla}\cdot(\lambda\vec{\nabla}T) - \frac{p}{\rho}\,\vec{\nabla}\cdot\vec{u} + 2\nu\left(S_{ij}S_{ij} - \frac{1}{3}S_{ii}S_{jj}\right) \tag{1.8}$$

with $\overline{\overline{S}} = [\vec{\nabla}\vec{u} + \vec{\nabla}\vec{u}|^t]/2$, $\dot{Q}$ characterizing the forcing, and λ being the thermal conductivity. Let $h = e_i + (p/\rho)$ be the enthalpy of the fluid. From the continuity equation, we have

$$\rho\frac{D}{Dt}\left(\frac{p}{\rho}\right) = \frac{Dp}{Dt} + p\vec{\nabla}\cdot\vec{u}, \tag{1.9}$$

and from the enthalpy equation, omitting $\dot{Q}$, we write

$$\rho\frac{Dh}{Dt} = \frac{Dp}{Dt} + \vec{\nabla}\cdot(\lambda\vec{\nabla}T) + 2\mu\left(S_{ij}S_{ij} - \frac{1}{3}S_{ii}S_{jj}\right). \tag{1.10}$$

It can now easily be shown that by taking the scalar product of the momentum equation (1.6) with $\vec{u}$ and adding the result to Eq. (1.10), we get

$$\rho \frac{D}{Dt}\left(h + \frac{1}{2}\vec{u}^2 + \Phi\right) = \frac{\partial p}{\partial t} + \vec{\nabla}\cdot(\lambda \vec{\nabla} T) + 2\mu\left(S_{ij}S_{ij} - \frac{1}{3}S_{ii}S_{jj}\right) + u_i \frac{\partial}{\partial x_j}\mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\vec{\nabla}\cdot\vec{u}\,\delta_{ij}\right]. \tag{1.11}$$

Indeed the geopotential Φ is time independent, and thus $D\Phi/Dt = \vec{u}\cdot\vec{\nabla}\Phi$. This gives us the generalized Bernoulli theorem stating that $h + \frac{1}{2}\vec{u}^2 + \Phi$ is an invariant of motion if the flow is time independent and if molecular diffusion is neglected.

For a perfect barotropic fluid (i.e., p is a function of ρ only) where rotation is neglected, the momentum equation reduces to

$$\frac{D\vec{u}}{Dt} = -\vec{\nabla}(h + \Phi). \tag{1.12}$$

Returning to the more general case, let us consider successively a liquid and a gas.

- For a liquid, we have approximately $e_i = C_p\, T$. However, we can check that the pressure and molecular viscous terms on the right-hand side (r.h.s.) of Eq. (1.8) are in general negligible, and thus we have

$$\frac{DT}{Dt} \approx \kappa \nabla^2 T, \qquad \frac{D\rho}{Dt} \approx \kappa \nabla^2 \rho, \tag{1.13}$$

  where $\kappa = \lambda/\rho\, C_p$ is the thermal diffusivity.[2]
- For an ideal gas, the state equation reads $p/\rho = RT$ (with $R = C_p - C_v$). We make a further assumption of identifying this thermodynamic pressure with the static pressure already introduced in the stress tensor. We suppose also that C_p and C_v are temperature independent. We now have $e_i = C_v T$. Introducing the potential temperature

$$\Theta = T\left(\frac{p_0}{p}\right)^{(\gamma-1)/\gamma}, \tag{1.14}$$

  where $\gamma = C_p/C_v$ and p_0 is the pressure at some reference level, we write

[2] Notice, however, that in Eq. (1.13) the density equation is obtained by assuming a linear relation between ρ and T such that ρ is a decreasing function of T. Because of mass conservation this implies that, if T decreases, ρ will increase and the volume of the fluid parcel will decrease. This is no longer true for water at temperatures close to 4 °C, where it will dilate when cooled (Balibar [11]). In this case, pressure effects in Eq. (1.8) have to be taken into account.

the thermodynamic equation as

$$\frac{D\Theta}{Dt} = \frac{\Theta}{C_p T}\left[\frac{1}{\rho}\vec{\nabla}\cdot(\lambda\vec{\nabla}T) + 2\nu\left(S_{ij}S_{ij} - \frac{1}{3}S_{ii}S_{jj}\right)\right]. \tag{1.15}$$

A good approximation of this equation for subsonic flows is

$$\frac{D\Theta}{Dt} \approx \kappa\frac{\Theta}{T}\nabla^2 T, \tag{1.16}$$

where the thermal diffusivity κ has the same definition as before for the liquid. We recall that if the motion is adiabatic ($\kappa = 0$), Θ is an invariant of motion, as are both the entropy and $p(\delta V)^\gamma$. If the ideal gas is barotropic (and perfect), it is isentropic.

Validation of these equations of motion comes from the very good comparison of theoretical solutions with laboratory experiments in laminar regimes for cases such as Poiseuille flow in a channel or a pipe, or boundary layers developing over a flat plate, or mixing layers. In the turbulent regimes, first- and second-order statistics of numerical solutions also compare favorably with experiments for the same flows. Only above Mach numbers of the order of 15–20 does the molecular-agitation scale catch up with the continuous-medium scales in such a way that the continuous-medium assumption no longer holds.

The generalized Bernoulli theorem allows us to understand why a hypersonic body heats during atmospheric reentry. Indeed, let us consider a frame fixed to the body and suppose that an upstream fluid parcel is at a velocity U_∞ and a temperature T_∞. Its enthalpy is $C_p T_\infty$. If the parcel hits the body, on which the velocity is zero, neglecting gravity, we get

$$C_p T_\infty + \frac{1}{2}U_\infty^2 = C_p T_{\mathrm{a}}, \tag{1.17}$$

where T_{a} is the temperature at the wall, which is higher than T_∞ owing to this exchange between kinetic energy and enthalpy. We will talk more of this adiabatic temperature in the section of Chapter 7 devoted to LES of a space-shuttle rear wing.

Let us finally consider Eq. (1.15) in the case of a compressible, parallel time-independant flow of ideal gas. The velocity-vector components are $[u(y), 0, 0]$. Let $Pr = C_p\mu(y)/\lambda(y)$ be the Prandtl number assumed constant. We have

$$\frac{d}{dy}\left(\mu\frac{dT}{dy}\right) = -\frac{Pr}{C_p}\mu\left(\frac{du}{dy}\right)^2, \tag{1.18}$$

which shows there is a temperature gradient of molecular-diffusion origin induced by the velocity gradient. This has analogies with the Crocco–Busemann equation. In fact, such a velocity profile is only possible if the pressure $p(x)$

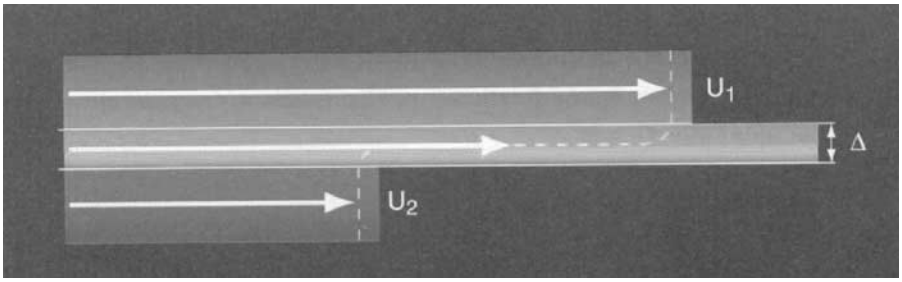

Figure 1.1. Schematic view of a vortex sheet.

depends only on x; then the pressure gradient dp/dx is constant with

$$\frac{dp}{dx} = \frac{d}{dy}\left(\mu \frac{du}{dy}\right). \tag{1.19}$$

In the weakly compressible case, this yields a parabolic velocity profile if $dp/dx \neq 0$ and a linear velocity profile if $dp/dx = 0$.

1.2.4 Vorticity

A very important quantity for characterizing turbulence (in the absense of entrainment rotation) is the vorticity vector $\vec{\omega} = \vec{\nabla} \times \vec{u}$. A quasi-discontinuity between two parallel flows of velocity $\vec{U}_1$ and $\vec{U}_2$ gives rise to a vortex sheet (see Figure 1.1). The latter is violently unstable under small perturbations (Kelvin–Helmholtz instability) and rolls up into spiral Kelvin–Helmholtz vortices into which vorticity has concentrated. These vortices may undergo secondary successive instabilities, leading to a violent direct kinetic-energy cascade toward small scales; they may also be responsible for inverse energy cascades through pairings (see Lesieur [170], Chapter III). In practive, Kelvin–Helmholtz-type instabilities are the source of turbulence in many hydrodynamic as well as external and internal aerodynamic applications. An illustration is provided by the famous helium–nitrogen mixing-layer experiment carried out at Caltech by Brown and Roshko [33] and presented in Figure 1.2 (top). Figure 1.2 (bottom) shows a "numerical dye" (with the passive scalar of the upstream distribution proportional to the upstream velocity) in a two-dimensional numerical simulation of a uniform-density mixing layer carried out in Grenoble by Normand [220]. We will return in detail to these vortex-dynamic aspects in Chapter 5. Let us focus now on small-scale–developed turbulence characteristics, which are very important to assess the potential of direct numerical simulations of flows in terms of practical applications. This is why we devote a section to very useful spectral tools in isotropic turbulence.

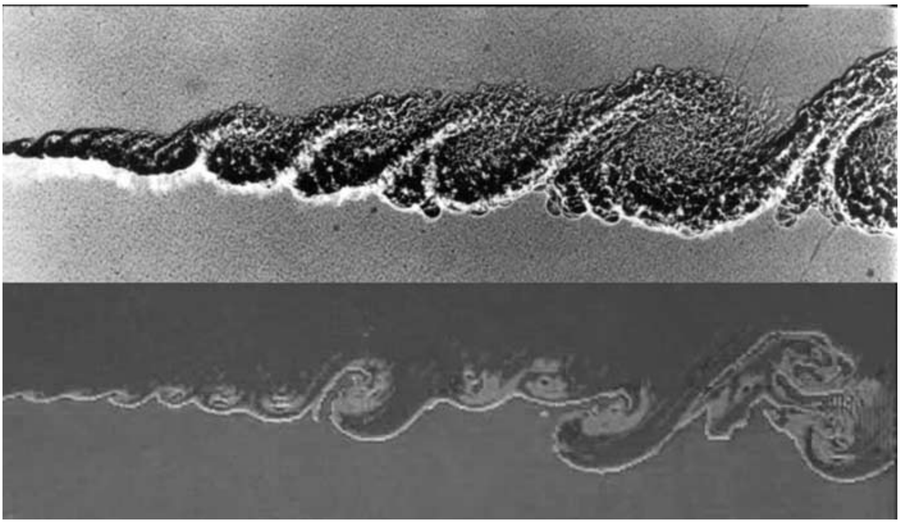

Figure 1.2. (Top) Experimental mixing layer of Brown and Roshko. (Courtesy A. Roshko.) (Bottom) Grenoble two-dimensional numerical simulation. (Courtesy X. Normand.)

1.3 Isotropic turbulence

1.3.1 Formalism

Isotropic turbulence is a model that may be relevant to small-scale–developed turbulent flows. We assume an infinite domain without boundaries. Turbulent quantities are represented by random functions for which averages are taken on ensembles of realizations and are denoted $\langle\ \rangle$. Turbulence is assumed to be statistically invariant under rotations about arbitrary axes (and hence translations). Thus the average velocity is zero. We restrict our attention to a flow of uniform density. The easiest mathematical way to deal with such turbulence is to use spatial Fourier space. Let us first introduce the spatial integral Fourier transform of a given function (scalar or vector) $f(\vec{x}, t)$ associated with turbulence

$$\hat{f}(\vec{k}, t) = \left(\frac{1}{2\pi}\right)^3 \int e^{-i\vec{k}.\vec{x}} \ f(\vec{x}, t)\, d\vec{x}, \tag{1.20}$$

where the integral is carried out over the entire three-dimensional space. Because turbulence is statistically homogeneous, its fluctuations cannot be expected to decrease at infinity. However, Eq. (1.20) does make sense in the framework of generalized-functions theory (distributions). In this context, the inverse relation

$$f(\vec{x}, t) = \int e^{i\vec{k}.\vec{x}} \ \hat{f}(\vec{k}, t) d\vec{k} \tag{1.21}$$