J. Fluid Mech. (2010), *vol.* 652, *pp.* 139–169.
doi:10.1017/S0022112009994174

Self-conditioned fields for large-eddy simulations of turbulent flows

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(Received 4 September 2009; revised 18 December 2009; accepted 18 December 2009; first published online 13 April 2010)

An alternative foundation is developed for the large-eddy simulation (LES) of turbulent flows. It is based on 'self-conditioned fields', for example, the mean velocity field conditional on a discrete representation of the filtered velocity field. It is shown that the self-conditioned velocity field minimizes the residual kinetic energy, and that, with the ideal model, the method yields the correct one-time behaviour as determined by the Navier–Stokes equations. The approach is extended to the self-conditioned probability density function (PDF) of compositions. Compared to LES formulations based on the filtered velocity and the filtered density function, the self-conditioned field approach has several advantages: for laminar flow, and in the direct-numerical-simulation limit, the residual fluctuations are zero or exponentially small; full account is taken of the probability distribution of turbulent fields; there are no commutation issues; and there are no issues with filtering at walls, where the self-conditioned velocity is zero. The exact evolution equations for the self-conditioned velocity and composition PDF are derived. Basic models are presented, and the development of improved models is discussed.

1. Introduction

Large-eddy simulation (LES) is a well-established approach for the simulation of turbulent flows (see e.g. Pope 2000; Sagaut 2001; Lesieur, Métais & Comte 2005; Grinstein, Margolin & Rider 2007). An essential idea in LES is to use a reduced-order description of the turbulent flow, so that the LES evolution equations remain computationally tractable even at high Reynolds number, for which case direct numerical simulation (DNS) is intractable (or at least extremely expensive). There are many variants of LES, differing in their definition of the reduced-order description, in the evolution equations solved and in their numerical implementation (see e.g. Schumann 1975; Rogallo & Moin 1985; Boris *et al.* 1992; Pope 2001; Bazilevs *et al.* 2007). Arguably, the dominant approach to the reduced-order description is 'filtering', so that LES evolution equations are solved for the spatially filtered velocity field.

Simply put, the present work offers an alternative to the filtering approach. LES evolution equations are instead solved for 'self-conditioned fields', which are defined and explored below. The motivation for introducing the self-conditioned field approach is to overcome some shortcomings and deficiencies of the filtering approach. (In describing the new approach as LES, the word 'large' should not be taken entirely literally, since (as discussed in § 6.2) the method can represent coherent small-scale features, such as laminar boundary layers and mixing layers.)

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To develop the ideas involved, we consider the turbulent flow of a fluid of constant and uniform density, ρ. The velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$ is solenoidal

$$\frac{\partial U_i}{\partial x_i} = 0, \tag{1.1}$$

and satisfies the momentum equation

$$\frac{\mathrm{D}U_i}{\mathrm{D}t} \equiv \left(\frac{\partial}{\partial t} + U_j \frac{\partial}{\partial x_j}\right) U_i = \frac{\partial \tau_{ij}}{\partial x_j} = \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{1}{\rho}\frac{\partial p}{\partial x_i}, \tag{1.2}$$

where $\rho\tau_{ij}$ is the stress tensor, ν is the uniform kinematic viscosity and $p(\boldsymbol{x}, t)$ is the pressure.

Let $\boldsymbol{W}(\boldsymbol{x}, t)$ denote the velocity field considered in an LES. Then, in nearly all LES approaches, the evolution equations solved are

$$\frac{\partial W_i}{\partial x_i} = 0 \tag{1.3}$$

and

$$\frac{\overline{\mathrm{D}}W_i}{\overline{\mathrm{D}}t} \equiv \left(\frac{\partial}{\partial t} + W_j \frac{\partial}{\partial x_j}\right) W_i = \frac{\partial \tilde{\tau}_{ij}}{\partial x_j}, \tag{1.4}$$

where $\rho\tilde{\tau}_{ij}$ is an 'effective' stress. The differences between LES approaches based on these fundamental equations are:

(a) how $\boldsymbol{W}(\boldsymbol{x}, t)$ is defined, interpreted and deemed to correspond to $\boldsymbol{U}(\boldsymbol{x}, t)$;

(b) how the effective stress is specified; and

(c) how (approximate) numerical solutions are obtained.

This work focuses on item (a), which has an impact on item (b). We do not consider item (c), except to discuss (in § 6.2) the spatial resolution necessary for the accurate numerical solution of (1.3) and (1.4).

1.1. *The filtering approach*

In the filtering approach, $\boldsymbol{W}(\boldsymbol{x}, t)$ is taken to be the spatially filtered velocity field, $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$, defined by

$$\overline{\boldsymbol{U}}(\boldsymbol{x}, t) = \int_{\mathscr{D}} \boldsymbol{U}(\boldsymbol{y}, t)\, G(\boldsymbol{x}, \boldsymbol{y} - \boldsymbol{x})\, \mathrm{d}\boldsymbol{y}, \tag{1.5}$$

where integration is over the flow domain $\mathscr{D}$, and $G(\boldsymbol{x}, \boldsymbol{r})$ is the specified filter function, satisfying the normalization condition

$$\int_{\mathscr{D}} G(\boldsymbol{x}, \boldsymbol{y} - \boldsymbol{x})\, \mathrm{d}\boldsymbol{y} = 1. \tag{1.6}$$

The residual velocity field is then defined by

$$\boldsymbol{U}'(\boldsymbol{x}, t) = \boldsymbol{U}(\boldsymbol{x}, t) - \overline{\boldsymbol{U}}(\boldsymbol{x}, t). \tag{1.7}$$

We consider two types of filtering. In 'spatial filtering', the filter function is taken to be positive, $G \geqslant 0$. Among other things, this condition ensures that filtered species mass fractions and the filtered density function are non-negative. This type of spatial filtering is generally used for inhomogeneous flows, and examples of positive filters are the top-hat and Gaussian filters. The characteristic filter width, $\Delta(\boldsymbol{x})$, is defined by

$$\Delta(\boldsymbol{x})^2 = 4 \int_{\mathscr{D}} G(\boldsymbol{x}, \boldsymbol{y} - \boldsymbol{x}) |\boldsymbol{y} - \boldsymbol{x}|^2\, \mathrm{d}\boldsymbol{y}. \tag{1.8}$$

For homogeneous turbulence, we consider 'spectral filtering' in which the filtered field corresponds to all Fourier modes of wavenumber less than the specified cutoff, κ_c. While this sharp spectral filter can be expressed as a spatial filter, the corresponding filter function, G, has negative portions, and its second moment does not exist. Instead of (1.8), the characteristic filter width is defined as $\Delta = \pi/\kappa_c$.

In this paper, we primarily consider spatial filtering applied to inhomogeneous flows. Some of the issues that arise in the spatial filtering approach (i.e. taking $\boldsymbol{W} = \overline{\boldsymbol{U}}$) are as follows:

(i) For a laminar flow, $\overline{\boldsymbol{U}}$ differs from $\boldsymbol{U}$ by an amount generally of order Δ^2; or, equivalently, the residual velocity $\boldsymbol{U}'$ is of order Δ^2.

(ii) The same applies to turbulent flows in the DNS limit (which is defined and examined in § 2).

(iii) In the filtering approach (as usually presented) no account is taken of the fact that, given a filtered velocity field $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$, there is a corresponding probability distribution of velocity fields $\boldsymbol{U}(\boldsymbol{x}, t)$. Consequently, for a given filtered field $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$, there is a probability distribution of rates of change $\partial\overline{\boldsymbol{U}}(\boldsymbol{x}, t)/\partial t$.

(iv) At best, the statistics of the LES velocity $\boldsymbol{W}$ correspond to statistics of the filtered velocity field $\overline{\boldsymbol{U}}$ (which depend on the non-physical filter function $G(\boldsymbol{x}, \boldsymbol{r})$), whereas it is the statistics of the (unfiltered) velocity field $\boldsymbol{U}$, which are of fundamental significance.

(v) For non-uniform filters (e.g. with spatial variation of $\Delta(\boldsymbol{x})$), the divergence of $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$ is, in general, non-zero. Hence, taking $\boldsymbol{W}$ to be solenoidal (1.3) incurs some error.

(vi) At points $\boldsymbol{x}^w$ on a stationary solid wall, where the no-slip and impermeability conditions $\boldsymbol{U}(\boldsymbol{x}^w, t) = 0$ apply, the filtered velocity $\overline{\boldsymbol{U}}(\boldsymbol{x}^w, t)$ is non-zero (unless the support of the filter function $G(\boldsymbol{x}^w, \boldsymbol{y} - \boldsymbol{x}^w)$ is confined to points on the wall).

1.2. *The self-conditioned field approach*

The idea of defining LES fields in terms of conditional means is due to Fox (2003). The present work is a substantial development and expansion of this idea.

Many previous works (e.g. Adrian 1990; Langford & Moser 1999; McComb, Hunter & Johnston 2001 and references therein) have considered conditional means of residual quantities (conditional on LES fields), as we do in this paper. Note, however, that this is different from Fox's idea (further developed here) of using conditional means to define the LES fields.

The simplest self-conditioned field approach is now outlined, with a fuller description provided in §§ 3 and 4. A set of n_c conditioning variables $\boldsymbol{C}(t) = \{C_1(t), C_2(t), \ldots, C_{n_c}(t)\}$ is defined, most simply as components of the filtered velocity at points on a mesh. Thus, in this case, $\boldsymbol{C}(t)$ provides a finite approximation to the filtered velocity field. Then the self-conditioned velocity field is defined as

$$\boldsymbol{W}(\boldsymbol{x}, t) \equiv \langle \boldsymbol{U}(\boldsymbol{x}, t) \mid \boldsymbol{C}(t) \rangle, \tag{1.9}$$

i.e. $\boldsymbol{W}$ is the mean over the probability distribution of turbulent velocity fields $\boldsymbol{U}(\boldsymbol{x}, t)$ for which the conditioning variables are $\boldsymbol{C}(t)$. (This definition is refined below; see (3.11) and (4.2).)

This construction is illustrated in figures 1 and 2 for a simple one-dimensional scalar test case described in Appendix A. Figure 1 shows four samples of a random process $U(x)$ which, by construction, have the same filtered values $\boldsymbol{C}$ at the $n_c = 5$ specified mesh points. This simply illustrates that, given the filtered field $\boldsymbol{C}$ at mesh points, the underlying field $U(x)$ is random with significant variations. The filter used

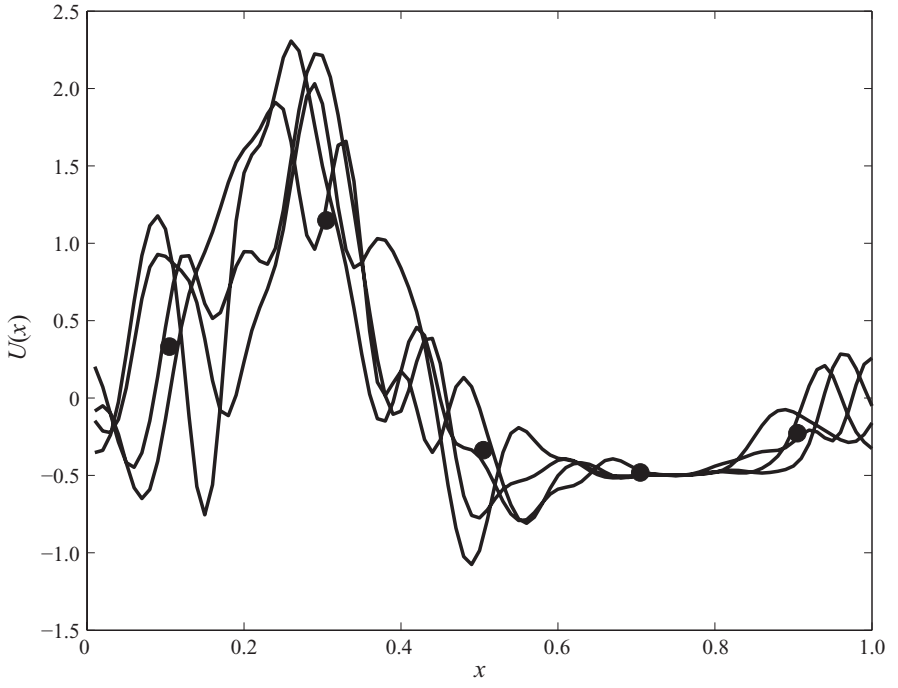

FIGURE 1. Four samples (lines) of a random process $U(x)$ and their filtered values $\boldsymbol{C}$ (symbols) at $n_c = 5$ mesh points. By construction, the four samples have the same value of $\boldsymbol{C}$.

is a top hat of width 1/5. Figure 2 shows the corresponding filtered fields $\overline{U}(x)$, and the conditional mean field $W(x)$ (conditional on the five filtered values), which is known exactly in this Gaussian test case. Note that, given $\boldsymbol{C}$, $\overline{U}(x)$ is also random (except at the mesh points), whereas $W(x)$ is non-random and differs from $\overline{U}(x)$ at the mesh points.

Returning to the general case, to expand on the description of the conditioning variables $\boldsymbol{C}(t)$, we consider a mesh with M points (e.g. the mesh used in the numerical solution of the LES equations), and hence there are $n_c = 3M$ conditioning variables, corresponding to the three components of the filtered velocity at each of the mesh points $\boldsymbol{x}^{(m)}$, $m = 1, 2, \ldots, M$. The value of the nth conditioning variable can then alternatively be expressed as

$$\begin{aligned} C_n(t) &= \overline{U}_{I_n}(\boldsymbol{x}^{(m_n)}, t) \\ &= \int_{\mathscr{D}} U_{I_n}(\boldsymbol{y}, t)\, G(\boldsymbol{x}^{(m_n)}, \boldsymbol{y} - \boldsymbol{x}^{(m_n)})\, \mathrm{d}\boldsymbol{y} \\ &= \int_{\mathscr{D}} U_i(\boldsymbol{y}, t)\, K_i^{(n)}(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}, \end{aligned} \tag{1.10}$$

where $I_n = 1$, 2 or 3 is the component of velocity, and $\boldsymbol{x}^{(m_n)}$ is the mesh point associated with C_n; and the last line identifies the nth 'conditioning kernel' as

$$K_i^{(n)}(\boldsymbol{y}) = \delta_{iI_n} G(\boldsymbol{x}^{(m_n)}, \boldsymbol{y} - \boldsymbol{x}^{(m_n)}). \tag{1.11}$$

The field $\boldsymbol{W}(\boldsymbol{x}, t)$ defined by (1.9) is referred to as being 'self-conditioned', because it contains full information about the conditioning variables. That is, (1.9) and (1.10)

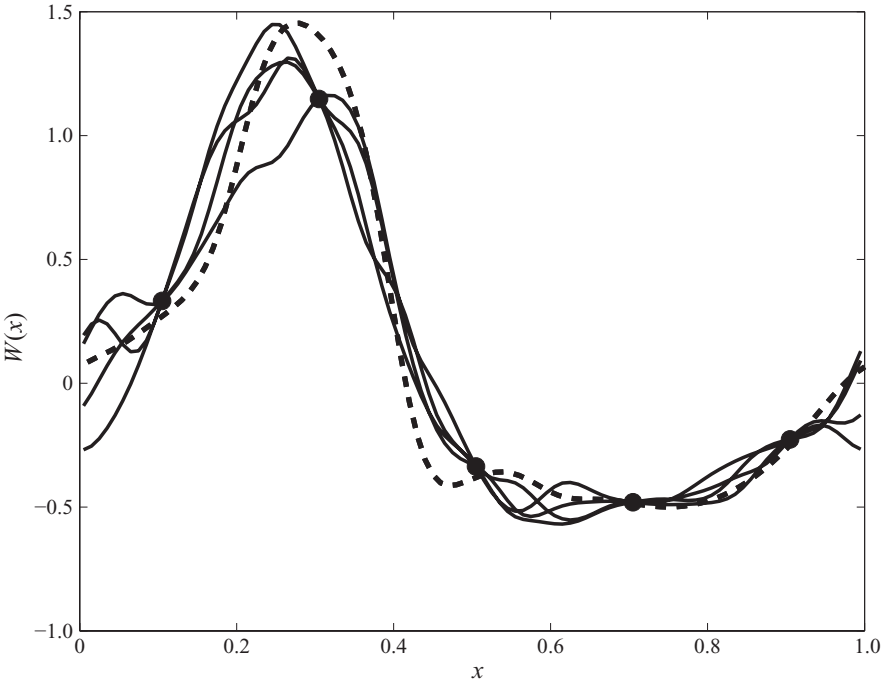

FIGURE 2. The filtered processes $\overline{U}(x)$ (solid lines) corresponding to the four sample processes $U(x)$ in figure 2 and the conditional mean $W(x) = \langle U(x) \mid \boldsymbol{C} \rangle$ (dashed line).

lead to

$$C_n(t) = \int_{\mathscr{D}} W_i(\boldsymbol{y}, t) K_i^{(n)}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}. \tag{1.12}$$

In comparison to the issues raised by the filtering approach (enumerated above), the self-conditioning field approach (i.e. taking $\boldsymbol{W} = \langle \boldsymbol{U} | \boldsymbol{C} \rangle$) has the following attributes:

(i) For a laminar flow, $\langle \boldsymbol{U} | \boldsymbol{C} \rangle$ is identical to $\boldsymbol{U}$; or, equivalently, the residual velocity $\boldsymbol{U}' \equiv \boldsymbol{U} - \langle \boldsymbol{U} | \boldsymbol{C} \rangle$ is zero.

(ii) In the DNS limit, the residual velocity is exponentially small (as explained and justified in § 2).

(iii) From its definition, $\langle \boldsymbol{U} | \boldsymbol{C} \rangle$ explicitly accounts for the probability distribution of turbulent velocity fields, and there is a unique rate of change $\partial \langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{C}(t) \rangle / \partial t$.

(iv) The mean $\langle \langle \boldsymbol{U} | \boldsymbol{C} \rangle \rangle$ is the Reynolds averaged (unfiltered) velocity field $\langle \boldsymbol{U} \rangle$. (This mean is over the distribution of conditioning variables.)

(v) The operations of spatial differentiation and taking the conditional mean commute, and hence $\langle \boldsymbol{U} | \boldsymbol{C} \rangle$, is solenoidal (for an incompressible flow).

(vi) At points $\boldsymbol{x}^w$ on a stationary solid wall, $\langle \boldsymbol{U}(\boldsymbol{x}^w, t) | \boldsymbol{C}(t) \rangle$ is zero.

Furthermore, the specification $\boldsymbol{W}(\boldsymbol{x}, t) = \langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{C}(t) \rangle$ minimizes the residual velocity. More precisely, out of all possible specifications of the LES velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ based on a knowledge of $\boldsymbol{C}(t)$, the self-conditioned velocity field yields the smallest residual, $\boldsymbol{U}'(\boldsymbol{x}, t) \equiv \boldsymbol{U}(\boldsymbol{x}, t) - \boldsymbol{W}(\boldsymbol{x}, t)$, in the sense that the specification $\boldsymbol{W} = \langle \boldsymbol{U} | \boldsymbol{C} \rangle$ minimizes the residual kinetic energy. It is readily shown that the conditional residual kinetic energy,

$$\tfrac{1}{2} \langle |\boldsymbol{U}(\boldsymbol{x}, t) - \boldsymbol{W}(\boldsymbol{x}, t)|^2 \mid \boldsymbol{C}(t) = \boldsymbol{c} \rangle, \tag{1.13}$$

is minimized (for each $\boldsymbol{x}, t$) by $\boldsymbol{W}(\boldsymbol{x}, t) = \langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{C}(t) \rangle$, and hence the mean residual kinetic energy,

$$k_r \equiv \tfrac{1}{2} \langle |\boldsymbol{U} - \boldsymbol{W}|^2 \rangle = \tfrac{1}{2} \langle \langle |\boldsymbol{U} - \boldsymbol{W}|^2 \mid \boldsymbol{C} \rangle \rangle, \tag{1.14}$$

is also minimized by the self-conditioned velocity field.

1.3. *Outline*

In § 2, we define the DNS limit and substantiate the claims made above concerning the behaviour of the filtering and self-conditioned field approaches in this limit. In § 3, we develop the basic concepts of self-conditioned fields and how they can be used for turbulent simulations. This development is performed in the phase space of the velocity field, drawing on the work of Temam (1991), in order to make explicit the distribution of turbulent velocity fields and related concepts.

In § 4, we describe the method to simulate turbulent flows using the self-conditioned velocity field, and the relevant equations are derived in Appendix B. The merits of this approach relative to the filtering approach are further discussed.

In § 5, the approach is extended to consider the self-conditioned probability density function (PDF) of composition, of particular relevance to reacting flows. Previously, several LES of reactive flows have been based on the filter density function (FDF) (Pope 1990; Gao & O'Brien 1993; Colucci *et al.* 1998; Raman & Pitsch 2007). Compared to the FDF approach, the self-conditioned PDF approach has similar advantages to those enumerated above. In particular, in laminar flow and in the DNS limit, the PDF has zero or exponentially small variance, whereas the FDF has variance of order Δ^2. These considerations are of some significance in turbulent combustion, where the DNS limit can be approached (given the strong increase of viscosity and diffusivity with temperature), and the differential diffusion of species can be influential. The self-conditioned PDF equation is derived in Appendix C.

In § 6, there is a discussion of modelling issues, the spatial resolution required by the self-conditioned fields, the near-wall behaviour, the use of spectral filtering, the choice of conditioning variables and various extensions of the approach. Conclusions are drawn in § 7.

The essential contribution of this paper is to provide a different and advantageous conceptual basis for LES. Significant new models are not proposed, but the self-conditioning approach provides simpler, more fundamental limiting behaviours (especially the DNS limit) that provide guidance and constraints on models.

2. The DNS limit

An important consideration in this work is the 'DNS limit', which is now defined and considered, first for the filtering approach and then for the self-conditioned field approach.

For a given turbulent flow, let $\Delta^\circ(\boldsymbol{x})$ be a specified reference filter width (with $0 < \Delta^\circ < \infty$). Then, the DNS limit corresponds to the specification $\Delta(\boldsymbol{x}) = \epsilon \Delta^\circ(\boldsymbol{x})$ and the limit $\epsilon \to 0$. For a simple spatial filter, a Taylor-series analysis of (1.5) shows that the residual velocity and the residual kinetic energy vary as ϵ^2 in this limit, thus substantiating the claims made above (items (i) and (ii) in § 1.1).

For spectral filtering the picture is different. We consider LES of homogeneous isotropic turbulence with a sharp spectral filter, with cutoff wavenumber $\kappa_c = \pi/\Delta = \pi/(\epsilon \Delta^\circ)$. It is well established (see e.g. Pope 2000) that at very high wavenumber (in the far dissipation range) the energy spectrum function $E(\kappa)$ decreases exponentially with wavenumber κ, approximately proportional to $\kappa^{-5/3} \exp(-\beta \kappa \eta)$,

where η is the Kolmogorov length scale and $\beta \approx 2$ is a constant. It follows that (for $\kappa_c \eta \gg 1$) the residual kinetic energy k_r varies with κ in the same way, and hence is proportional to $\epsilon^{5/3} \exp(-\gamma/\epsilon)$, where $\gamma \equiv \pi\beta\eta/\Delta^\circ$. Thus, in the DNS limit $\epsilon \to 0$, the residual kinetic energy k_r tends to zero much faster than any power of ϵ; and we describe it as being 'exponentially small'.

To examine the DNS limit in the self-conditioned field approach, we consider the simplest base case, in which the conditioning variables are defined as the filtered velocities (with filter width Δ°) at the M_o mesh points (with mesh spacing comparable to Δ°). For the DNS limit $\epsilon \to 0$, we require that both the filter width and the mesh spacing scale with ϵ: hence the number of conditioning variables increases as ϵ^{-3}. We can consider, for example, approaching the limit by successively halving ϵ (starting with $\epsilon = 1$). At each halving of ϵ, the filter width Δ and the mesh spacing are halved, and the number of conditioning variables, n_c, increases by a factor of 8.

We claim that for the self-conditioned field approach in the DNS limit, the residual kinetic energy is exponentially small. To provide some evidence for this claim, we consider homogeneous isotropic turbulence, with the uniform mesh spacing being equal to the filter width $\Delta = \epsilon\Delta^\circ$, and with ϵ being sufficiently small that Δ is very small compared to η. The mesh is capable of representing Fourier modes up to the cutoff wavenumber $\kappa_c = \pi/\Delta$. Consider, first, the hypothetical case of the velocity field being composed solely of the $n_c = 3M$ Fourier modes represented on the mesh. Then, there is a one-to-one correspondence between these n_c Fourier modes and the n_c constraints, and so $\langle \boldsymbol{U}|\boldsymbol{C}\rangle$ equals $\boldsymbol{U}$, and the residual velocity is zero. It follows, then, that for the case of a turbulent velocity field, the residual kinetic energy arises from Fourier modes of $\boldsymbol{U}$ of wavenumber larger than κ_c. These high-wavenumber modes contribute directly to k_r, and also indirectly as they affect $\boldsymbol{C}(t)$ and hence $\langle \boldsymbol{U}|\boldsymbol{C}\rangle$. However, the energy in the high-wavenumber modes is exponentially small, and hence so also is k_r. While this argument pertains to the simplest case, there is reason to suppose that the conclusion is true in general, namely, that for the self-conditioned field approach in the DNS limit, the residual kinetic energy k_r is exponentially small.

3. Formulation in function space

In this section, we develop the necessary concepts by considering a turbulent flow described by its velocity field $u(t)$ in a function space $\mathscr{H}$, which is the appropriate phase space of incompressible velocity fields. The conditioning variables $\boldsymbol{C}(t)$ are defined by a specified mapping from $\mathscr{H}$ to the n_c-dimensional conditioning space $\mathscr{C}$. The reduced description considered consists of the self-conditioned velocity field $\langle u(t)|\boldsymbol{C}(t) = \boldsymbol{c}\rangle$ and the PDF of $\boldsymbol{C}(t)$, denoted by $f_c(\boldsymbol{c}; t)$.

The simulation approach is based on the observation that the same information (i.e. $\langle u(t)|\boldsymbol{c}\rangle$ and f_c) can be obtained by solving a deterministic evolution equation for a self-conditioned velocity field, $w(t)$, from a distribution of initial conditions, $w(0)$.

3.1. *The distribution of turbulent velocity fields*

The self-conditioned velocity field $\langle \boldsymbol{U}(\boldsymbol{x}, t)|\boldsymbol{C}(t)\rangle$ is defined as a conditional mean over the distribution of turbulent velocity fields. The purpose of this section is to clarify the nature of this distribution. In practice, turbulent flows are random, because of the randomness inherent in initial conditions, boundary conditions, material property variations, etc. For such random flows, we can consider the probability distribution of the velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$. However, this probability distribution is determined

not only by the sources of randomness but also by the chaotic nature of the solutions of the Navier–Stokes equations. Arguably, the essence of turbulent flows is more concerned with the latter. Consequently, in this subsection and the next, we examine the appropriate distribution for the case in which all randomness is removed. We do so by drawing on the picture developed by Temam (1991) for the deterministic (chaotic) solutions to the Navier–Stokes equations for channel flow. (A similar development is described in Foias *et al.* 2001.) We then address the general, random case in § 3.3.

We consider the constant-property Navier–Stokes equations applied to the spatially periodic channel flow. The smooth channel walls are located at $y = 0$ and $y = L_y$. The velocity field is periodic in the mean-flow direction, x, and in the spanwise direction, z, with periods L_x and L_z large compared to L_y. The density ρ, kinematic viscosity ν and mean pressure gradient $\mathrm{d}\langle p\rangle/\mathrm{d}x$ are specified. For fixed aspect ratios L_x/L_y and L_z/L_y, the problem specification involves a single non-dimensional parameter, which can be taken to be the friction Reynolds number $Re_\tau = (|\mathrm{d}\langle p\rangle/\mathrm{d}x|L_y^3/(8\rho\nu^2))^{1/2}$. A non-trivial deterministic initial condition is specified at time $t = 0$. The solution for the velocity field at time t, ($t \geqslant 0$) is denoted by $u(t)$, and is an element of the appropriate function space, $\mathscr{H}$, which is the phase space of incompressible flow fields satisfying these boundary conditions.

Temam (1991) shows that there is an invariant attractor $\mathscr{A}$ in $\mathscr{H}$ of finite dimension, n_A, such that, at all large times, $u(t)$ is arbitrarily close to $\mathscr{A}$. The attractor $\mathscr{A}$ and its dimension n_A depend solely on Re_τ. For sufficiently small Re_τ, n_A is zero, and $\mathscr{A}$ is the single fixed point corresponding to steady laminar flow. But we consider sufficiently large Re_τ (corresponding to fully turbulent flow) so that n_A is large (but finite) and $\mathscr{A}$ is most likely fractal.

We now modify the problem statement by requiring that the initial condition $u(0)$ be on the attractor. Then, since $\mathscr{A}$ is invariant, the solution $\{u(t),\ t \geqslant 0\}$ is a trajectory in $\mathscr{H}$, which remains on the n_A-dimensional attractor $\mathscr{A}$ for all time.

It is assumed that the system is ergodic, so that long time averages converge, and are independent of the initial condition. A measure μ_u can then be defined such that, with δu being a region of the function space $\mathscr{H}$, $\mu_u(\delta u)$ is the fraction of time that $u(t)$ spends in δu, i.e. μ_u is the frequency distribution. The measure μ_u is non-zero only on the attractor $\mathscr{A}$, and its integral $\int_{\mathscr{H}} \mathrm{d}\mu_u$ over the entire space is unity.

3.2. *Conditioning variables*

As described in the Introduction and exemplified by (1.10), we define $\boldsymbol{C}$ to be a set of n_c conditioning variables. In general, we consider n_c to be small compared to n_A, since we are seeking a reduced-order description of the flow. However, we also consider the limiting cases of laminar flow, and the DNS limit, for which n_c exceeds n_A. Let $\mathscr{C}$ denote the n_c-dimensional conditioning space, and let $\boldsymbol{c}$ be the sample-space variable (i.e. a general point in $\mathscr{C}$). As a generalization of (1.10), the conditioning variables can be written as

$$\boldsymbol{C}(t) = \mathscr{K}(u(t)), \tag{3.1}$$

where $\mathscr{K}$ is a specified linear function from the infinite-dimensional function space $\mathscr{H}$ to the n_c-dimensional conditioning space $\mathscr{C}$. We require that the conditioning variables be linearly independent (so that every point in $\mathscr{C}$ is mapped from $\mathscr{H}$).

With $\delta\boldsymbol{c}$ being a region in $\mathscr{C}$, we denote by $\mathscr{A}(\delta\boldsymbol{c})$ all velocity fields u on the attractor which are mapped to $\delta\boldsymbol{c}$ by $\mathscr{K}$:

$$\mathscr{A}(\delta\boldsymbol{c}) \equiv \{u \in \mathscr{A} : \mathscr{K}(u) \in \delta\boldsymbol{c}\}. \tag{3.2}$$

Note that $\mathscr{A}$ is n_A-dimensional and $\mathscr{C}$ is n_c-dimensional so that for $n_A > n_c$, $\mathscr{A}(\boldsymbol{c})$ may be composed of multiple $(n_A - n_c)$-dimensional regions corresponding to multiple

leaves of the attractor. The frequency measure in $\mathscr{C}$ is

$$\mu_c(\delta \boldsymbol{c}) = \int_{u \in \mathscr{A}(\delta \boldsymbol{c})} \mathrm{d}\mu_u. \tag{3.3}$$

For a region $\delta \boldsymbol{c}$ of positive measure, the conditional mean of u is

$$\langle u \mid \boldsymbol{C} \in \delta \boldsymbol{c} \rangle = \frac{\displaystyle\int_{u \in \mathscr{A}(\delta \boldsymbol{c})} u \, \mathrm{d}\mu_u}{\displaystyle\int_{u \in \mathscr{A}(\delta \boldsymbol{c})} \mathrm{d}\mu_u} = \frac{1}{\mu_c(\delta \boldsymbol{c})} \int_{u \in \mathscr{A}(\delta \boldsymbol{c})} u \, \mathrm{d}\mu_u. \tag{3.4}$$

By shrinking $\delta \boldsymbol{c}$ to the point $\boldsymbol{c}$ and assuming the necessary continuity properties, we can define the conditional mean field $\langle u | \boldsymbol{C} = \boldsymbol{c} \rangle$. This conditional velocity field ($\langle u | \boldsymbol{c} \rangle$ in an abbreviated notation) is an n_c-dimensional manifold in the function space $\mathscr{H}$ (e.g. parameterized by $C_1, C_2, \ldots, C_{n_c}$): $\langle u | \boldsymbol{c} \rangle$ need not be on the attractor.

The measure μ_c can be re-expressed in terms of a density function $f_c(\boldsymbol{c})$, such that, for any region $\delta \boldsymbol{c}$ of $\mathscr{C}$,

$$\int_{\delta \boldsymbol{c}} f_c(\boldsymbol{c}) \, \mathrm{d}\boldsymbol{c} = \int_{\delta \boldsymbol{c}} \mathrm{d}\mu_c. \tag{3.5}$$

Then the unconditional (Reynolds) mean of u can be obtained as

$$\langle u \rangle = \int_{\mathscr{H}} u \, \mathrm{d}\mu_u = \int_{\mathscr{C}} \langle u | \boldsymbol{c} \rangle \, f_c(\boldsymbol{c}) \, \mathrm{d}\boldsymbol{c}. \tag{3.6}$$

For the deterministic case under consideration, we re-define the DNS limit as being achieved when n_c is sufficiently large ($n_c \geqslant n_A$), and the conditioning variables are so chosen that each velocity field u in $\mathscr{A}$ is mapped by (3.1) to a distinct value of $\boldsymbol{c}$. In this limit, we have $\langle u | \boldsymbol{c} \rangle = u$, and so the residual velocity is zero.

The space $\mathscr{H}$ can be decomposed into two subspaces, $\widetilde{\mathscr{H}}$ and $\widehat{\mathscr{H}}$, which are mutually orthogonal with respect to the inner product of $\mathscr{H}$, where $\widehat{\mathscr{H}}$ is the kernel of $\mathscr{K}$ (so that $\mathscr{K}(\widehat{u}) = 0$ for all $\widehat{u}$ in $\widehat{\mathscr{H}}$). Correspondingly, u can be decomposed as $u = \widetilde{u} + \widehat{u}$ with $\widetilde{u} \in \widetilde{\mathscr{H}}$ and $\widehat{u} \in \widehat{\mathscr{H}}$. Note that $\widetilde{\mathscr{H}}$ is n_c-dimensional. The upshot of this development is the observation that conditioning on $\boldsymbol{c}$ is equivalent to conditioning on $\widetilde{u}$, and that it is the subspace $\widetilde{\mathscr{H}}$ which is of fundamental significance, rather than the particular choice of conditioning kernels. (The decomposition $u = \widetilde{u} + \widehat{u}$ and the choice of conditioning variables is discussed further in Appendix D.)

3.3. *Generalization*

The development above pertains to the long-time behaviour of a particular deterministic flow. We wish to generalize some of the results to turbulent flows with random initial conditions and to flows which are not statistically stationary. For this case, a finite-dimensional attractor may not exist, but there nevertheless appears to be no inherent difficulty in considering the following generalizations.

The flow field $u(t)$ evolves deterministically in a phase space $\mathscr{H}$ from an initial condition $u(0)$ drawn from a specified probability distribution. At time t there is a probability measure $\mu_u(t)$; there are conditioning variables $\boldsymbol{C}(t)$, defined by (3.1), which have a PDF $f_c(\boldsymbol{c}; t)$; and the conditional velocity field is $\langle u(t) | \boldsymbol{C}(t) = \boldsymbol{c} \rangle$.

For simplicity of the subsequent development, we exclude randomness in boundary conditions and material properties, so that the velocity field evolves deterministically. However, there does not appear to be any difficulty, in principle, in including these additional sources of randomness.

3.4. *Equivalent deterministic reduced system*

We write the Navier–Stokes equation as

$$\frac{\mathrm{d}u}{\mathrm{d}t} = a(u(t)), \tag{3.7}$$

thus implicitly defining the function $a(u)$. It follows from the definition of the conditioning variables $\boldsymbol{C}(t)$ (3.1) that they evolve by

$$\frac{\mathrm{d}\boldsymbol{C}}{\mathrm{d}t} = \mathscr{K}\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right) = \mathscr{K}\left(a(u(t))\right). \tag{3.8}$$

Note that, while $\mathrm{d}u/\mathrm{d}t$ is determined by u, in contrast $\mathrm{d}\boldsymbol{C}/\mathrm{d}t$ is not determined by $\boldsymbol{C}$.

We now draw on the ideas of 'equivalent systems' (Pope 1985) and 'ideal LES' (Langford & Moser 1999; Pope 2000) to construct a system that evolves deterministically with the same one-time statistics as $\boldsymbol{C}(t)$ and $\langle u(t)|\boldsymbol{C}(t)=\boldsymbol{c}\rangle$. First, we define $\widehat{\boldsymbol{C}}(t)$ to evolve by the deterministic equation

$$\frac{\mathrm{d}\widehat{\boldsymbol{C}}}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}\boldsymbol{C}}{\mathrm{d}t} \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle, \tag{3.9}$$

from the random initial condition $\widehat{\boldsymbol{C}}(0)$, sampled from the initial PDF, $f_c(\boldsymbol{c};0)$. It follows that $\boldsymbol{C}(t)$ and $\widehat{\boldsymbol{C}}(t)$ have identical one-time distributions, since their PDFs evolve by the same Liouville equation

$$\frac{\partial f_c}{\partial t} + \frac{\partial}{\partial c_i}\left[f_c \left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c} \right\rangle\right] = 0, \tag{3.10}$$

from the same initial condition. (This result requires that $\mathrm{d}\widehat{\boldsymbol{C}}/\mathrm{d}t$ does not vanish anywhere, which is the case for a turbulent flow with a reasonable specification of the conditioning variables.)

We now define the self-conditioned velocity field $w(t)$ by

$$w(t) = \langle u(t) \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t)\rangle. \tag{3.11}$$

Since $\widehat{\boldsymbol{C}}(t)$ has the same distribution as $\boldsymbol{C}(t)$, it follows that $w(t)$ has the same distribution as $\langle u(t)|\boldsymbol{C}(t)\rangle$. Given that $\widehat{\boldsymbol{C}}(0)$ is random, the initial condition $w(0)$ is random, but subsequently $w(t)$ evolves deterministically, by an equation of the form

$$\frac{\mathrm{d}w}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}u}{\mathrm{d}t} \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle + R(\widehat{\boldsymbol{C}}(t), t). \tag{3.12}$$

A specific form of this equation is derived in Appendix B, where the term R is identified (see (B 12)–(B 15)).

From (3.11) we obtain

$$\mathscr{K}(w(t)) = \mathscr{K}(\langle u(t) \mid \mathscr{K}(u(t)) = \widehat{\boldsymbol{C}}(t)\rangle) = \widehat{\boldsymbol{C}}(t), \tag{3.13}$$

showing that $w(t)$ is indeed a self-conditioned field. Hence, it is unnecessary to solve (3.9) for $\widehat{\boldsymbol{C}}(t)$, since it can be obtained from the solution to (3.12) for $w(t)$ and the application of (3.13). Likewise, $\widehat{\boldsymbol{C}}(t)$ can be eliminated from (3.12) in favour of $w(t)$ to yield an evolution equation of the form

$$\frac{\mathrm{d}w}{\mathrm{d}t} = B(w(t), t), \tag{3.14}$$

where B is defined by the right-hand side of (3.12).

Based on the ideas developed above, the use of the self-conditioned velocity fields to simulate the turbulent flow is now explained and the central result is stated.

We denote by $\widehat{w}(t)$ the model for $w(t) = \langle u(t)|\boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t)\rangle$, which is specified to evolve by

$$\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} = \widehat{B}(\widehat{w}(t), t), \tag{3.15}$$

from a random initial condition $\widehat{w}(0)$, drawn from a specified distribution, where $\widehat{B}$ is a specified model for B. Solving (3.15) for one initial condition is analogous to performing a large-eddy simulation. We denote by $\langle\ \ \rangle_{\widehat{w}(0)}$ the mean over the distribution of initial conditions, which can be approximated by the ensemble mean of multiple simulations (with independent initial conditions).

The model is deemed to be ideal if (a) the initial condition $\widehat{w}(0)$ has the same distribution as $w(0)$ (and hence also the same as that of $\langle u(0)|\boldsymbol{C}(0)\rangle$), and ($b$) the modelled rate of change $\widehat{B}(w, t)$ equals $B(w, t)$. It follows from this definition that, for the ideal model, the distributions of $\widehat{w}(t)$ and $w(t)$ are identical, because $\widehat{w}(t)$ and $w(t)$ evolve identically (deterministically) from initial conditions with the same distribution. Furthermore, since $w(t)$ has the same distribution as $\langle u(t)|\boldsymbol{C}(t)\rangle$, it follows that the model $\widehat{w}(t)$ is identically distributed to the self-conditioned velocity field, $\langle u(t)|\boldsymbol{C}(t)\rangle$. Thus, for the ideal model we have

$$\langle u(t) \mid \boldsymbol{C}(t) = \boldsymbol{c}\rangle = \langle \widehat{w}(t) \mid \mathscr{K}(\widehat{w}(t)) = \boldsymbol{c}\rangle_{\widehat{w}(0)}, \tag{3.16}$$

and that the distribution of $\mathscr{K}(\widehat{w}(t))$ is identical to that of $\boldsymbol{C}(t)$ (and $\widehat{\boldsymbol{C}}(t)$).

Given that there are n_c conditioning variables, it follows that $\langle u(t)|\boldsymbol{c}\rangle$ lies in a (possibly time-dependent) manifold of dimension at most n_c. For an ideal model, $\widehat{w}(t)$ lies in the same manifold. The deficiencies of a non-ideal model may be manifest in two ways: first, (3.16) may not be satisfied; second, $\widehat{w}(t)$ may lie in a different manifold of different dimension.

3.5. *Distinction between self-conditioned fields*

This subsection emphasizes the distinction between three different self-conditioned velocity fields, $\langle u(t)|\boldsymbol{c}\rangle$, $\langle u(t)|\widehat{\boldsymbol{C}}(t)\rangle$ and $\langle u(t)|\boldsymbol{C}(t)\rangle$. The primary distinction is between their time rates of change.

To clarify issues, we define the deterministic function $u_c(t, \boldsymbol{c})$ by

$$u_c(t, \boldsymbol{c}) \equiv \langle u(t) \mid \boldsymbol{C}(t) = \boldsymbol{c}\rangle = \langle u(t) \mid \boldsymbol{c}\rangle, \tag{3.17}$$

where the last part is simply an abbreviated notation. This function has partial derivatives $\partial u_c/\partial t$ and $\partial u_c/\partial c_i$, where of course $\partial u_c/\partial t$ is the time rate of change at fixed $\boldsymbol{c}$. Thus

$$\langle u(t) \mid \boldsymbol{c}\rangle = u_c(t, \boldsymbol{c}), \tag{3.18}$$

is a determined quantity with determined time rate of change

$$\frac{\partial\langle u(t) \mid \boldsymbol{c}\rangle}{\partial t} = \frac{\partial u_c(t, \boldsymbol{c})}{\partial t}. \tag{3.19}$$

By definition, $\langle u(t)|\widehat{\boldsymbol{C}}(t)\rangle$ is

$$\langle u(t) \mid \widehat{\boldsymbol{C}}(t)\rangle = u_c(t, \widehat{\boldsymbol{C}}(t)). \tag{3.20}$$

Note that $\widehat{\boldsymbol{C}}(t)$ evolves deterministically from a random initial condition (by (3.9)), so that $\mathrm{d}\widehat{\boldsymbol{C}}/\mathrm{d}t$ is a determined function of $\widehat{\boldsymbol{C}}(t)$. Thus we obtain

$$\left(\frac{\partial\langle u(t)\mid\widehat{\boldsymbol{C}}(t)\rangle}{\partial t}\right)_{\widehat{\boldsymbol{C}}(t)=\boldsymbol{c}}=\frac{\partial u_c(t,\boldsymbol{c})}{\partial t}+\left(\frac{\mathrm{d}\widehat{C}_i}{\mathrm{d}t}\right)_{\widehat{\boldsymbol{C}}(t)=\boldsymbol{c}}\frac{\partial u_c(t,\boldsymbol{c})}{\partial c_i}$$
$$=\frac{\partial u_c(t,\boldsymbol{c})}{\partial t}+\left\langle\frac{\mathrm{d}C_i}{\mathrm{d}t}\mid\boldsymbol{C}(t)=\boldsymbol{c}\right\rangle\frac{\partial u_c(t,\boldsymbol{c})}{\partial c_i},\qquad(3.21)$$

showing that, given $\widehat{\boldsymbol{C}}(t)$, $\partial\langle u(t)|\widehat{\boldsymbol{C}}(t)\rangle/\partial t$ is a determined quantity, which differs from $\partial u_c/\partial t$ by the final terms in (3.21).

By definition, $\langle u(t)|\boldsymbol{C}(t)\rangle$ is

$$\langle u(t)\mid\boldsymbol{C}(t)\rangle=u_c(t,\boldsymbol{C}(t)).\qquad(3.22)$$

Note that $\boldsymbol{C}(t)$ is random, and the rate of change $\mathrm{d}\boldsymbol{C}(t)/\mathrm{d}t$ is 'not' determined by $\boldsymbol{C}(t)$. Thus, the rate of change

$$\left(\frac{\partial\langle u(t)\mid\boldsymbol{C}(t)\rangle}{\partial t}\right)_{\boldsymbol{C}(t)=\boldsymbol{c}}=\frac{\partial u_c(t,\boldsymbol{c})}{\partial t}+\frac{\mathrm{d}C_i(t)}{\mathrm{d}t}\frac{\partial u_c(t,\boldsymbol{c})}{\partial c_i}\qquad(3.23)$$

is random, even given $\boldsymbol{C}(t)$.

In summary, while we have

$$\langle u(t)\mid\boldsymbol{c}\rangle=\left\langle u(t)\mid\widehat{\boldsymbol{C}}(t)\right\rangle_{\widehat{\boldsymbol{C}}(t)=\boldsymbol{c}}=\langle u(t)\mid\boldsymbol{C}(t)\rangle_{\boldsymbol{C}(t)=\boldsymbol{c}},\qquad(3.24)$$

the rates of change

$$\frac{\partial\langle u(t)\mid\boldsymbol{c}\rangle}{\partial t},\quad\left(\frac{\partial\langle u(t)\mid\widehat{\boldsymbol{C}}(t)\rangle}{\partial t}\right)_{\widehat{\boldsymbol{C}}(t)=\boldsymbol{c}}\text{ and }\quad\left(\frac{\partial\langle u(t)\mid\boldsymbol{C}(t)\rangle}{\partial t}\right)_{\boldsymbol{C}(t)=\boldsymbol{c}}\qquad(3.25)$$

are different: the first two are determined, while the third is random.

In the self-conditioned approach to LES, the velocity field considered is

$$w(t)\equiv\langle u(t)\mid\widehat{\boldsymbol{C}}(t)\rangle.\qquad(3.26)$$

This is more fully described as 'the self-conditioned velocity field, with conditional mean evolution'.

3.6. *Summary*

The self-conditioned field approach for simulating turbulent flows consists of solving a deterministic model equation, (3.15), for the field $\widehat{w}(t)$, which is a model for the self-conditioned velocity field with conditional mean evolution, $w(t)=\langle u(t)|\widehat{\boldsymbol{C}}(t)\rangle$. For the ideal model, the one-time statistics of $\widehat{w}(t)$ are identical to those of the self-conditioned velocity field $\langle u(t)|\boldsymbol{C}(t)\rangle$. For statistically stationary flows, these statistics can be obtained from long time averages. For non-stationary flows, they can be obtained from ensemble averages over simulations with initial conditions drawn from the distribution of $\langle u(0)|\boldsymbol{C}(0)\rangle$.

4. The self-conditioned velocity field

The ideas introduced in the previous section are developed here in a more definite form by invoking the Navier–Stokes equations ((1.1) and (1.2)) governing the velocity field $\boldsymbol{U}(\boldsymbol{x},t)$ in a turbulent flow of a constant-property fluid.

The nth conditioning variable is defined by (1.10) as

$$C_n(t) = \int_{\mathscr{D}} U_i(\boldsymbol{y}, t) K_i^{(n)}(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}, \tag{4.1}$$

where $K_i^{(n)}$ is a specified conditioning kernel and integration is over the flow domain. The self-conditioned velocity field is

$$\boldsymbol{W}(\boldsymbol{x}, t) \equiv \left\langle \boldsymbol{U}(\boldsymbol{x}, t) \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle, \tag{4.2}$$

which is simply written as $\boldsymbol{W} = \langle \boldsymbol{U} | \widehat{\boldsymbol{C}} \rangle$.

The equations governing $\boldsymbol{W}(\boldsymbol{x}, t)$, derived from the Navier–Stokes equations in Appendix B, are described here. First, we discuss some of the properties of $\boldsymbol{W}(\boldsymbol{x}, t)$.

Because the conditioning variables $\boldsymbol{C}(t)$ do not depend upon $\boldsymbol{x}$, it follows that the operations of taking the conditional mean and spatial differentiation commute (as is explicitly confirmed by (B 5)). Mass conservation then yields

$$\frac{\partial W_i}{\partial x_i} = 0. \tag{4.3}$$

Let Q denote any function of the turbulent velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$. The conditional mean of Q, $\langle Q | \widehat{\boldsymbol{C}} \rangle$, can be decomposed as

$$\langle Q \mid \widehat{\boldsymbol{C}} \rangle = Q^W(\widehat{\boldsymbol{C}}) + Q^R(\widehat{\boldsymbol{C}}), \tag{4.4}$$

where $Q^W(\widehat{\boldsymbol{C}})$ denotes the contribution that is known in terms of $\boldsymbol{W}$, and $Q^R(\widehat{\boldsymbol{C}})$ denotes the residual contribution (due to conditional variations of the residual velocity $\boldsymbol{U}'(\boldsymbol{x}, t) \equiv \boldsymbol{U}(\boldsymbol{x}, t) - \langle \boldsymbol{U}(\boldsymbol{x}, t) | \widehat{\boldsymbol{C}} \rangle$). The unconditional mean can be obtained by integrating over the PDF, f_c:

$$\begin{aligned} \langle\langle Q \mid \widehat{\boldsymbol{C}} \rangle\rangle &= \int_{\mathscr{C}} \langle Q \mid \boldsymbol{c} \rangle f_c(\boldsymbol{c})\, \mathrm{d}\boldsymbol{c} \\ &= \langle Q^W(\widehat{\boldsymbol{C}}) \rangle + \langle Q^R(\widehat{\boldsymbol{C}}) \rangle. \end{aligned} \tag{4.5}$$

We consider three informative examples. First, let $Q = Q_0$ be non-random or a deterministic function of $\boldsymbol{c}$, $Q = Q_0(\boldsymbol{c})$. Then

$$\langle Q \mid \boldsymbol{c} \rangle = Q_0(\boldsymbol{c}), \quad Q^W(\boldsymbol{c}) = Q_0(\boldsymbol{c}), \quad Q^R(\boldsymbol{c}) = 0. \tag{4.6}$$

This observation substantiates several of the claims made in the Introduction: in laminar flows $\langle \boldsymbol{U} | \boldsymbol{c} \rangle$ equals $\boldsymbol{U}$, and there are no residual fluctuations, and on a stationary solid wall $\langle \boldsymbol{U}(\boldsymbol{x}^w, t) | \boldsymbol{c} \rangle$ is zero.

Second, we consider the viscous term $Q = \nu \partial^2 U_i / \partial x_j \partial x_j$ in the Navier–Stokes equations. For this we have

$$\left\langle \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} \mid \widehat{\boldsymbol{C}} \right\rangle = \nu \frac{\partial^2 \left\langle U_i \mid \widehat{\boldsymbol{C}} \right\rangle}{\partial x_j \partial x_j} = \nu \frac{\partial^2 W_i}{\partial x_j \partial x_j}, \tag{4.7}$$

so, again, there is no residual contribution. This result applies to all linear operations on $\boldsymbol{U}$ (at fixed time).

Third, we consider the two-point velocity product $Q = U_i(\boldsymbol{x}, t) U_j(\boldsymbol{y}, t)$. In this case, we have

$$\left\langle U_i(\boldsymbol{x}, t) U_j(\boldsymbol{y}, t) \mid \widehat{\boldsymbol{C}} \right\rangle = W_i(\boldsymbol{x}, t) W_j(\boldsymbol{y}, t) + \mathrm{cov}(U_i(\boldsymbol{x}, t), U_j(\boldsymbol{y}, t) \mid \widehat{\boldsymbol{C}}), \tag{4.8}$$

where for any two quantities P and Q, the 'conditional covariance' is defined by

$$\mathrm{cov}(P, Q \mid \boldsymbol{c}) \equiv \langle PQ \mid \boldsymbol{c}\rangle - \langle P \mid \boldsymbol{c}\rangle \langle Q \mid \boldsymbol{c}\rangle . \tag{4.9}$$

On the right-hand side of (4.8), the first term corresponds to Q^W and the second term corresponds to Q^R.

The momentum equation for $\boldsymbol{W}(\boldsymbol{x}, t)$, derived from the Navier–Stokes equations in Appendix B ((B 12)–(B 17)), can be written as

$$\left(\frac{\partial}{\partial t} + W_j \frac{\partial}{\partial x_j}\right) W_i = \nu \frac{\partial^2 W_i}{\partial x_j \partial x_j} - \frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tau_{ij}^R}{\partial x_j} + R_i, \tag{4.10}$$

where $\tilde{p}$ is the conditional pressure $\langle p|\widehat{\boldsymbol{C}}\rangle$, which can be determined from a Poisson equation in the usual way; τ_{ij}^R is the residual stress, defined by

$$\tau_{ij}^R = -\mathrm{cov}(U_i, U_j \mid \widehat{\boldsymbol{C}}); \tag{4.11}$$

and the term $\boldsymbol{R}$, identified and discussed more fully in Appendix B, represents a transfer of momentum in conditioning space.

In order to use (4.3) and (4.10) in a simulation, it is necessary to model the unknown quantities τ_{ij}^R and $\boldsymbol{R}$. A discussion of modelling in deferred to § 6.1, save to say:

(i) In a model, there is every reason to take $\boldsymbol{R}$ to be zero (see (B 17) for further discussion).

(ii) Standard models and approaches (e.g. the dynamic Smagorinsky model) can be applied.

(iii) A difference, compared to the filtering approach, is the behaviour imposed on τ_{ij}^R is limiting cases such as laminar flow and the DNS limit.

5. The self-conditioned composition PDF

We now extend the discussion to consider a single composition variable $\phi(\boldsymbol{x}, t)$ governed by the conservation equation

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \Gamma \nabla^2 \phi + S(\phi), \tag{5.1}$$

where Γ is the constant molecular diffusivity, and S is the chemical source term, which is a known function of ϕ. This suffices to develop the concepts involved in the self-conditioned PDF. (It is straightforward to extend the concepts and equations to the more general case of a set of compositions with different diffusivities in a variable-density flow.)

The conditioning variables $\boldsymbol{C}(t)$ are extended to include variables of the form

$$C_m(t) = \int_{\mathscr{D}} L^{(m)}(\phi(\boldsymbol{x}, t)) K_\phi^{(m)}(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}, \tag{5.2}$$

where $L^{(m)}(\phi)$ is any specified function of ϕ, and $K_\phi^{(m)}(\boldsymbol{x})$ is a specified conditioning kernel. Thus $C_m(t)$ can include filtered values of nonlinear functions of ϕ.

The quantities considered in the simulation are $\boldsymbol{W}(\boldsymbol{x}, t)$, the self-conditioned velocity field (as previously), and $g(\psi; \boldsymbol{x}, t)$, the (one-point, one-time) self-conditioned PDF of $\phi(\boldsymbol{x}, t)$. Let $f_{\phi|c}(\psi|\boldsymbol{c}; \boldsymbol{x}, t)$ denote the PDF of $\phi(\boldsymbol{x}, t)$ conditional on $\boldsymbol{C}(t) = \boldsymbol{c}$. Then $g(\psi; \boldsymbol{x}, t)$ is defined by

$$g(\psi; \boldsymbol{x}, t) = f_{\phi|c}(\psi \mid \widehat{\boldsymbol{C}}(t); \boldsymbol{x}, t). \tag{5.3}$$

It is verified in Appendix C that $\boldsymbol{W}(\boldsymbol{x}, t)$ and $g(\psi; \boldsymbol{x}, t)$ are self-conditioned, that is, given $\boldsymbol{W}$ and g, conditioning variables of the form of (4.1) and (5.2) can be evaluated.

It follows from its definition that g is a PDF, and hence has the properties

$$g(\psi; \boldsymbol{x}, t) \geqslant 0, \tag{5.4}$$

$$\int_{\psi_-}^{\psi_+} g(\psi; \boldsymbol{x}, t)\, \mathrm{d}\psi = 1, \tag{5.5}$$

$$g(\psi; \boldsymbol{x}, t) = 0 \quad \text{for} \quad \psi < \psi_- \quad \text{and} \quad \psi > \psi_+, \tag{5.6}$$

where ψ_- and ψ_+ are the lower and upper bounds on ϕ. The conditional mean and variance are

$$\widetilde{\phi}(\boldsymbol{x}, t) \equiv \langle \phi(\boldsymbol{x}, t) \mid \widehat{\boldsymbol{C}}(t) \rangle = \int_{\psi_-}^{\psi_+} \psi g(\psi; \boldsymbol{x}, t)\, \mathrm{d}\psi, \tag{5.7}$$

and

$$\begin{aligned} \widetilde{\phi''^2}(\boldsymbol{x}, t) &\equiv \operatorname{cov}\left(\phi(\boldsymbol{x}, t), \phi(\boldsymbol{x}, t) \mid \widehat{\boldsymbol{C}}(t)\right) \\ &= \int_{\psi_-}^{\psi_+} \left(\psi - \widetilde{\phi}(\boldsymbol{x}, t)\right)^2 g(\psi; \boldsymbol{x}, t)\, \mathrm{d}\psi. \end{aligned} \tag{5.8}$$

Very importantly, for a laminar flow we have

$$\widetilde{\phi}(\boldsymbol{x}, t) \equiv \langle \phi \mid \widehat{\boldsymbol{C}} \rangle = \phi, \tag{5.9}$$

$$\widetilde{\phi''^2} = 0, \tag{5.10}$$

$$g(\psi; \boldsymbol{x}, t) = \delta\left(\widetilde{\phi}(\boldsymbol{x}, t) - \psi\right). \tag{5.11}$$

These results ((5.9)–(5.11)) are in contrast to those for the filter density function, for which the variance is of order Δ^2.

To expand on this observation, figure 3 shows a profile $\phi(x)$ corresponding to a thin, laminar diffusive layer. As may be seen, the filtered profile $\overline{\phi}(x)$ is much broader, and the second moment of the FDF $\overline{\phi^2} - \overline{\phi}^2$ is large (over 80 % of its maximum possible value of 1/4). Both of these undesirable characteristics are due to spatial smearing, which is completely avoided in the self-conditioned approach (viz. (5.9)–(5.11)).

The evolution equation for the self-conditioned PDF is derived in Appendix C (C 10). It is of standard form, except for a source term R_ϕ (analogous to $\boldsymbol{R}$), which represents a flux in the conditioning space. The simplest closed model equation is given as (C 11).

6. Discussion

6.1. *Modelling*

We consider the modelling of the residual stress τ_{ij}^R appearing in the momentum equation for the self-conditioned velocity and compare it to the analogous task in the filtering approach. Similar considerations apply to the modelling in the self-conditioned PDF equation.

The momentum equation for the self-conditioned velocity, (4.10), is of the standard LES form (once the term $\boldsymbol{R}$ is neglected). The conditioning variables do not appear explicitly in the momentum equation, (4.10): they enter through the definition of the residual stress, τ_{ij}^R, (4.11). (The same is true of the filter in the filtering approach.)

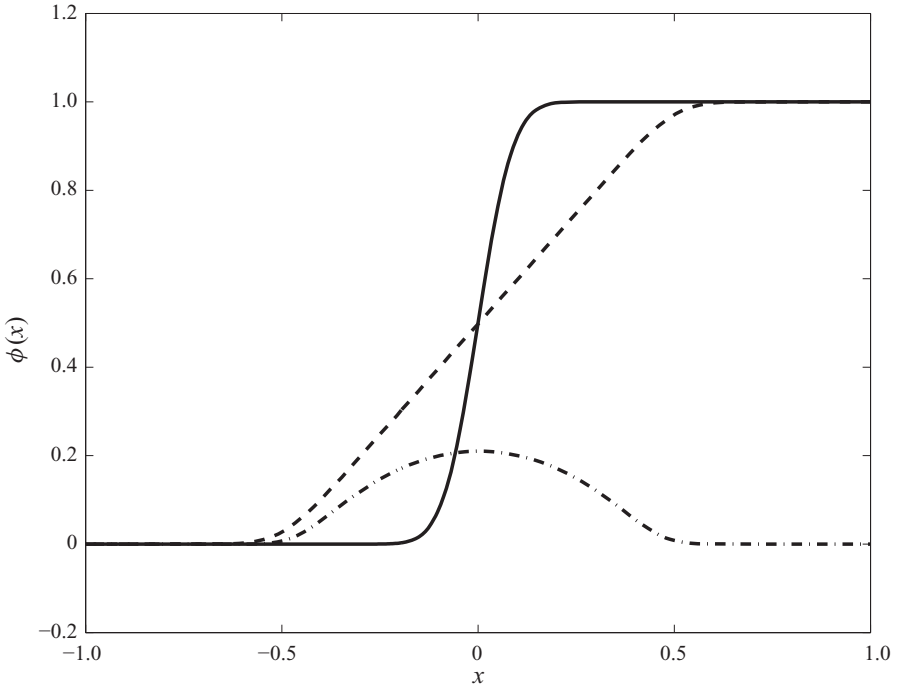

FIGURE 3. Scalar profile $\phi(x)$ (solid line) in a thin, laminar diffusive layer; the corresponding filtered profile $\overline{\phi}(x)$ (dashed line); and the second moment of the FDF $\overline{\phi^2} - \overline{\phi}^2$ (dot-dashed line). The unit top-hat filter is used.

The difference between the momentum equations used in DNS, Reynolds-averaged Navier–Stokes (RANS) and LES is solely in the way the effective stress $\widetilde{\tau}_{ij}$ is related to the velocity field being considered. Obviously, how the stress is modelled is crucial to the success of the method.

We consider now, in general terms, the approaches used to develop and test LES models for the residual stress, and how these can be used with the self-conditioned approach, in contrast to the filtering approach. The approaches include:

(i) The derivation of exact (unclosed) evolution equations and the identification of conservation and invariance properties.

(ii) The determination of the behaviour of the stress $\widetilde{\tau}_{ij}$ in limiting cases, especially for laminar flow, the DNS limit and the RANS limit.

(iii) *A posteriori* testing in which statistical results from a simulation are compared with measurements (or DNS).

(iv) *A priori* testing in which modelled and measured values of $\widetilde{\tau}_{ij}$ are compared.

(v) A spectral analysis in which properties of the stress and its model are deduced from a model turbulence spectrum (e.g. Lilly 1967).

(vi) Dynamic procedures based on scale invariance (Germano *et al.* 1991) or deduced scale dependence (Meneveau, Lund & Cabot 1996).

(vii) Deconvolution techniques, which provide estimates of part of the residual motions, based on the resolved velocity field.

With respect to (i), the evolution equation for the self-conditioned fields have been derived. The term in $\boldsymbol{R}$ in (4.10) indicates that the momentum of the velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ may not be exactly conserved, although it is in the mean. In a model, given the

current state of knowledge, there is every reason to take $\boldsymbol{R}$ to be zero. Nevertheless, a possible model is mentioned in Appendix B (B 19). Apart from the term in $\boldsymbol{R}$, the self-conditioning approach appears advantageous in that the mass conservation equation is more straightforward, with $\nabla \cdot \boldsymbol{W}(\boldsymbol{x}, t) = 0$ for incompressible flows. It may also be observed that the stress τ_{ij}^R is Galilean invariant and contains no cross terms.

As already discussed, the self-conditioned approach is advantageous with respect to (ii). In particular, in laminar flow $\boldsymbol{W}$ equals $\boldsymbol{U}$ (i.e. the residual velocity is zero), and in the DNS limit the residual velocity is exponentially small. In contrast, $\overline{\boldsymbol{U}}$ differs from $\boldsymbol{U}$ in a way that depends on the specification of the filter, with the residual velocity scaling as Δ^2.

A posteriori testing is the ultimate test of any LES model, and its application is similar for the self-conditioned and filtering approaches. Note, however, that in the self-conditioned approach, the unconditional mean $\langle \boldsymbol{W}(\boldsymbol{x}, t) \rangle$ models $\langle \boldsymbol{U}(\boldsymbol{x}, t) \rangle$, independent of the conditioning variables, whereas in the filtering approach, $\langle \boldsymbol{W}(\boldsymbol{x}, t) \rangle$ depends on the filter. Also, with the self-conditioned approach, it is possible to perform *a posteriori* testing of conditioned quantities, e.g. $\langle \boldsymbol{W}(\boldsymbol{x}, t) \mid C_1 = c_1 \rangle$ compared to $\langle \boldsymbol{U}(\boldsymbol{x}, t) \mid C_1 = c_1 \rangle$ for a single condition such as the filtered velocity at a point (or for a small number of conditions). As demonstrated by Wang, Tong & Pope (2004), it is feasible to extract such conditional statistics from experiments, as it is from DNS.

An apparent disadvantage of the self-conditioning approach is that in practice it is extremely difficult, if not impossible, to measure or even explicitly represent quantities conditioned on many variables. This represents an obstacle to *a priori* testing. It should be appreciated, however, that *a priori* testing of filtered models on a realization-by-realization basis is dubious at best, and appropriate testing requires significant conditioning (Pope 2000).

Spectral analysis, dynamic procedures and deconvolution techniques are most likely applicable to the self-conditioned approach, but the underlying theories have yet to be developed.

The pragmatic approach to the initial modelling of the self-conditioned equations is to use existing LES models that have proved successful in *a posteriori* tests, modified as necessary to conform to DNS and other limits. The filter width $\Delta(\boldsymbol{x})$ appearing in such models is interpreted as the characteristic width of the kernel used to define the conditioning variables (4.1).

6.2. *Spatial resolution*

In the numerical solution of the LES equations for the filtered velocity, $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$, the usual practice is to specify the filter width $\Delta(\boldsymbol{x})$ to be proportional to the local numerical mesh spacing, denoted by $h(\boldsymbol{x})$, for example, $\Delta(\boldsymbol{x}) = 2h(\boldsymbol{x})$. The spatial filtering attenuates scales smaller than Δ, so that the resulting filtered fields can indeed be resolved (to a level deemed acceptable) on a mesh of spacing h. A 'good' LES model for the residual stress ensures that the 'modelled' filtered velocity field has the same resolution requirements.

For the self-conditioned velocity field the picture is different. Consider, for example, the turbulent mixing layer that develops behind a splitter plate on which there are laminar boundary layers of characteristic thickness δ_L. Some distance downstream, the characteristic thickness of the turbulent mixing layer, δ_T, may be very large compared to δ_L, and the conditioning variables $\boldsymbol{C}(t)$ may be defined based on kernels of width $\Delta \approx (1/10)\delta_T$, say, which may be large compared to δ_L. Regardless of how the conditioning variables are defined, in a region of steady laminar flow, we have

$$\langle \boldsymbol{U} \mid \boldsymbol{c} \rangle = \boldsymbol{U}. \tag{6.1}$$

Thus, the self-conditioned velocity field varies on scales as small as δ_L, and hence requires spatial resolution of this order. In other words, as this example illustrates, the spatial resolution h needed to resolve the self-conditioned fields can be small compared to the length scale Δ associated with the conditioning variables.

Is this good or bad?

The answer is a matter of viewpoint. From the viewpoint that an LES should consider only 'large eddies', and that the LES velocity field should be resolvable on a specified grid, then this behaviour of $\langle \boldsymbol{U}|\boldsymbol{c}\rangle$ is undesirable. We, however, take the different viewpoint that there is merit in a reduced-order model representing the dynamically most important processes, regardless of scale. For fully developed turbulent free shear flows, the dynamically most important motions are indeed the large eddies. However, it is well appreciated that even the gross features of turbulent flows can be strongly influenced by the details of fine-scale features connected to the initiation of the flow and the turbulence – such as the states of the boundary layers on the splitter plate for the mixing layer.

As a second example, in turbulent jet flames, immediately downstream of the jet exit, there is a very thin diffusive mixing layer (possibly reacting) between the fuel in the jet and the air in the co-flow, which, depending on the conditions, may resemble a mildly wrinkled laminar mixing layer. The details of this fine-scale mixing process are likely to have a significant influence on the downstream development of the flame. There is merit, therefore, in representing and resolving these fine-scale processes, as is done by the self-conditioned composition PDF (but not by the FDF) even for Δ large compared to the diffusive-layer thickness.

The fact that self-conditioned fields may have smaller length scales than the specified kernel width, Δ, means that the appropriate resolution is not known *a priori*. Consequently, adaptive mesh refinement (or a similar methodology) is required, or at least a methodology to assess the adequacy of a specified mesh.

For the case of the thin viscous or diffusive layers in the two examples discussed above, fine resolution is needed only in the gradient direction. Consequently, the number of mesh points required is essentially independent of Reynolds number.

6.3. *Near-wall behaviour*

To examine the self-conditioned velocity field for wall-bounded turbulent flows, we consider again a fully developed channel flow (as in § 3).

For LES based on filtering applied to near-wall flows, Pope (2000) distinguishes between LES–NWR (with near-wall resolution) and LES–NWM (with near-wall modelling). In LES–NWR, the filter width Δ at the wall is of order the viscous length scale δ_ν, and it increases no more than linearly with the wall-normal distance y, so that the principal three-dimensional unsteady near-wall structures (which scale with δ_ν) are resolved (to some extent). An LES based on the self-conditioned velocity with conditioning variables having the same specification of $\Delta(y)$ is likely to be essentially the same (although issues related to filtering at the wall are avoided). In LES–NWR, with either filtering or self-conditioning approaches, the computational cost increases as a power of Reynolds number, and hence the method is infeasible at high Reynolds number.

In the alternative LES–NWM, which is applicable at high Reynolds number, the filter width Δ scales with the mean flow length scale (e.g. channel width or boundary-layer thickness), and hence Δ/δ_ν is large and increases with Reynolds number. In this case the behaviour of the filtered and self-conditioned velocity fields is different. For example, $\langle \boldsymbol{U}|\boldsymbol{c}\rangle$ includes the steep variation in the wall-normal (y) direction of the

velocity U_1 in the mean-flow (x) direction. Hence, close to the wall, a mesh spacing in y of order δ_v is required to resolve $\langle U_1|\boldsymbol{c}\rangle$.

A crucial question is the resolution requirement in the tangent plane (x–z) of the wall, and this may depend on the specification of the conditioning variables. If the required resolution in the tangent plane scales with Δ, then the computational cost scales as the logarithm of Reynolds number, so that the method is applicable at high Reynolds number.

To a large extent, this application of self-conditioned LES is similar to a hybrid LES/RANS method. Far from the wall it is dominantly LES, with the bulk of the turbulent kinetic energy and shear stress being in the three-dimensional, unsteady, resolved motions. However, as the wall is approached, the bulk of the stress is modelled (as τ_{12}^R) or is viscous ($\nu\partial\langle U_1|\boldsymbol{c}\rangle/\partial y$), and the unsteadiness and three-dimensionality are strongly attenuated.

6.4. *Spectral filtering*

We have primarily considered spatial filtering and the self-conditioned field approach based on positive conditioning kernels. In this subsection, we make some observations on spectral filtering.

With a spectral filter (or with any other filter for which the filter function G contains negative portions), the filtered species mass fractions $\phi(\boldsymbol{x},t)$ can be negative, as can the filter density function. In contrast, the self-conditioned species $\tilde{\phi}(\boldsymbol{x},t)\equiv\langle\phi(\boldsymbol{x},t)|\widehat{\boldsymbol{C}}(t)\rangle$ is non-negative, because it is the mean of non-negative fields. Similarly, the self-conditioned PDF is non-negative, irrespective of the conditioning variables.

Following Fox (2003), we can consider homogeneous turbulence and represent the velocity field $\boldsymbol{U}(\boldsymbol{x},t)$ as the infinite sum of Fourier modes with coefficients denoted by $\widehat{\boldsymbol{U}}(\boldsymbol{\kappa},t)$. With the sharp spectral filter with cutoff wavenumber κ_c, the Fourier modes of the filtered field $\overline{\boldsymbol{U}}(\boldsymbol{x},t)$ are $\widehat{\boldsymbol{U}}(\boldsymbol{\kappa},t)H(\kappa_c-|\boldsymbol{\kappa}|)$, where H is the Heaviside function. With the self-conditioned field approach, the Fourier coefficients of the residual velocity field are

$$\langle\widehat{\boldsymbol{U}}(\boldsymbol{\kappa},t)H(|\boldsymbol{\kappa}|-\kappa_c)\mid\boldsymbol{C}(t)\rangle, \tag{6.2}$$

where $\boldsymbol{C}(t)$ consists of all of the Fourier coefficients with $|\boldsymbol{\kappa}|<\kappa_c$. It may be observed that the residual field is zero:

(i) if the Fourier modes above the cutoff are statistically independent of those below the cutoff, or

(ii) if the field is Gaussian, or

(iii) according to the linear mean-square approximation.

The last two results stem from the fact that different Fourier modes are uncorrelated.

Since turbulent velocity fields are not Gaussian, it appears that the residual velocity field is not exactly zero (as suggested by Fox 2003). But it may be relatively small, since it arises solely because of nonlinear, non-Gaussian effects.

6.5. *The choice of conditioning variables*

The optimal choice of conditioning variables is discussed in Appendix D, and three possible definitions of 'optimal' are considered. These are based on a decomposition of the velocity field (D 11) and the associated kinetic energies (D 13).

The first possibility is, for a given value of n_c, to choose the conditioning kernels to minimize the residual kinetic energy k' (D 14). Roughly, this has the benefits of maximizing the resolved energy, minimizing the modelling required and minimizing the value of n_c required to achieve the DNS limit.

The second possibility is to employ 'eigen-conditioning' such that the self-conditioned velocity field $\langle \boldsymbol{U} \mid \boldsymbol{C} \rangle$ is in the n_c-dimensional subspace $\widetilde{\mathscr{H}}$ defined by the conditioning kernels. The benefit is that $\langle \boldsymbol{U} \mid \boldsymbol{C} \rangle$ is of the smallest possible dimension (i.e. n_c). Whether such eigen-conditioning exists is an open question.

The third possibility is to maximize the energy $\widetilde{k}$ associated with the component of the self-conditioned velocity in the subspace $\widetilde{\mathscr{H}}$. This is achieved by choosing the conditioning kernels such that $\widetilde{\mathscr{H}}$ is the subspace spanned by the first n_c proper orthogonal decomposition (POD) modes.

6.6. *Extensions*

We have described two specific methods based on the self-conditioned velocity, $\langle \boldsymbol{U} | \widehat{\boldsymbol{C}} \rangle$, and the self-conditioned composition PDF, $g(\psi; \boldsymbol{x}, t)$. As with other LES approaches, other fields can be considered, including the residual kinetic energy, the residual stress tensor, the PDF of velocity, and the joint PDF of velocity and a set of composition variables.

Furthermore, different types of conditioning variables can be considered, based on the different quantities mentioned (velocity, energy, PDFs), with a different spatial structure (which enters through the kernels $K_i^{(n)}(\boldsymbol{x})$ in (4.1)). These kernels can be based on filtering, wavelets, Fourier modes, POD modes, and other orthogonal and non-orthogonal basis functions. However, this conditioning information enters solely into the modelling, and current models typically admit only a simple specified length scale $\Delta(\boldsymbol{x})$.

7. Conclusions

An alternative basis for large-eddy simulation has been developed based on self-conditioned fields. In the simplest case, the n_c conditioning variables, $\boldsymbol{C}(t)$, provide an approximate representation of the filtered velocity field $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$. The reduced description of the flow is provided not by $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$ but by $\langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{c} \rangle$, which is the mean velocity field conditioned on $\boldsymbol{C}(t) = \boldsymbol{c}$. This field is said to be self-conditioning, because the value of the conditioning variables can be deduced from the field itself.

The velocity field considered in the LES is

$$\boldsymbol{W}(\boldsymbol{x}, t) \equiv \left\langle \boldsymbol{U}(\boldsymbol{x}, t) \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle, \tag{7.1}$$

where $\widehat{\boldsymbol{C}}(t)$ is defined to evolve by

$$\frac{\mathrm{d}\widehat{\boldsymbol{C}}(t)}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}\boldsymbol{C}(t)}{\mathrm{d}t} \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle. \tag{7.2}$$

The field $\boldsymbol{W}(\boldsymbol{x}, t)$ evolves deterministically from random initial conditions. A fundamental result justifying the approach is that the one-time distribution of $\boldsymbol{W}(\boldsymbol{x}, t)$ and $\widehat{\boldsymbol{C}}(t)$ is identical to that of $\langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{C}(t) \rangle$ and $\boldsymbol{C}(t)$. An exact (unclosed) evolution equation for $\boldsymbol{W}(\boldsymbol{x}, t)$, (B 12), is deduced from the Navier–Stokes equations.

The approach is extended to composition fields, relevant to turbulent reactive flows, by considering the self-conditioned PDF of composition $g(\psi; \boldsymbol{x}, t)$, for which an exact evolution equation is derived (C 10). Further extensions are discussed in § 6.6.

Some characteristics of the self-conditioned field approach, which distinguish it from the filtering approach, are the following:

(i) For laminar flow, $\boldsymbol{W}(\boldsymbol{x}, t)$ is identical to $\boldsymbol{U}(\boldsymbol{x}, t)$: there are no residual fluctuations.

(ii) In the DNS limit, the residual velocity field is exponentially small.

(iii) Full account is taken of the probability distribution of turbulent velocity fields.

(iv) The means (over initial conditions) of $\boldsymbol{W}(\boldsymbol{x}, t)$ and $g(\psi; \boldsymbol{x}, t)$ are the (Reynolds) mean velocity, $\langle \boldsymbol{U}(\boldsymbol{x}, t) \rangle$, and the (unconditional) composition PDF (not their filtered counterparts).

(v) The operations of spatial differentiation and taking the conditional mean commute, so that $\boldsymbol{W}(\boldsymbol{x}, t)$ is divergence free in incompressible flow.

(vi) Repeated application of the conditional mean has no effect, and hence conditional variances (and the residual stress) contain no'cross terms'.

(vii) At points $\boldsymbol{x}^w$ on a stationary solid wall, $\boldsymbol{W}(\boldsymbol{x}, t)$ satisfies the no-slip and impermeability conditions $\boldsymbol{W}(\boldsymbol{x}^w, t) = 0$.

(viii) Laminar boundary layers (and other non-random fine structures) are resolved by the self-conditioned fields, even if the length scale $\Delta(\boldsymbol{x})$ associated with the conditioning variables is much larger. Hence, for the accurate numerical solution of the equations for self-conditioned fields, the mesh spacing $h(\boldsymbol{x})$ may need to be smaller than $\Delta(\boldsymbol{x})$ (locally, and in the gradient direction).

As in most approaches to LES, the modelling of the residual terms is crucial. The general issues related to modelling are discussed in § 6.1. As a starting point, existing models can be used, with modifications as necessary to conform to the DNS limit.

The residual stress τ_{ij}^R is strongly dependent on the choice of conditioning variables $\boldsymbol{C}(t)$. Two opportunities for future research are to make this dependence more explicit, so that models for τ_{ij}^R can incorporate directly information about the conditioning variables, and to develop tractable methodologies for determining near-optimal conditioning variables.

For discussions on this work and for comments on a draft of this paper, I am grateful to Rodney Fox, John Guckenheimer, Konstantin Kemenov, Alex Klimenko, Robert Moser, Heinz Pitsch, Pavel Popov, Dale Pullin and Alex Vladimirsky. This work is supported by the Air Force Office of Scientific Research under grant FA-9550-09-1-0047.

Appendix A. Conditioned Gaussian process

To provide illustrative examples of conditioned random processes, we describe here a simple, one-dimensional, Gaussian process. The results obtained are used to generate the processes shown in figures 1 and 2.

We consider a periodic Gaussian random process $U(x)$ in the interval [0, 1], which is completely characterized by its mean $\widetilde{U}(x)$ and autocovariance $R(x, y) \equiv \langle U'(x)U'(y) \rangle$, where $U'(x) \equiv U(x) - \widetilde{U}(x)$ is the fluctuation. It is simplest to consider a finite representation of the process, so we consider a fine, uniform grid in x, consisting of m grid points $x_1, x_2, \ldots, x_m$, and we represent the process by

$$\boldsymbol{u} = \widetilde{\boldsymbol{u}} + \boldsymbol{u}', \tag{A 1}$$

where $\boldsymbol{u}$ is the m-vector of the values of $U(x)$ sampled at the grid points (i.e. $u_i = U(x_i)$), and similarly the m-vectors $\widetilde{\boldsymbol{u}}$ and $\boldsymbol{u}'$ are the values of $\widetilde{U}$ and U' on the grid.

Since $U(x)$ is a Gaussian process, both $\boldsymbol{u}$ and $\boldsymbol{u}'$ are Gaussian random vectors, and we can express $\boldsymbol{u}'$ as

$$\boldsymbol{u}' = \boldsymbol{V}^{1/2}\boldsymbol{\xi}, \tag{A 2}$$

where $\boldsymbol{V}$ is the covariance matrix $V_{ij} = R(x_i, x_j)$, and $\boldsymbol{\xi}$ is an m-vector of independent standardized Gaussians ($\langle \xi_i \rangle = 0$, $\langle \xi_i \xi_j \rangle = \delta_{ij}$). It is convenient to work in terms of $\boldsymbol{u}'$ (since it has zero mean) and then $\boldsymbol{u}$ is readily recovered from (A 1).

The n_c conditioning variables $\boldsymbol{C}$ are defined by

$$\boldsymbol{C} = \boldsymbol{K}\boldsymbol{u}', \tag{A 3}$$

where $\boldsymbol{K}$ is a specified, full-rank $n_c \times m$ matrix. If C_i represents a filtered value of the process, then the ith row of $\boldsymbol{K}$ contains the corresponding quadrature weights at the grid points.

With $\boldsymbol{c}$ being a specified n_c-vector, the conditioned process considered is $(\boldsymbol{u}' \mid \boldsymbol{C} = \boldsymbol{c})$. Since this process is also Gaussian, it depends linearly on $\boldsymbol{c}$ and can be written as

$$(\boldsymbol{u}' \mid \boldsymbol{C} = \boldsymbol{c}) = \boldsymbol{M}\boldsymbol{c} + \boldsymbol{D}^{1/2}\boldsymbol{\eta}, \tag{A 4}$$

where $\boldsymbol{M}$ is an $m \times n_c$ matrix, $\boldsymbol{D}$ is the positive semi-definite $m \times m$ conditional covariance matrix, and $\boldsymbol{\eta}$ is an m-vector of independent standardized Gaussians (which is independent of $\boldsymbol{\xi}$). The matrices $\boldsymbol{M}$ and $\boldsymbol{D}$ are determined below. Thus, (A 4) can be used to generate random samples of the conditioned Gaussian process, and the conditional mean of the process is

$$\langle \boldsymbol{u} \mid \boldsymbol{C} = \boldsymbol{c} \rangle = \widetilde{\boldsymbol{u}} + \boldsymbol{M}\boldsymbol{c}. \tag{A 5}$$

The matrices $\boldsymbol{M}$ and $\boldsymbol{D}$ are uniquely determined by equating the expressions for $\langle \boldsymbol{u}'\boldsymbol{c}^{\mathrm{T}} \rangle$ and $\langle \boldsymbol{u}'\boldsymbol{u}'^{\mathrm{T}} \rangle$ obtained from (A 2) and (A 4). From (A 2) and (A 3) we obtain

$$\langle \boldsymbol{u}'\boldsymbol{C}^{\mathrm{T}} \rangle = \boldsymbol{V}\boldsymbol{K}^{\mathrm{T}}, \tag{A 6}$$

while from (A 4) we obtain

$$\langle \boldsymbol{u}'\boldsymbol{C}^{\mathrm{T}} \rangle = \langle (\boldsymbol{u}' \mid \boldsymbol{C})\boldsymbol{C}^{\mathrm{T}} \rangle = \boldsymbol{M}\boldsymbol{K}\boldsymbol{V}\boldsymbol{K}^{\mathrm{T}}. \tag{A 7}$$

Thus, equating the right-hand sides of these two equations, we obtain

$$\boldsymbol{M} = \boldsymbol{V}\boldsymbol{K}^{\mathrm{T}}(\boldsymbol{K}\boldsymbol{V}\boldsymbol{K}^{\mathrm{T}})^{-1}. \tag{A 8}$$

Similarly, we have

$$\langle \boldsymbol{u}'\boldsymbol{u}'^{\mathrm{T}} \rangle = \boldsymbol{V} = \boldsymbol{M}\boldsymbol{K}\boldsymbol{V}\boldsymbol{K}^{\mathrm{T}}\boldsymbol{M}^{\mathrm{T}} + \boldsymbol{D}, \tag{A 9}$$

where the latter two parts stem from (A 2) and (A 4), respectively. Hence $\boldsymbol{D}$, is determined as

$$\boldsymbol{D} = \boldsymbol{V} - \boldsymbol{M}\boldsymbol{K}\boldsymbol{V}\boldsymbol{K}^{\mathrm{T}}\boldsymbol{M}^{\mathrm{T}}. \tag{A 10}$$

The particular case shown in figures 1 and 2 has the following specifications:

$$\widetilde{U}(x) = \tfrac{1}{2}\sin(2\pi x), \tag{A 11}$$

$$\sigma(x) \equiv R(x, x)^{1/2} = \tfrac{1}{2}[1 + \sin(2\pi x)], \tag{A 12}$$

$$R(x, y) = \sigma(x)\sigma(y)\exp(-[20(x - y)]^2), \tag{A 13}$$

and with $\boldsymbol{K}$ corresponding to top-hat filters of width 1/5 at $n_c = 5$ equally spaced locations.

Appendix B. Derivation of the self-conditioned momentum equation

The equation governing the evolution of the self-conditioned velocity field $\langle \boldsymbol{U}(\boldsymbol{x},t)|\boldsymbol{C}(t)=\boldsymbol{c}\rangle$ and

$$\boldsymbol{W}(\boldsymbol{x},t) \equiv \left\langle \boldsymbol{U}(\boldsymbol{x},t) \mid \boldsymbol{C}(t) = \widehat{\boldsymbol{C}}(t) \right\rangle, \tag{B 1}$$

are derived, using the delta-function technique from PDF methods (see e.g. Appendix H of Pope 2000).

The PDF of the conditioning variables $\boldsymbol{C}(t)$ can be expressed as

$$f_c(\boldsymbol{c};t) = \langle \delta(\boldsymbol{C}(t)-\boldsymbol{c}) \rangle . \tag{B 2}$$

For any quantity $Q(\boldsymbol{x},t)$, its conditional mean $\langle Q|\boldsymbol{c}\rangle$ is given by

$$f_c(\boldsymbol{c};t)\,\langle Q(\boldsymbol{x},t) \mid \boldsymbol{C}(t)=\boldsymbol{c}\rangle = \langle Q(\boldsymbol{x},t)\,\delta(\boldsymbol{C}(t)-\boldsymbol{c})\rangle . \tag{B 3}$$

Since $\boldsymbol{C}(t)$ and $f_c(\boldsymbol{c};t)$ have no dependence on $\boldsymbol{x}$, differentiation of (B 3) with respect to x_i yields

$$f_c \frac{\partial}{\partial x_i}\langle Q \mid \boldsymbol{c}\rangle = \left\langle \frac{\partial Q}{\partial x_i}\,\delta(\boldsymbol{C}-\boldsymbol{c}) \right\rangle, \tag{B 4}$$

and hence

$$\frac{\partial}{\partial x_i}\langle Q \mid \boldsymbol{c}\rangle = \left\langle \frac{\partial Q}{\partial x_i} \mid \boldsymbol{c} \right\rangle . \tag{B 5}$$

Thus, the operations of spatial differentiation and taking the condition mean commute. Applying this result to the continuity equation (1.1) yields

$$\frac{\partial}{\partial x_i}\langle U_i \mid \boldsymbol{c}\rangle = 0. \tag{B 6}$$

A result needed in the sequel is that repeated conditioning has no effect, i.e.

$$\langle\langle Q \mid \boldsymbol{C}=\boldsymbol{c}\rangle \mid \boldsymbol{C}=\boldsymbol{c}'\rangle = \langle Q \mid \boldsymbol{C}=\boldsymbol{c}\rangle. \tag{B 7}$$

This follows simply because $\langle Q|\boldsymbol{C}=\boldsymbol{c}\rangle$ is non-random.

For any two quantities P and Q, the conditional covariance is defined as

$$\begin{aligned}\operatorname{cov}\left(P, Q \mid \boldsymbol{c}\right) &= \langle PQ \mid \boldsymbol{c}\rangle - \langle P \mid \boldsymbol{c}\rangle\langle Q \mid \boldsymbol{c}\rangle \\ &= \left\langle \left(P - \langle P \mid \boldsymbol{c}\rangle\right)\left(Q - \langle Q \mid \boldsymbol{c}\rangle\right) \mid \boldsymbol{c} \right\rangle,\end{aligned} \tag{B 8}$$

where the last line follows from (B 7). Thus, in contrast with the case for filtering, repeated conditioning has no effect, and there are no 'cross terms' in the conditional covariance.

Since $\boldsymbol{C}(t)$ and $f_c(\boldsymbol{c};t)$ depend on t, taking the temporal derivative of (B 3) is more involved, and yields

$$\frac{\partial}{\partial t}\left[f_c\,\langle Q \mid \boldsymbol{c}\rangle\right] = f_c\left\langle \frac{\partial Q}{\partial t} \mid \boldsymbol{c} \right\rangle - \frac{\partial}{\partial c_i}\left[f_c\left\langle Q\frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c}\right\rangle\right], \tag{B 9}$$

which, for $Q=1$, yields the Liouville equation

$$\frac{\partial f_c}{\partial t} + \frac{\partial}{\partial c_i}\left[f_c\left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c}\right\rangle\right] = 0. \tag{B 10}$$

From the above two equations, we obtain

$$\left(\frac{\partial}{\partial t} + \left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c}\right\rangle \frac{\partial}{\partial c_i}\right)\langle Q \mid \boldsymbol{c}\rangle = \left\langle \frac{\partial Q}{\partial t} \mid \boldsymbol{c}\right\rangle - \frac{1}{f_c}\frac{\partial}{\partial c_i}\left[f_c \operatorname{cov}\left(Q, \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c}\right)\right]. \tag{B 11}$$

Two important observations are, first, that the left-hand side of (B 11) evaluated for $\boldsymbol{c}=\widehat{\boldsymbol{C}}(t)$ is the rate of change of $\langle Q(\boldsymbol{x},t)|\boldsymbol{C}=\widehat{\boldsymbol{C}}(t)\rangle$, where $\widehat{\boldsymbol{C}}(t)$ evolves by $\langle \mathrm{d}\boldsymbol{C}/\mathrm{d}t|\widehat{\boldsymbol{C}}\rangle$, (3.9); and, second, that the conditional covariance (on the right-hand side of (B 11)) is zero if the conditional fluctuations, $Q-\langle Q|\boldsymbol{c}\rangle$ and $\mathrm{d}\boldsymbol{C}/\mathrm{d}t-\langle \mathrm{d}\boldsymbol{C}/\mathrm{d}t|\boldsymbol{c}\rangle$, are uncorrelated, or if either one is zero.

We mention in passing that (B 11) is a new and rather fundamental equation, which may have uses in other contexts and fields. In the conditional moment closure (CMC; Klimenko & Bilger 1999), the evolution of quantities like $\langle Q|\boldsymbol{c}\rangle$ are considered for fixed values of the conditioning variable $\boldsymbol{c}$. In contrast, (B 11) shows the evolution of $\langle Q|\widehat{\boldsymbol{C}}(t)\rangle$, that is, with the conditioning variable evolving at its conditional mean rate.

The evolution for the self-conditioned velocity field $\boldsymbol{W}(\boldsymbol{x},t)\equiv\langle \boldsymbol{U}(\boldsymbol{x},t)|\boldsymbol{C}(t)=\widehat{\boldsymbol{C}}(t)\rangle$ is obtained from (B 11) (with the substitution $Q=U_i$) and with $\partial U_i/\partial t$ obtained from the momentum equation (1.2). The result can be expressed as

$$\left(\frac{\partial}{\partial t}+W_j\frac{\partial}{\partial x_j}\right)W_i=\frac{\partial\widetilde{\tau}_{ij}}{\partial x_j}+R_i, \tag{B 12}$$

where the effective stress is

$$\widetilde{\tau}_{ij}=\langle\tau_{ij}\mid\widehat{\boldsymbol{C}}\rangle+\tau_{ij}^R, \tag{B 13}$$

where τ_{ij}^R is the residual stress

$$\tau_{ij}^R\equiv-\mathrm{cov}(U_i,U_j\mid\widehat{\boldsymbol{C}}), \tag{B 14}$$

and the final term is

$$R_i=-\frac{1}{f_c}\frac{\partial}{\partial c_j}\left[f_c\,\mathrm{cov}\left(U_i,\frac{\mathrm{d}C_j}{\mathrm{d}t}\mid\boldsymbol{c}\right)\right], \tag{B 15}$$

evaluated at $\boldsymbol{c}=\widehat{\boldsymbol{C}}$.

For the constant-property Navier–Stokes equation, the stress is

$$\tau_{ij}=\nu\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{p}{\rho}\delta_{ij}, \tag{B 16}$$

where ν is the kinematic and $p(\boldsymbol{x},t)$ is the pressure. Since differentiation and taking the conditional mean commute, we obtain, simply,

$$\langle\tau_{ij}\mid\widehat{\boldsymbol{C}}\rangle=\nu\left(\frac{\partial W_i}{\partial x_j}+\frac{\partial W_j}{\partial x_i}\right)-\frac{\delta_{ij}}{\rho}\langle p\mid\widehat{\boldsymbol{C}}\rangle. \tag{B 17}$$

Substitution of these results into (B 12) leads to the final form for the momentum equation for the self-conditioned velocity, which is (4.10).

We make the following comments and observations about $\boldsymbol{R}$, the final term in the momentum equation, defined by (B 15).

(i) The term appears as a specific force and hence is a source or sink of momentum.

(ii) The term does not appear as the divergence of a stress, and consequently it can cause the conditional momentum of the field $\int_{\mathscr{D}}\rho\boldsymbol{W}(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}$ to change.

(iii) From the definition of $\boldsymbol{R}$ we have

$$\int_{\mathscr{C}}f_c\,\boldsymbol{R}\,\mathrm{d}\boldsymbol{c}=0, \tag{B 18}$$

showing that the term does not affect the mean momentum $\rho\langle\boldsymbol{W}(\boldsymbol{x},t)\rangle$. Thus, the terms represent a flux of momentum in conditioning space.

(iv) In a model, it is expedient to take $\boldsymbol{R}$ to be zero, and, given the current state of knowledge, there is no reason to do otherwise.

(v) The previous point notwithstanding, the simplest non-trivial model satisfying (B 18) is the linear relaxation model

$$\boldsymbol{R}(\boldsymbol{x},t) = -(\boldsymbol{W}(\boldsymbol{x},t) - \langle \boldsymbol{W}(\boldsymbol{x},t)\rangle)/\tau_R(\boldsymbol{x},t), \tag{B 19}$$

where τ_R is a specified relaxation time scale. This model could be implemented by performing simultaneously an ensemble of simulations (with initial conditions drawn from the specified distribution), so that the mean $\langle \boldsymbol{W}(\boldsymbol{x},t)\rangle$ can be approximated as an ensemble average.

The simplest model equation for $\boldsymbol{W}(\boldsymbol{x},t)$ is obtained by (a) using a turbulent viscosity model for the residual stress τ_{ij}^R and (b) neglecting the term $\boldsymbol{R}$.

The result is the standard model LES equation

$$\left(\frac{\partial}{\partial t} + W_j\frac{\partial}{\partial x_j}\right) W_i = \frac{\partial}{\partial x_j}\left[(\nu+\nu_R)\left(\frac{\partial W_i}{\partial x_j} + \frac{\partial W_j}{\partial x_i}\right)\right] - \frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i}, \tag{B 20}$$

where ν_R is the modelled turbulent residual viscosity, and $\tilde{p}$ is the modified pressure, which is determined by a Poisson equation.

Next, we verify that $\langle \boldsymbol{U}(\boldsymbol{x},t)|\boldsymbol{c}\rangle$ is self-conditioning, and hence so also is $\boldsymbol{W}(\boldsymbol{x},t)$. The nth condition is (4.1)

$$C_n(t) = \int_{\mathscr{D}} U_i(\boldsymbol{x},t) K_i^{(n)}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{B 21}$$

and (B 3) with the substitution $Q = U_i$ is

$$f_c(\boldsymbol{c};t)\langle U_i(\boldsymbol{x},t) \mid \boldsymbol{C}(t) = \boldsymbol{c}\rangle = \langle U_i(\boldsymbol{x},t)\,\delta(\boldsymbol{C}(t)-\boldsymbol{c})\rangle. \tag{B 22}$$

Multiplying this last equation by $K_i^{(n)}(\boldsymbol{x})$ and integrating over all $\boldsymbol{x}$, we obtain

$$\begin{aligned} f_c \int_{\mathscr{D}} K_i^{(n)}(\boldsymbol{x})\langle U_i \mid \boldsymbol{c}\rangle\,\mathrm{d}\boldsymbol{x} &= \left\langle \int_{\mathscr{D}} K_i^{(n)}(\boldsymbol{x}) U_i(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}\;\delta(\boldsymbol{C}(t)-\boldsymbol{c})\right\rangle \\ &= \langle C_n(t) \mid \boldsymbol{c}\rangle f_c = c_n f_c. \end{aligned} \tag{B 23}$$

This equation (when divided by f_c) yields the required, consistent result

$$c_n = C_n(t) = \int_{\mathscr{D}} K_i^{(n)}(\boldsymbol{x})\langle U_i \mid \boldsymbol{c}\rangle\,\mathrm{d}\boldsymbol{x}. \tag{B 24}$$

This result is not completely trivial: it depends on the conditioning operation being independent of t and the conditioning variables being independent of $\boldsymbol{x}$.

Finally, we mention an alternative technique that can be used to derive the above equations and more. Let the velocity field be written as

$$\boldsymbol{U}(\boldsymbol{x},t) = \sum_{n=1}^{n_b} \boldsymbol{b}^{(n)}(\boldsymbol{x}) u_n(t), \tag{B 25}$$

where $\{\boldsymbol{b}^{(n)}(\boldsymbol{x}), n = 1,\ldots,n_b\}$ is a set of vector-valued basis functions and $\boldsymbol{u}(t) = \{u_1(t), u_2(t), \ldots, u_{n_b}(t)\}$ are basis function coefficients. This representation is certainly possible for n_b sufficiently large, possibly infinite.

The conditioning variables $\boldsymbol{C}(t)$ (defined by (4.1)) are given by

$$\boldsymbol{C}(t) = \boldsymbol{K}\boldsymbol{u}(t), \tag{B 26}$$

where $\boldsymbol{K}$ is the constant $n_c \times n_b$ matrix with components

$$K_{nm} = \int_{\mathscr{D}} K_i^{(n)}(\boldsymbol{x}) b_i^{(m)}(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}. \tag{B 27}$$

Standard techniques can be used to derive the evolution equation for the joint PDF of $\boldsymbol{u}$ and $\boldsymbol{C}$, and hence of the PDF of $\boldsymbol{u}$ conditioned on $\boldsymbol{C} = \boldsymbol{c}$. This equation is of interest in its own right, and can also be integrated to obtain the evolution equation for $\langle \boldsymbol{U}(\boldsymbol{x}, t) | \boldsymbol{c} \rangle$.

Appendix C. Derivation of the self-conditioned composition PDF equation

In addition to the velocity field, we consider a single composition variable $\phi(\boldsymbol{x}, t)$ evolving by

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = -\frac{\partial J_i}{\partial x_i} + S(\phi), \tag{C 1}$$

where S is the chemical source term, and $\boldsymbol{J}$ is the molecular flux

$$J_i = -\Gamma \frac{\partial \phi}{\partial x_i}, \tag{C 2}$$

where Γ is the molecular diffusivity. A single composition is considered for simplicity, but there is no difficulty in extending the analysis to multiple compositions.

The conditioning variables are extended to include variables of the form of (5.2).

In addition to the PDF, $f_c(\boldsymbol{c}; t)$, of the conditioning variables, (B 2), we consider the joint PDF $f_{\phi c}(\psi, \boldsymbol{c}; \boldsymbol{x}, t)$ of $\phi(\boldsymbol{x}, t)$ and $\boldsymbol{C}(t)$:

$$f_{\phi c}(\psi, \boldsymbol{c}; \boldsymbol{x}, t) = \langle \delta(\phi(\boldsymbol{x}, t) - \psi)\, \delta(\boldsymbol{C}(t) - \boldsymbol{c}) \rangle, \tag{C 3}$$

and the PDF of $\phi(\boldsymbol{x}, t)$ conditional on $\boldsymbol{C}(t) = \boldsymbol{c}$:

$$f_{\phi|c}(\psi \mid \boldsymbol{c}; \boldsymbol{x}, t) = f_{\phi c}(\psi, \boldsymbol{c}; \boldsymbol{x}, t) / f_c(\boldsymbol{c}; t). \tag{C 4}$$

The standard delta-function technique is used to derive the evolution equation for $f_{\phi c}$, and then the equation for $f_{\phi|c}$ is obtained from (C 4). Similar to (B 11), the equation for $f_{\phi|c}$ is

$$\left(\frac{\partial}{\partial t} + \left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c} \right\rangle \frac{\partial}{\partial c_i} \right) f_{\phi|c} = -\frac{\partial}{\partial \psi} \left[f_{\phi|c} \left\langle \frac{\partial \phi}{\partial t} \mid \phi, \boldsymbol{c} \right\rangle \right] + R_\phi, \tag{C 5}$$

where R_ϕ is defined by

$$R_\phi \equiv -\frac{1}{f_c} \frac{\partial}{\partial c_i} \left[f_c f_{\phi|c} \left(\left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \phi, \boldsymbol{c} \right\rangle - \left\langle \frac{\mathrm{d}C_i}{\mathrm{d}t} \mid \boldsymbol{c} \right\rangle \right) \right]. \tag{C 6}$$

The term R_ϕ represents a source due to a flux in conditioning space, and it satisfies

$$\int_{\mathscr{C}} f_c R_\phi \, \mathrm{d}\boldsymbol{c} = 0, \tag{C 7}$$

(similar to (B 18)), and

$$\int_{\psi_-}^{\psi_+} R_\phi \, \mathrm{d}\psi = 0, \tag{C 8}$$

(where ψ_- and ψ_+ are the lower and upper bounds on ϕ) so that the normalization of $f_{\phi|c}$ is preserved.

We now define $g(\psi;\boldsymbol{x},t)$ to be the PDF of composition conditioned on $\widehat{\boldsymbol{C}}(t)$,

$$g(\psi;\boldsymbol{x},t) \equiv f_{\phi|c}(\psi \mid \widehat{\boldsymbol{C}}(t);\boldsymbol{x},t), \tag{C 9}$$

so that the left-hand side of (C 5) (evaluated at $\boldsymbol{c}=\widehat{\boldsymbol{C}}(t)$) is simply $\partial g/\partial t$. Then substituting (C 1) for $\partial\phi/\partial t$, we obtain

$$\left(\frac{\partial}{\partial t}+W_i\frac{\partial}{\partial x_i}\right)g = -\frac{\partial}{\partial x_i}\left[g(\langle U_i \mid \psi,\widehat{\boldsymbol{C}}(t)\rangle - \langle U_i \mid \widehat{\boldsymbol{C}}(t)\rangle)\right] - \frac{\partial}{\partial\psi}\left[g\left(S(\psi)-\left\langle\frac{\partial J_i}{\partial x_i}\mid\psi,\widehat{\boldsymbol{C}}(t)\right\rangle\right)\right]+R_\phi. \tag{C 10}$$

The simplest model equation for g is obtained by (a) using a gradient diffusion model for the spatial flux due to residual velocity (the first term on the right-hand side of (C 10)), (b) modelling the molecular term by the interaction by exchange with the mean (IEM) mixing model plus a mean diffusion, and (c) neglecting R_ϕ. The result is the model equation

$$\left(\frac{\partial}{\partial t}+W_i\frac{\partial}{\partial x_i}\right)g = \frac{\partial}{\partial x_i}\left(\Gamma_R\frac{\partial g}{\partial x_i}\right) - \frac{\partial}{\partial\psi}\left[g\left(S(\psi)-\omega_R(\psi-\tilde{\phi})+\Gamma\frac{\partial^2\tilde{\phi}}{\partial x_i\partial x_i}\right)\right], \tag{C 11}$$

where Γ_R and ω_R are the modelled residual diffusivity and mixing rate, and $\tilde{\phi}(\boldsymbol{x},t)$ is the conditional mean field

$$\tilde{\phi}(\boldsymbol{x},t) \equiv \langle\phi(\boldsymbol{x},t)\mid\widehat{\boldsymbol{C}}(t)\rangle = \int_{\psi_-}^{\psi_+}\psi g(\psi;\boldsymbol{x},t)\,\mathrm{d}\psi. \tag{C 12}$$

Finally, we verify that $g(\psi;\boldsymbol{x},t)$ is self-conditioning, for conditioning given by (5.2). Taking the conditional mean of this equation, we obtain

$$\begin{aligned}\langle C_m(t)\mid\boldsymbol{C}(t)=\widehat{\boldsymbol{C}}(t)\rangle &= \widehat{C}_m(t)\\ &= \int_{\mathscr{D}}\langle L^{(m)}(\phi(\boldsymbol{x},t))\mid\boldsymbol{C}(t)=\widehat{\boldsymbol{C}}(t)\rangle\,K_\phi^{(m)}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\\ &= \int_{\mathscr{D}}\int_{\psi_-}^{\psi_+} g(\psi;\boldsymbol{x},t)L^{(m)}(\psi)\,\mathrm{d}\psi\,K_\phi^{(m)}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},\end{aligned} \tag{C 13}$$

showing that $\widehat{C}_m(t)$ is determined by $g(\psi;\boldsymbol{x},t)$.

For the simplest case of $L^{(m)}$ being the identity (i.e. $L^{(m)}(\psi)=\psi$), then the corresponding conditioning variable is

$$\widehat{C}_m(t) = \int_{\mathscr{D}}\tilde{\phi}(\boldsymbol{x},t)K_\phi^{(m)}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}. \tag{C 14}$$

Appendix D. The choice of conditioning variables

In this appendix, we consider the optimal choice of conditioning variables and make some related observations. We consider deterministic, ergodic, channel flow (as introduced in § 3.1), in which the velocity field $\boldsymbol{U}(\boldsymbol{x},t)$ is on an n_A-dimensional attractor $\mathscr{A}$ in the function space $\mathscr{H}$. These considerations are based on a decomposition of the velocity field (D 11) which is now described.

The n_c conditioning variables $\boldsymbol{C}(t)$ are defined by the n_c-vector of conditioning kernels $\boldsymbol{K}(\boldsymbol{x})$ (whose components, $\boldsymbol{K}_1(\boldsymbol{x}), \boldsymbol{K}_2(\boldsymbol{x}), \ldots, \boldsymbol{K}_{n_c}(\boldsymbol{x})$ are vectors in physical space). Specifically, we have that the n_c-vector of conditioning variables is

$$\boldsymbol{C}(t) = \int_{\mathscr{D}} \boldsymbol{K}(\boldsymbol{x}) \cdot \boldsymbol{U}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x}. \tag{D 1}$$

We require that the n_c conditioning kernels be linearly independent on the attractor $\mathscr{A}$, which implies that n_c is no larger than n_A.

As in § 3.2, we decompose the function space $\mathscr{H}$ into two mutually orthogonal subspaces $\widetilde{\mathscr{H}}$ and $\widehat{\mathscr{H}}$, and correspondingly the velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$ is decomposed as $\boldsymbol{U} = \widetilde{\boldsymbol{U}} + \widehat{\boldsymbol{U}}$ (with $\widetilde{\boldsymbol{U}} \in \widetilde{\mathscr{H}}$ and $\widehat{\boldsymbol{U}} \in \widehat{\mathscr{H}}$). The defining property of the infinite-dimensional subspace $\widehat{\mathscr{H}}$ is

$$\int_{\mathscr{D}} \boldsymbol{K}(\boldsymbol{x}) \cdot \widehat{\boldsymbol{U}}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} = 0 \quad \text{for all} \quad \widehat{\boldsymbol{U}} \in \widehat{\mathscr{H}}, \tag{D 2}$$

so that $\widehat{\boldsymbol{U}}$ makes no contribution to the conditioning variables. Given $\boldsymbol{U}$, both $\boldsymbol{C}$ and $\widehat{\boldsymbol{U}}$ can be determined, and then $\widehat{\boldsymbol{U}}$ can be decomposed as

$$\widehat{\boldsymbol{U}}(\boldsymbol{x}, t) = \langle \widehat{\boldsymbol{U}}(\boldsymbol{x}, t) \mid \boldsymbol{C}(t) \rangle + \boldsymbol{U}'(\boldsymbol{x}, t, \boldsymbol{C}(t)), \tag{D 3}$$

i.e. into its conditional mean $\langle \widehat{\boldsymbol{U}}(\boldsymbol{x}, t) \mid \boldsymbol{C}(t) \rangle$ and the conditional deviation $\boldsymbol{U}'(\boldsymbol{x}, t, \boldsymbol{C}(t))$, which is implicitly defined by the above equation.

The subspace $\widetilde{\mathscr{H}}$ is n_c-dimensional, it is orthogonal to $\widehat{\mathscr{H}}$, and we introduce for it an orthonormal basis $\widetilde{\boldsymbol{b}}(\boldsymbol{x})$. We treat $\widetilde{\boldsymbol{b}}(\boldsymbol{x})$ as an n_c-vector, but note that its components $(\widetilde{\boldsymbol{b}}_1(\boldsymbol{x}), \widetilde{\boldsymbol{b}}_2(\boldsymbol{x}), \ldots, \widetilde{\boldsymbol{b}}_{n_c}(\boldsymbol{x}))$ are divergence-free vector-valued functions in physical space. The orthonormality conditions are

$$\int_{\mathscr{D}} \widetilde{\boldsymbol{b}}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}}\, \mathrm{d}\boldsymbol{x} = \boldsymbol{I} \int_{\mathscr{D}} \mathrm{d}\boldsymbol{x}, \tag{D 4}$$

where $\boldsymbol{I}$ is the $n_c \times n_c$ identity matrix. In this basis, $\widetilde{\boldsymbol{U}}$ can be expressed as

$$\widetilde{\boldsymbol{U}}(\boldsymbol{x}, t) = \widetilde{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}} \widetilde{\boldsymbol{u}}(t), \tag{D 5}$$

where $\widetilde{\boldsymbol{u}}(t)$ is an n_c-vector of scalar-valued basis-function coefficients. Pre-multiplying this equation by $\boldsymbol{K}(\boldsymbol{x})\cdot$ and integrating over the domain, we obtain

$$\boldsymbol{C}(t) = \int_{\mathscr{D}} \boldsymbol{K}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{U}}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} = \int_{\mathscr{D}} \boldsymbol{K}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}} \widetilde{\boldsymbol{u}}(t)\, \mathrm{d}\boldsymbol{x} = \widetilde{\boldsymbol{L}}\, \widetilde{\boldsymbol{u}}(t), \tag{D 6}$$

where $\widetilde{\boldsymbol{L}}$ is the non-singular $n_c \times n_c$ matrix defined by

$$\widetilde{\boldsymbol{L}} \equiv \int_{\mathscr{D}} \boldsymbol{K}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}}\, \mathrm{d}\boldsymbol{x}. \tag{D 7}$$

Equation (D 6) shows that there is a one-to-one linear relation between $\boldsymbol{C}$ and $\widetilde{\boldsymbol{u}}$, so that we can re-express $\widetilde{\boldsymbol{U}}$ as

$$\widetilde{\boldsymbol{U}}(\boldsymbol{x}, t) = \bar{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{C}(t), \tag{D 8}$$

where the n_c-vector of basis functions $\bar{\boldsymbol{b}}(\boldsymbol{x})$ is defined by

$$\bar{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}} = \widetilde{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}} \widetilde{\boldsymbol{L}}^{-1}, \tag{D 9}$$

and is uniquely determined by $\boldsymbol{K}$ (independent of the particular choice of the basis $\widetilde{\boldsymbol{b}}$). Equation (D 8) shows the non-trivial result that $\widetilde{\boldsymbol{U}}$ is a determined linear function of $\boldsymbol{C}$. It then follows simply that the conditional mean of $\widetilde{\boldsymbol{U}}$ is the known linear function:

$$\langle \widetilde{\boldsymbol{U}}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)=\boldsymbol{c}\rangle = \bar{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{c}. \tag{D 10}$$

From (D 8) and (D 3) we obtain the decomposition

$$\boldsymbol{U}(\boldsymbol{x},t) = \bar{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{C}(t) + \langle \widehat{\boldsymbol{U}}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)\rangle + \boldsymbol{U}'(\boldsymbol{x},t,\boldsymbol{C}(t)). \tag{D 11}$$

On the right-hand side, the first term is the known linear component in $\widetilde{\mathscr{H}}$; the first and second terms together give the conditional mean $\langle \boldsymbol{U}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)\rangle$; and the third term gives the deviation of $\boldsymbol{U}(\boldsymbol{x},t)$ from this conditional mean.

The volume-average mean kinetic energy is

$$k \equiv \int_{\mathscr{D}} \frac{1}{2}\langle |\boldsymbol{U}(\boldsymbol{x},t)|^2\rangle \,\mathrm{d}\boldsymbol{x} \Big/ \int_{\mathscr{D}} \mathrm{d}\boldsymbol{x}, \tag{D 12}$$

which can be decomposed as

$$k = \widetilde{k} + \widehat{k} + k', \tag{D 13}$$

where the three terms on the right-hand side correspond to the three terms on the right-hand side of (D 11), e.g.

$$k' \equiv \int_{\mathscr{D}} \frac{1}{2}\langle |\boldsymbol{U}'(\boldsymbol{x},t,\boldsymbol{C}(t))|^2\rangle \,\mathrm{d}\boldsymbol{x} \Big/ \int_{\mathscr{D}} \mathrm{d}\boldsymbol{x}. \tag{D 14}$$

On the basis of this decomposition, we consider three possible definitions of optimal conditioning variables, namely, those which minimize k', $\widehat{k}$ and $k'+\widehat{k}$.

Minimizing the residual kinetic energy k' may be optimal from a modelling viewpoint. The maximum possible energy is explicitly represented in the self-conditioned field, and the residual stresses requiring modelling are in some sense minimized. Minimizing k' is also optimal in the sense that, as n_c is increased, the DNS limit is achieved with the smallest possible value of n_c.

An interesting question is: for a given value of n_c, can the conditioning kernels be chosen such that the n_c-dimensional manifold $\langle \boldsymbol{U}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)=\boldsymbol{c}\rangle$ is in the n_c-dimensional subspace $\widetilde{\mathscr{H}}$? For such 'eigen-conditioning' (if it exists), $\widehat{k}$ is zero, and the self-conditioned velocity field is a known linear function of the conditioning variables, i.e.

$$\langle \boldsymbol{U}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)\rangle = \bar{\boldsymbol{b}}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{C}(t). \tag{D 15}$$

On the basis of this observation, the choice of conditioning variables that yields $\widehat{k}=0$, or which minimizes $\widehat{k}$, or which minimizes the dimension of $\langle \boldsymbol{U}(\boldsymbol{x},t) \mid \boldsymbol{C}(t)=\boldsymbol{c}\rangle$ may be optimal from the viewpoint of numerical simulations, since it requires the smallest number of basis functions to accurately represent the self-conditioned velocity field.

Finally, we consider minimizing the sum $k'+\widehat{k}$ of the two quantities previously considered for minimization, to yield a compromise between the benefits of minimizing either one alone. This is equivalent to maximizing $\widetilde{k}$, which is a well-known property of the POD basis (see e.g. Holmes, Lumley & Berkooz 1996). That is, given n_c,

the energy $\widetilde{k}$ associated with the velocity field $\widetilde{\boldsymbol{U}}$ in $\widetilde{\mathscr{H}} = \mathrm{span}(\widetilde{\boldsymbol{b}})$ is maximized by $\widetilde{\boldsymbol{b}}$ spanning the same subspace as the first n_c POD modes.

Of the three minimization problems considered, only for the last one is there an established minimization procedure, i.e. the POD methodology; and even this is unlikely to be tractable except for simple model problems (since the computational work involved scales as the cube of the number of basis functions required to resolve $\boldsymbol{U}(\boldsymbol{x}, t)$). Nevertheless, it is a useful, if not surprising, conclusion that the POD modes provide a good basis for the conditioning variables.

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