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# Optimal large eddy simulation in one dimension

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How the optimal choice of the filter function in large eddy simulations is related to the spectrum of the turbulent flow is shown. A new formula for the subgrid residuals, which ensures that the exact and filtered flow have the same energy decay profile, is also derived.

Turbulent flows contain motions in various scales. Because of this fact the computation of such flows on a finite step grid (in more than one spatial dimension) is not within the computational ability of present-day computers. Large eddy simulation (LES) attempts to resolve this difficulty by proper modeling of the subgrid motions and their interaction

with the resolvable flow.<sup>1</sup>

In brief, the essence of LES is to introduce a filter function<sup>2</sup>  $G(x)$  and define the filtered flow as

$$\mathbf{u} = \int G(x - x')u(x')dx. \quad (1)$$

(To simplify notation we use  $\mathbf{u}$  for  $\bar{u}$ .) By applying this filter to Navier–Stokes equations we then derive an equation for  $\mathbf{u}$  after proper modeling of the subgrid terms.

To illustrate this process we consider Burger’s equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}. \quad (2)$$

Applying the filter operation to this equation we obtain, after obvious algebra,

$$\frac{\partial \mathbf{u}}{\partial t} + \overline{\mathbf{u} \frac{\partial \mathbf{u}}{\partial x}} + \frac{\partial \tau}{\partial x} = \nu \frac{\partial^2 \mathbf{u}}{\partial x^2}, \quad (3)$$

where

$$\tau = u' \mathbf{u} + (\mathbf{u}')^2 \quad (4)$$

and  $u'$  are the subgrid residuals

$$u' = u - \mathbf{u}. \quad (5)$$

Various prescriptions are available in the literature to model  $\tau$  in terms of  $\mathbf{u}$ , e.g., the Smagorinski eddy viscosity model<sup>3</sup> or the mixed model proposed by Bardina *et al.*<sup>4</sup> and Piomelli *et al.*<sup>5</sup>

In one dimension these models are given, respectively, by<sup>2,4</sup>

$$\tau = -2\nu_T \frac{\partial \mathbf{u}}{\partial x}, \quad \nu_T = k \frac{\partial \mathbf{u}}{\partial x}$$

and

$$\tau = \mathbf{u}^2 - \bar{\mathbf{u}}^2 - 2\nu_T \frac{\partial \mathbf{u}}{\partial x},$$

where  $k$  is a constant.

As to the filter function, three principal choices are available in the literature. These are the Gaussian filter,<sup>2,5</sup>

$$G(x) = (6/\pi\Delta^2)^{1/2} \exp(-6x^2/\Delta^2); \quad (6)$$

the sharp Fourier cutoff filter,<sup>2,5</sup>

$$G(x) = 2 \sin(x/\Delta)/x; \quad (7)$$

and the top-hat filter.<sup>1,6</sup> These different choices for  $G$  and  $\tau$  lead us naturally to examine whether an optimal filter function and a subgrid model can be constructed for LES. Motivated by the properties of the filter functions [(6) and (7)] we require this optimal filter function  $G$  to be a smooth even function defined on  $(-\infty, \infty)$ . Furthermore,  $G$  has to be determined so that for a large class of flows the solutions of the filtered equations (using some fixed subgrid model) “resembles” as much as possible the characteristics of the original flow. This last requirement, however, can have different interpretations. For example, we may use it to derive an optimal model that is based on the structure of the Reynold’s stress tensor. Another possibility is to require that the turbulence statistics, including the effect of the subgrid scales obtained from LES, represents a “good approximation” to those obtained from direct simulation. We also observe that from a formal point of view (1) represents a change of variable and if this transformation is exactly invertible then we can obtain  $u$  back from  $\mathbf{u}$ .<sup>7</sup> In practice, however,  $\tau$  is not known exactly and the inversion on a finite precision machine will lead to further discrepancies between  $u$  and  $\mathbf{u}$ .

Our objective in this Brief Communication is to derive an optimal (Gaussian-like) filter function that is based on

the requirement that the spectral decomposition of  $u$  and  $\mathbf{u}$  (with respect to some complete set of orthogonal functions) is the same up to order  $n$ . Furthermore, we shall derive a new model for  $\tau$  that is based on the requirement that the flow energy represented by  $u$  and  $\mathbf{u}$  have the same decay profile.

We begin by performing a spectral analysis of LES in one dimension.

Since  $G$  must be defined on  $(-\infty, \infty)$  it is natural to expand it in terms of an orthogonal basis of  $L_2(-\infty, \infty)$ . Such a basis is given by the Hermite polynomials  $H_n(x)$ ,<sup>8</sup> which are orthogonal to each other with respect to the weight function  $e^{-x^2}$ , i.e.,

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi} \delta_{m,n}. \quad (8)$$

Moreover, since  $H_{2k+1}(x)$ ,  $k=0,1,\dots$ , are odd it follows that an expansion for  $G$  (which is even) in terms of these functions can take, without loss of generality, the form

$$G(x) = e^{-x^2} \sum_{k=0}^{\infty} b_{2k} H_{2k}(x). \quad (9)$$

Assuming that  $u$ ,  $\mathbf{u}$  are also defined on  $(-\infty, \infty)$  we introduce the spectral decomposition

$$u(x,t) = \sum_{n=0}^{\infty} a_n(t) H_n(x), \quad (10)$$

$$\mathbf{u}(x,t) = \sum_{n=0}^{\infty} \mathbf{a}_n(t) H_n(x). \quad (11)$$

Substituting (10) in (2) we can use the identities

$$H'_n(x) = 2nH_{n-1}(x), \quad (12)$$

$$H_m(x)H_n(x) = 2^m m! n! \sum_{k=0}^m \frac{H_{n-m+2k}(x)}{2^k k! (k+n-m)! (m-k)!}, \quad (13)$$

$n \geq m$

to simplify and linearize the products of Hermite polynomials that appear. Multiplying the resulting expression by  $e^{-x^2} H_m(x)$ ,  $m=0,1,\dots$ , and integrating over  $(-\infty, \infty)$  we obtain an infinite system of ordinary differential equations for  $a_n(t)$ ,

$$\frac{\partial a_0}{\partial t} = 8\nu a_2 - 2a_1(a_0 + 4a_2) - 48a_2 a_3 + \dots, \quad (14a)$$

$$\frac{\partial a_1}{\partial t} = -2a_1^2 - a_2(16a_2 - 4a_0) + 24(\nu - a_1 - 6a_3) + \dots, \quad (14b)$$

etc.

Similarly, by substituting (11) in (3) we can linearize the products of Hermite polynomials in the expression

$$I = \int_{-\infty}^{\infty} G(x-x') \mathbf{u}(x',t) \frac{\partial \mathbf{u}(x',t)}{\partial x'} dx', \quad (15)$$

which appear in this equation. To this end we first linearize the products in the term  $\mathbf{u}(\partial \mathbf{u}/\partial x)$  by using the identities (12) and (13). Then we make use of the identity

$$H_n(x') = \frac{1}{2^{n/2}} \sum_{k=0}^n \binom{n}{k} H_{n-k}[(x'-x)\sqrt{2}] H_k(x\sqrt{2}), \quad (16)$$

to replace  $H_n(x')$  in  $I$ . Expressing  $H_n[(x' - x)\sqrt{2}]$  in terms of  $H_n(x' - x)$  we can evaluate the resulting integrals using (8). Substituting this result in Eq. (3) we obtain, as before, a system of ordinary differential equations for  $\mathbf{a}_n(t)$ ,

$$\begin{aligned} \frac{d\mathbf{a}_0}{dt} &= 8\nu_T\mathbf{a}_2 + \sqrt{\pi}\{2\mathbf{a}_1(2b_1\mathbf{a}_1 - b_0\mathbf{a}_0) \\ &\quad + 4\mathbf{a}_2[2b_1\mathbf{a}_0 - \mathbf{a}_1(5b_0 + 12b_2) \\ &\quad + 16\mathbf{a}_2(5b_1 + 12b_3)]\} + \dots, \end{aligned} \quad (17a)$$

$$\begin{aligned} \frac{d\mathbf{a}_1}{dt} &= 24\nu_T\mathbf{a}_3 + \sqrt{\pi}\{2\mathbf{a}_1(12b_1\mathbf{a}_2 - b_0\mathbf{a}_1) \\ &\quad - 4\mathbf{a}_2[b_0\mathbf{a}_0 + 2\mathbf{a}_2(5b_0 + 12b_2)]\} + \dots, \end{aligned} \quad (17b)$$

etc.

In these equations  $\nu_T$  represents the sum of molecular and eddy viscosity (but no specific model is assumed). It follows then that the exact and filtered equations yield the same spectral approximation for the flow up to order  $n$  if  $\mathbf{a}_n(t)$  and  $\mathbf{a}_n(t)$  satisfy the same differential equations up to that order. For this to happen we should be able to solve the algebraic equations,

$$(14k) - (17k) = 0, \quad k = 0, 1, \dots, n \quad (18)$$

(after setting  $a_i = \mathbf{a}_j = 0$  for  $i, j > n$  and  $a_i = \mathbf{a}_i$  for  $i \leq n$ ) for the  $b_{2k}$ 's in terms of the  $a_k$ 's and obtain scalar expressions, i.e., expressions that are time independent.

It turns out that the maximal order of  $n$  for which this program can be carried out is  $n = 3$ , and we obtain

$$\begin{aligned} b_0 &= 1/\sqrt{\pi}, \quad b_2 = -1/4\sqrt{\pi}, \\ b_4 &= (15a_3 + \nu_T - \nu)/480\sqrt{\pi}a_3 \end{aligned} \quad (19)$$

(the expression for  $b_4$  is time independent only if we let  $\nu_T = \nu$ ). For  $n > 3$  the solution of the linear system (18) for  $b_{2k}$  contains polynomials of  $\mathbf{a}_n(t)$  and it is impossible to obtain exact agreement between  $u$  and  $\mathbf{u}$  with scalar  $b$ 's. This discrepancy between  $u$  and  $\mathbf{u}$  will increase as the number of degrees of freedom in the flow increases and the modes with  $n > 3$  make significant contributions to the overall flow. Thus we demonstrated that under present assumptions and constraints the approximation for  $u$  obtained through any filter function will break down as the Reynolds number increases. Moreover, even for Reynold numbers that are not large, Eq. (19) shows that the optimal filter function is not purely Gaussian and should contain contributions from higher-order terms.

Finally, we observe that  $u$  and  $\mathbf{u}$  are assumed to satisfy the same boundary conditions and therefore (19) is independent of these.

We now present an energy model for  $\tau$ .

Let  $u$  be the solution of Burger's equation on some region  $\Omega$  subject to some boundary conditions. By multiplying (2) and (3) by  $u$  and  $\mathbf{u}$ , respectively, and integrating over  $\Omega$  we obtain the energy equations

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} u^2 dx + \nu \int_{\Omega} \left(\frac{\partial u}{\partial x}\right)^2 &= \left(\nu u \frac{\partial u}{\partial x} - \frac{u^3}{3}\right) \Big|_{\partial\Omega}, \quad (20) \\ \frac{d}{dt} \int_{\Omega} \mathbf{u}^2 dx + \nu \int_{\Omega} \left(\frac{\partial \mathbf{u}}{\partial x}\right)^2 dx &+ \int_{\Omega} (\bar{\mathbf{u}}\mathbf{u} - \tau) \frac{\partial \mathbf{u}}{\partial x} dx \\ &= \left(\nu \mathbf{u} \frac{\partial \mathbf{u}}{\partial x} - \mathbf{u}\tau\right) \Big|_{\partial\Omega}. \end{aligned} \quad (21)$$

Our objective is to determine an expression for  $\tau$  so that the energy represented by  $u$  and  $\mathbf{u}$  have the same decay profile for a large class of flows. Because of this "universality" requirement  $\tau$  must be independent of the boundary conditions imposed on the flow and we may therefore disregard these terms in Eqs. (20) and (21).

From these assumptions it is easy to infer from (20) and (21) that an attractive model for  $\tau$  that yields similar evolution equations for the energy of  $u$  and  $\mathbf{u}$  is

$$\tau = \bar{\mathbf{u}}\cdot\mathbf{u} - k \frac{\partial \mathbf{u}}{\partial x}. \quad (22)$$

In fact, with this choice of  $\tau$  we can apply the Poincaré inequality<sup>9</sup> to (20) and (21) to obtain

$$\int_0^a u^2 dx \leq e^{-(\nu\pi^2/4a)t}, \quad (23)$$

$$\int_0^a \mathbf{u}^2 dx \leq e^{-[(\nu+k)\pi^2/4a]t}. \quad (24)$$

Although the prescription (22) for  $\tau$  did not appear in the literature (to our knowledge) it is reminiscent of the mixed model of Bardina *et al.* as  $\bar{\mathbf{u}}$  appears naturally in the modeling of  $\tau$ .

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<sup>1</sup>A review and complete list of references on the subject are given in J. H. Ferziger, in *Computational Methods for Turbulent, Transonic and Viscous Flow*, edited by J. A. Essers (Springer, New York, 1983), p. 93; M. D. Love and D. C. Leslie, in *Turbulent Shear Flows I*, edited by F. Durst, D. E. Launder, F. W. Schmidt, and J. H. Whitelaw (Springer, New York, 1979), p. 353.

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