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A new approach to LES based on explicit filtering

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Abstract

A new model for large eddy simulation is derived by considering a formal extension to the deconvolution method of Stolz et al. [Stolz, S., Adams, N., 1999. An approximate deconvolution procedure for large-eddy simulation. Phys. Fluids 11, 1699–1701] as interpreted in Mathew et al. [Mathew, J., Lechner, R., Foysi, H., Sesterhenn, J., Friedrich, R., 2003. An explicit filtering method for LES of compressible flows. Phys. Fluids 15(8), 2279–2289]. The new model terms are shown to reduce the error in approximating the governing differential equations, and are evaluated with a simple, additional filtering step. This approach holds special promise for compressible flows, which have several kinds of nonlinearities besides convection, because all nonlinearities are treated in a uniform, mathematically consistent way without recourse to heuristic modeling. The method was assessed by computing supersonic channel flows with passive scalar transport at high Reynolds numbers and found to give excellent results.

Keywords: Large-eddy-simulation; Explicit filtering; Approximate deconvolution; Error estimation; Compressible flow

1. Introduction

A large eddy simulation (LES) contains only a range of the largest scales of a turbulent flow. The omitted small scales have an effect on the large scales because the problem is nonlinear. LES models are needed to account for this effect. A heuristic LES model, like the Smagorinsky model, follows from the nature of the additional terms which appear in the LES equations due to the omitted scales. For incompressible flow these are stresses which the model evaluates from known large-scale strain rates. Other heuristic approaches incorporate features expected in an LES such as the transfer of energy between the computed and omitted scales. An accurate LES should require that all properties, known and unknown, be represented accurately in the simulation. However, explicit provisions are not always made, nor have they proved to be necessary. For example, there are several LES approaches without explicit models, termed ILES, which argue that the numerical method provides the required properties implicitly (Boris et al., 1992; Visbal and Rizzetta, 2002). An extension of the ILES concept which combines the LES formalism with an adapted numerical method is discussed in Adams et al. (2004). In this paper, we propose a new approach in which the LES model terms are derived rigorously from the basic equations without any heuristic modeling. The method turns out to be easy to implement as it requires only a few explicit filtering operations.

The equations for an LES field are derived by applying a low-pass filter to the equations for the unfiltered field. New terms, often called sub-grid-scale (SGS) terms, which are functions of the unfiltered field appear. Models like the Smagorinsky model replace such terms with others that depend on the LES field alone. A different approach is to estimate the unfiltered field, use the estimate to compute the SGS terms, and thus close the LES equations. Shah and Ferziger (1995) assumed the implied filter to be a top-hat filter and related the LES variable implicitly to the unfiltered variable through local Taylor series expansions and

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finite difference formulas. The estimated unfiltered field was found by inverting the relation. Geurts (1997) also assumed the implied filter to be a top-hat and constructed inverse filters of various orders such that polynomials could be inverted exactly. In the approximate deconvolution method (ADM) of Stolz and Adams (1999), filters were explicitly defined. A low-order Padé formula (Gaussian-like filter) related the unfiltered variable to the LES variable. During the simulations, approximate deconvolution of the LES field using the van Cittert formula gave an estimate of the unfiltered field. An expectation in these methods is that the deconvolution or inversion yields a field which is accurate over a large part of the computed large scales. In turn, the SGS terms are also accurate over a similar range which ensures the accurate evolution of the LES field. An essential requirement is that the numerical integration scheme is of high resolution so that it does not add its own filtering of large scales. Spectral or compact schemes are good candidates. The scale similarity model of Bardina (1983) is also an example of this approach where the LES field itself is taken as an estimate of the unfiltered field. Another related approach is the velocity estimation model introduced in Domaradzki and Saiki (1997). They perform a supplementary simulation over twice the LES scale range to find an estimate of the unfiltered field which is accurate over the LES scales.

Although deconvolution can be used to compute the SGS terms, a stable LES requires a treatment for the energy transfer to the smaller omitted scales. Excessive transfer will reduce the content of the computed scales resulting in a less accurate solution whereas inadequate transfer will cause the solution to diverge. Methods to handle this requirement are termed regularizations. In mixed models the Smagorinsky part provides for this energy transfer. In ADM, an *ad hoc* low-order term was added, with a free coefficient to provide regularization. A new class of SGS models called high-pass filtered (HPF) models have appeared recently. Using HPF fields with eddy viscosity models provides a regularization and allows LES to be performed without any special wall damping. This type of model has been proposed independently by Vreman (2003) and Stolz et al. (2004). Schlatter et al. (2005) have further improved these models and successfully applied them to transitional flows. Its use for the prediction of compressible flows was suggested by Stolz et al. (2004).

Mathew et al. (2003) interpreted ADM as a nearly equivalent procedure of explicit, low-pass filtering of the solution between integration time-steps. It was shown that the formally separate components of ADM (primary filtering, deconvolution and regularization by a secondary filtering) could all be combined into a single filtering step with a composite filter. This composite filter has a response function which is unity over a large part of the represented wavenumbers and then, beyond an effective cut-off, falls off smoothly to zero at high wavenumbers ensuring that the high wavenumber content is suppressed. The results were found to be accurate and, more importantly for general application, reliable and consistent: solutions improved monotonically when grid spacing or filter cut-off length was reduced.

In this paper, the analysis has been extended to find new model terms which are derived directly from nonlinear terms in the original equations. *All* aspects of this model have been obtained without recourse to heuristics. For a given problem, the simulation may benefit from or even require, some understanding of the flow, but even laminar flows have such requirements. As an added attraction, the model can be implemented in high-resolution direct numerical simulation (DNS) codes easily, using simple, explicit filtering procedures.

As in Mathew et al. (2003), the present model was also applied to supersonic channel flows and found to give good results. Dramatic improvements are not possible when the previous solutions are themselves very close to the corresponding DNS. The uniqueness of the present proposal is that it is a completely non-heuristic LES model, but its advantages may become apparent only with wider application. In the following sections, first, a derivation of the new model is given. After a short description of the numerical method used, results of large-eddy simulations of supersonic channel flow at a bulk Reynolds number $Re = 6000$ and Mach number $Ma = 3$ are discussed. Transport of a passive scalar has also been included. A comparison of LES with the new method, the previous filtering method (with and without regularization) and the corresponding DNS demonstrates the power of the new method.

2. New LES model

The essential aspects of the new method can be understood by applying it to the generic, one-dimensional transport equation for $u(x,t)$,

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \tag{1}$$

where $f(u)$ is a nonlinear function. Computing a low wavenumber solution, as in an LES, implies a filtering of Eq. (1):

$$\frac{\partial \bar{u}}{\partial t} + G * \frac{\partial f(u)}{\partial x} = 0. \tag{2}$$

Here, G is a low-pass filter and filtered quantities are obtained by convolution: $\bar{u} = G * u = \int G(x - x')u(x')\mathrm{d}x'$. Eq. (2) can be written as

$$\frac{\partial \bar{u}}{\partial t} + \frac{\partial f(\bar{u})}{\partial x} = \frac{\partial f(\bar{u})}{\partial x} - G * \frac{\partial f(u)}{\partial x} \tag{3}$$

by introducing the quantity $\partial f(\bar{u})/\partial x$. Eq. (3) is the LES equation, i.e., the equation for the variable $\bar{u}(x,t)$, which is usually considered as the LES variable. The terms on the rhs arise iff $f(u)$ is nonlinear, and require an LES model because u is not known. We can rewrite Eq. (3) as

$$\frac{\partial \bar{u}}{\partial t} + \frac{\partial f(\bar{u})}{\partial x} = \frac{\partial f(\bar{u})}{\partial x} - G * \frac{\partial f(u^*)}{\partial x} + G * \left[\frac{\partial f(u^*)}{\partial x} - \frac{\partial f(u)}{\partial x}\right] \tag{4}$$

by introducing the quantity $\partial f(u^*)/\partial x$. Here $u^*(x,t) = Q * \bar{u}$ is an approximation to $u(x,t)$ obtained by approximate deconvolution. Q is an approximate inverse of the filter G such that $Q * G \approx I$ (identity operator) over most of the large scales considered. When the field $u(x,t)$ has little content beyond these large scales, it follows that

$$G * u^* \approx G * u. \tag{5}$$

Condition (5) is an expectation for an LES performed with the present explicit filtering approach to be successful. If $u(x,t)$ has significant content at computed small scales, which would be suppressed by this method, the LES may be viewed as a strongly smoothed solution. If there is content at very fine scales which are not computed in the LES, the effect of these small scale processes (such as thin fronts/flames) must be accounted for separately. Only then will condition (5) be met.

2.1. Basic model

In the ADM of Stolz and Adams (1999), and the explicit filtering method presented before (Mathew et al., 2003), the model $u = u^*$ was used. Then, the last two terms in Eq. (4) drop out. The resulting LES problem is

$$\frac{\partial \bar{u}}{\partial t} + G * \frac{\partial f(u^*)}{\partial x} = 0; \quad u^* = Q * \bar{u}.$$

To derive the solution procedure, we use the forward Euler scheme just to demonstrate the numerical integration of this LES problem from $\bar{u}^n$ to $\bar{u}^{n+1}$:

$$\bar{u}^{n+1} = \bar{u}^n - \Delta t G * \frac{\partial f(u^{*(n)})}{\partial x}. \tag{6}$$

The timestep is Δt. We can approximate the rhs of Eq. (6) as

$$\bar{u}^n - \Delta t G * \frac{\partial f(u^{*(n)})}{\partial x} = G * \left[u^{*(n)} - \Delta t \frac{\partial f(u^{*(n)})}{\partial x} \right] \tag{7}$$

because we expect condition (5) to hold. Then, the quantity within the square brackets on the rhs of Eq. (7) is the field $u^{*(n+1)}$ that is obtained by integrating Eq. (1) for the unfiltered variable taken to be u^*. The integration of the LES problem can now be written as three steps:

(1) Deconvolution: $u^{*(n)} = Q * \bar{u}^n$.
(2) Integration: $u^{*(n+1)} = u^{*(n)} - \Delta t\ \partial f(u^{*(n)})/\partial x$.
(3) Filtering: $\bar{u}^{n+l} = G * u^{*(n+1)}$.

Since these three steps are executed repeatedly, step (1) follows step (3) and can be combined into the single filtering step

$$u^{*(n+1)} \leftarrow Q * G * u^{*(n+1)}$$

after every integration (step (2)). Over a range of computed large scales, there is no filtering because $QG \approx I$. Over this range, the numerical integration should not cause any filtering either. The filtering characteristics of the composite filter QG on the smallest computed scales are important in determining the efficiency of the LES. If the filtering is too strong, a finer grid (larger range of computed scales) is necessary. If it is too weak, additional filtering is needed. For example, Stolz and Adams (1999) added an *ad hoc* term with a free parameter which was chosen dynamically. This term models the transfer of energy to small scales and is nearly equivalent to a filter which suppresses the high wavenumber part of u^*. In Mathew et al. (2003) it was noted that this additional filtering is not distinct in any meaningful way from moving the cut-off of the composite filter QG to a slightly larger scale, for the filters that they considered.

To summarize: an LES technique with the basic model is obtained by integrating the given differential equation for the unfiltered variable and filtering after every time-step with a composite filter QG. $QG \approx I$ over a range of computed large scales and suppresses content in the high wavenumber part of this range. Any filtering due to the numerical scheme is restricted to the scales which are suppressed by the QG filter.

2.2. Refined model

A refined LES technique is obtained by estimating the two terms on the rhs of Eq. (4) which had vanished in the basic model. By definition, $u^* = Q * \bar{u} = Q * G * u$. Then, the sub-filter-scale (SFS) quantity is

$$f(u^*) - f(u) = f(Q * G * u) - f(u). \tag{8}$$

An *estimate* of this SFS quantity can be obtained by setting $u = u^*$ in the expression on the right hand side of Eq. (8). The differential equation for the LES problem with new terms reads

$$\frac{\partial \bar{u}}{\partial t} + G * \frac{\partial f(u^*)}{\partial x} = G * \frac{\partial}{\partial x}[f(Q * G * u^*) - f(u^*)],$$
$$u^* = Q * \bar{u}.$$

The method proposed above for the basic model applies here. So, the LES is performed by integrating the equation

$$\frac{\partial u^*}{\partial t} + \frac{\partial f(u^*)}{\partial x} = \frac{\partial}{\partial x}[f(Q * G * u^*) - f(u^*)],$$

which is essentially Eq. (1) augmented with model terms, and filtering after each time-step with filter QG. Model terms are found easily by computing each nonlinear term with a further filtered field $Q * G * u^*$. Implementation in direct numerical simulation codes is thus straightforward.

2.3. Model error estimate

Before applying any model, the LES equation is (4). When the approximate deconvolution model $u = u^*$ is applied, the last two terms in (4), which drop out, measure the error in approximating the differential equation

$$\epsilon_0 = G * \left[\frac{\partial f(u^*)}{\partial x} - \frac{\partial f(u)}{\partial x} \right].$$

By using relation (8), and keeping only the leading terms in a Taylor series expansion about u^*, we get

$$\epsilon_0 \approx G * \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial u}\bigg|_{u=u^*}(Q * G - I) * u\right]. \tag{9}$$

In the new model, since an estimate of ϵ_0 has been retained in the LES equation, the approximation error is

$$\epsilon_1 = -G * \frac{\partial}{\partial x}[2f(u^*) - f(Q * G * u^*) - f(u)].$$

Using leading terms in the Taylor series about u^*, and the definition $u^* = Q * G * u$, we get

$$\epsilon_1 \approx -G * \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial u}\bigg|_{u=u^*}(Q * G - I)^2 * u\right]. \tag{10}$$

We can expect that $\|\epsilon_1\| < \|\epsilon_0\|$ when the filter $Q * G$ is such that $\|Q * G * u\| < \|u\|$ or its Fourier transform $0 < \widehat{Q}\widehat{G} < 1$($\|\cdot\|$ is, say, the 2-norm.). This is an a priori expectation that the error in approximating the differential equation reduces when the new model is used. The error falls in the range of represented scales (where $\|G * u\| \neq 0$) only. If there is significant content at smaller scales, this reduction in error does not give an improved solution.

3. Numerical method

The LES equations are derived from the Navier–Stokes equations for compressible flow and the transport equation for a passive scalar (see, for example, Bird et al., 1960). They are written in the usual divergence form for the conservative variables ρ, ρu_1, ρu_2, ρu_3, ρe and $\rho\theta$, where the u_i are the Cartesian velocity components in the streamwise (x_1), wall-normal (x_2) and spanwise (x_3) directions and $\rho\theta$ is the mass concentration of the passive scalar. The density ρ is related to the pressure p and temperature T by the perfect gas equation of state: $p = \rho RT$; R is the gas constant. The specific total energy is $e = p/((\gamma - 1)\rho) + u_iu_i/2$. The viscous stress tensor reads $\tau_{ij} = 2\mu s_{ij} - (2/3)\mu s_{kk}\delta_{ij}$ with $s_{ij} = (1/2)(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$, and the heat flux vector $q_i = -\lambda\partial T/\partial x_i$. Effects of bulk viscosity are neglected. The dynamic viscosity μ follows the power law

$$\frac{\mu}{\mu_{\text{ref}}} = \left(\frac{T}{T_{\text{ref}}}\right)^{0.7}$$

and the heat conductivity reads $\lambda = \mu c_p/Pr$. The Prandtl number Pr and $\gamma = c_p/c_v$ have the constant values 0.7 and 1.4, respectively. Spatial derivatives were obtained with sixth-order, compact difference formulae. The solution was advanced in time using a third-order, optimized Runge–Kutta scheme of Williamson (1980).

3.1. Filters

The nature of the required explicit filter $Q * G$ can be understood with a specific example. For any quantity u to be filtered, we use a simple one-parameter family of Padé filters, defined by the relation (Lele, 1992)

$$\bar{u}_j + \alpha(\bar{u}_{j-1} + \bar{u}_{j+1}) = \left(\alpha + \frac{1}{2}\right)\left[u_j + \frac{1}{2}(u_{j-1} + u_{j+1})\right].$$

$\bar{u}_j$ and u_j are discrete values on an equidistant grid at points $x = x_j$. For a given α, the filter width decreases and the LES includes an increasing range of scales as the grid is refined. We write $\bar{u} = G * u$ and, for periodic functions, obtain the filter response function

$$\widehat{G}(\xi) = \frac{\hat{\bar{u}}(\xi)}{\hat{u}(\xi)} = \left(\alpha + \frac{1}{2}\right)\frac{1 + \cos\xi}{1 + 2\alpha\cos\xi}. \tag{11}$$

The caret denotes Fourier coefficients and ξ is a scaled wavenumber. All represented wavenumbers lie in $[0, \pi]$. The approximate inverse Q is obtained from the finite van Cittert series (see, for example, Stolz and Adams, 1999)

$$Q = \sum_{m=0}^{M}(I - G)^m, \tag{12}$$

where I is the identity operator. This approximation gives an excellent inverse over a range of low wavenumbers, and the range increases with M. Fig. 1(a) shows the filter

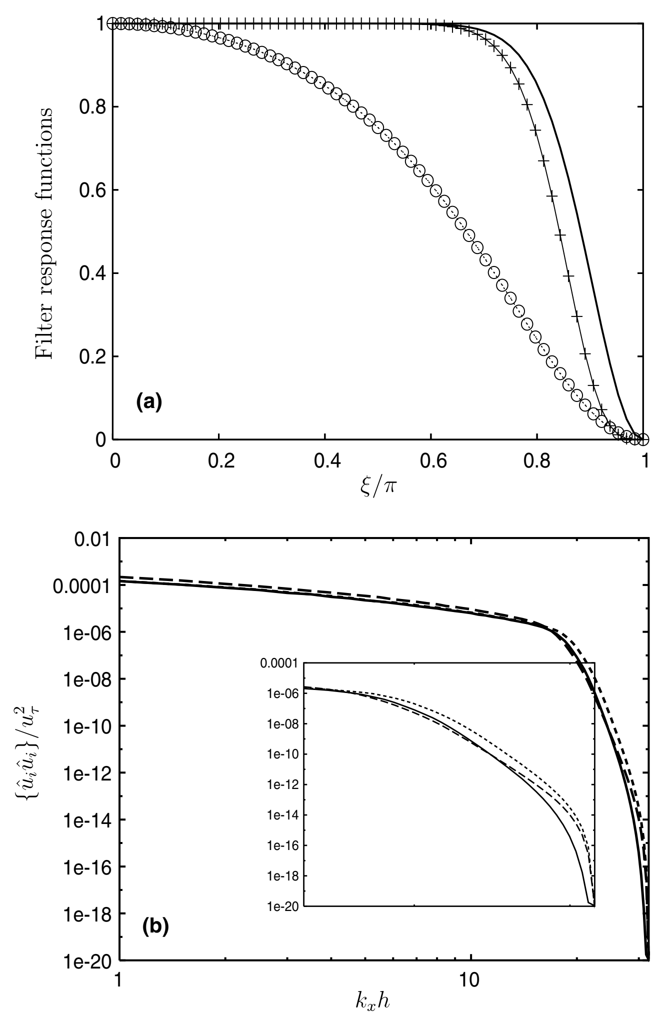

Fig. 1. (a) Filter response functions for $\alpha = 0.25$, $M = 6$. —○—: $\widehat{G}(\xi)$; —: $\widehat{Q}_M(\xi)\widehat{G}(\xi)$; −+−: $\widehat{Q}_M(\xi)\widehat{G}(\xi)\widehat{Q}_M(\xi)\widehat{G}(\xi)(QGR)$; (b) wall-normal-integrated, kinetic energy spectrum - - -: LESnew; – – –: LES$_{QG}$; —: LES$_{QGR}$.

response function $\widehat{G}(\xi)$ for $\alpha = 0.25$. The resultant filter $Q * G$, with $M = 6$, is a perfect low-pass filter for ξ less than 0.6π and then falls off smoothly. This is the required characteristic of the deconvolution operator since we require $u^* \approx u$ over low wavenumbers. Regularization in ADM is obtained by adding a term with a free parameter χ and filter G_2. When $\chi = 1/(m\Delta t)$, this is nearly equivalent to a secondary filtering every m time-steps with filter G_2. Mathew et al. (2003) had applied secondary filtering after every time-step with $G_2 = Q * G$. This composite filter $(Q * G)^2$ is similar to $Q * G$ but has a lower effective cut-off wavenumber (see Fig. 1(a)). So this type of *ad hoc* regularization is only formally present, and cannot be distinguished from the primary deconvolution method. In Stolz et al. (2001), the regularization is distinct because the parameter χ is determined dynamically by measuring the growth of energy at small scales.

Since the present channel flow simulations are periodic in the streamwise and spanwise coordinates, filtering was performed in Fourier space in these directions. For filtering in the wall-normal direction on the non-uniform grid, the filter recommended by Stolz et al. (2001) (see their appendices A.1 and A.2) has been used. The deconvolution is now performed by iteration with the primary filter G. It is more expensive since repeated filtering is required, but still requires only O(N) operations. The error estimates (9) and (10) for ϵ_0 and ϵ_1 can be written in terms of filter widths as follows. Using a Taylor series expansion, filtering can be written as a series (Sagaut, 2002)

$$\bar{u} = G * u = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \overline{\Delta}^k M_k(x) \frac{\partial^k}{\partial x^k} u(x) = \sum_{k=0}^{\infty} \overline{\Delta}^k A_k u(x), \tag{13}$$

where M_k are the moments of the filter and $\overline{\Delta}$ is the filter width. When Q is obtained from the finite sum (12), we have after rearranging

$$Q * G * u = (I - (I - G)^{M+1}) * u.$$

To leading order, using the series form (13) for G,

$$(Q * G - I) * u = \overline{\Delta}^{M+1} A_1^{M+1} u.$$

Now, inserting the expressions for the operator into Eqs. (9) and (10), we have the estimates

$$\epsilon_0 = G * \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial u}\bigg|_{u=u^*} \overline{\Delta}^{M+1} A_1^{M+1} u\right]$$

and

$$\epsilon_1 = G * \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial u}\bigg|_{u=u^*} \overline{\Delta}^{2(M+1)} A_1^{M+1} u\right].$$

Clearly, filter width ($\overline{\Delta}$) and the approximation of the inverse (M) control the error in approximating the governing equation.

4. Results

The simulations were performed to predict turbulent, supersonic channel flow between isothermal walls and transport of a passive scalar introduced from one side and removed from the other. The bulk density ρ_m, velocity u_m and wall temperature T_w were held constant. These quantities and the channel half-width h are used to define the Mach number $\text{Ma} = u_m/c_w$ and the Reynolds number $\text{Re} = \rho_m u_m h/\mu_w$. $Re_\tau = \rho_w u_\tau h/\mu_w$ is the Reynolds number based on the friction velocity $u_\tau = (\tau_w/\rho_w)^{1/2}$. It is a result of the computation. To enforce streamwise periodic boundary conditions in the simulation, the mean pressure gradient $\langle \partial p/\partial x\rangle$ has been replaced by a body force $-F$. During the simulation the body force was controlled to achieve constant mass flux. At time level n

$$F = \frac{\{\rho u_1\}^0 - \{\rho u_1\}^n}{\Delta t} + \frac{\{\tau_{12}\}}{h}.$$

Here, the braces indicate spatial averaging over the two homogeneous (or periodic) directions.

A mean scalar gradient is imposed on the flow, using an initial profile of the form (Johansson and Wikström, 1999)

$$\theta(x_1, x_2, x_3) = \log_{10}\left[\frac{y_0 + x_2}{y_0 - x_2}\bigg/\frac{y_0 + 1}{y_0 - 1}\right], \quad y_0 = 1.007$$

and the boundary conditions $\theta(x_1/h, 0, x_3/h, t) = 1$ and $\theta(x_1/h, 2, x_3/h, t) = -1$.

DNS of supersonic channel flow at $Re_\tau = 221$ had been done previously by Coleman et al. (1995) and Lechner (2001). Foysi et al. (2004) simulated flows with Reynolds numbers up to $Re_\tau = 1030$. With the DNS of Foysi et al. (2004) as a reference, three LES have been performed using the new model (LESnew) and the previous filtering method of Mathew et al. (2003) with secondary filtering (LES_{QGR}) and without (LES_{QG}). The flows are at $Ma = 3$ and $Re = 6000$. The wall temperature is $T_w = 500$ K. The simulations return a Reynolds number of $Re_\tau \approx 560$. In all cases, the $Q * G$ filter is specified by the two parameters $\alpha = 0.25$ in Eq. (11) and $M = 6$ in Eq. (12). Regularized filtering (LES_{QGR}) denotes filtering with $(Q * G)^2$.

The simulations extend over the region $4\pi h \times 2h \times 4/3\pi h$ in the streamwise, wall normal and spanwise directions. Grid sizes for all cases are listed in Table 1. The LES grid has about 32 times fewer points. Data presented here were obtained by averaging over durations of $24h/u_\tau$ for the DNS and $35h/u_\tau$ or more for the LES cases.

Fig. 1(b) gives a first impression of how the different filtering approaches behave in terms of the kinetic energy

Table 1
Number of grid points and mesh sizes

	N_{x_1}	N_{x_2}	N_{x_3}	Δx_1^+	$\Delta x_{2\,\min}^+$	Δx_3^+
DNS560	512	221	256	13.88	0.889	9.25
LESnew	128	111	64	55.48	1.246	36.99
LES_{QGR}	128	111	64	55.39	1.244	36.93
LES_{QG}	128	111	64	54.76	1.230	36.51

spectrum, integrated over the wall-normal x_2-direction. Here, and in the following plots, predictions are based on u_i^* rather than $\bar{u}_i$. As can be expected LES$_{QGR}$ is the lowest curve because there is more filtering loss compared to LES$_{QG}$. With the new model terms, energy levels are higher over most of the wavenumbers but fall off more sharply in the high wavenumber part (see inset).

In this paper, LES results are compared with filtered DNS data. The DNS fields have been filtered with filter QG. We have considered LES to be a computation of a large scale part of a turbulent flow. So the present comparison is with DNS fields of the same spectral range. LES quantities will differ from the actual turbulent flow because of the omitted part, and this must be accounted for separately when LES is used for prediction. Some measures of the overall accuracy are listed in Table 2. The small differences are consistent with the differences in spectral distributions of the energy shown in Fig. 1(b).

Table 2
Mean quantities from LES and DNS solutions

	$\bar{u}_\tau/u_m$	$\bar{\rho}_w/\bar{\rho}_m$	Re_τ
DNS560	0.0373	2.54	565.4
LESnew	0.0371	2.53	562.2
LES$_{QGR}$	0.0370	2.53	562.1
LES$_{QG}$	0.0368	2.53	556.5

Fig. 2(a) shows the distribution of the Van Driest transformed mean stream-wise velocity component

$$u_{\mathrm{VD}}^+ = \int_0^{\bar{u}+} \sqrt{\frac{\bar{\rho}}{\rho_w}} \mathrm{d}\bar{u}^+.$$

Present and previous methods result in excellent agreement with the filtered DNS results. The slope of u_{VD}^+ in the log-region is slightly steeper for the LES results compared to the DNS. It should be emphasized that in compressible flow τ_w is a result of the simulation and is not prescribed through a constant pressure gradient like in incompressible flow. Resolving the viscous sublayer is therefore crucial to getting a good agreement between DNS and LES. This graph may suggest that the simple explicit filtering step is sufficient (LES$_{QGR}$). Such an approach is in general incom-

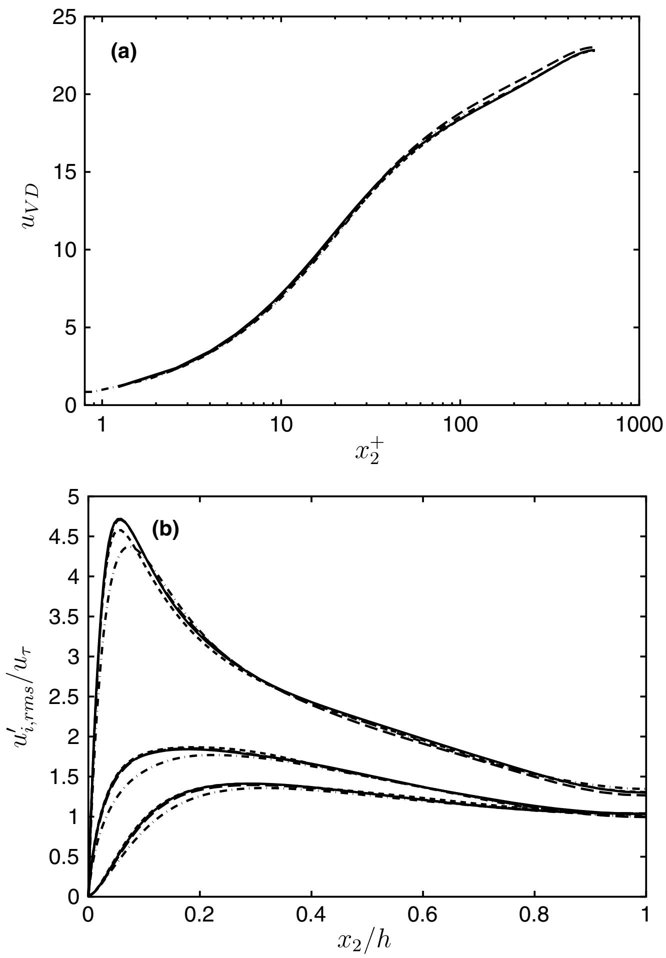

Fig. 2. (a) Van Driest transformed velocity; (b) rms velocity fluctuations. Filtered DNS (dash-dot), LESnew (short dash), LES$_{QG}$ (long dash) and LES$_{QGR}$ (solid).

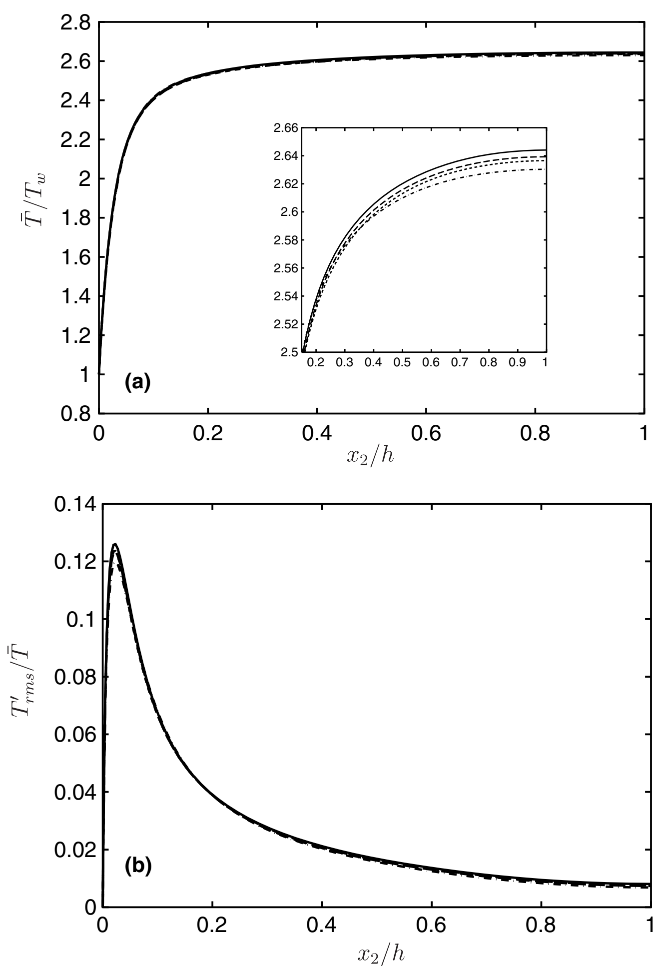

Fig. 3. (a) Mean temperature; (b) rms of temperature fluctuation (line-types as in Fig. 2).

plete. The new method is complete and the result shows that the new model terms are both sufficient for performing the computations on LES grids and that the solution remains accurate. Fig. 2(b) shows results for the rms velocity fluctuations. Again the agreement between DNS and LES is very good. Note that solid and long-dashed lines coincide. It is generally observed that the velocity rms values are larger for the LES results compared to the filtered DNS results, with the peaks being closer to the wall. The new model offers an improvement in reducing the peak value of the streamwise rms velocity and comes closer to the DNS result. Mean temperature and its fluctuations from all the LES are in very close agreement with DNS (Fig. 3). The inset in Fig. 3(a) which magnifies the differences shows that these small differences remain consistent with expectations. The regularized filtering results in a greater departure from the DNS solution compared to just filtering with $Q * G$. And, the new model brings the solution slightly closer to filtered DNS.

It is interesting to see how the models perform in calculating higher-order statistical quantities, even though a full discussion is outside the scope of this paper (details are available elsewhere Foysi, 2005). For example, Figs. 4(a) and (b) show the dissipation rates in the balance equations for the streamwise and wall normal turbulent stresses $\langle \rho u_i'' u_j'' \rangle$, where the primes indicate Favre fluctuations. The dissipation rates show higher values in the viscous sublayer and lower values in the logarithmic region for the LES data compared to the DNS data. The basic filtering approach shows the lowest dissipation rate whereas the present new model shows the best performance. For completeness, the prediction of the passive scalar field has been included in Fig. 5. Small differences are found in the rms of scalar fluctuations. This quantity has two peaks as a result of mean scalar gradient-production in the wall layer and in the channel core. Again, the new model shows the best performance in the wall layer and in the core. A similar behaviour is observed for the streamwise and wall-normal scalar fluxes in Fig. 6. The fairly large deviations of the LES from the filtered DNS data are, perhaps, due to the smoothing of the scalar ramp and cliff structures in the LES.

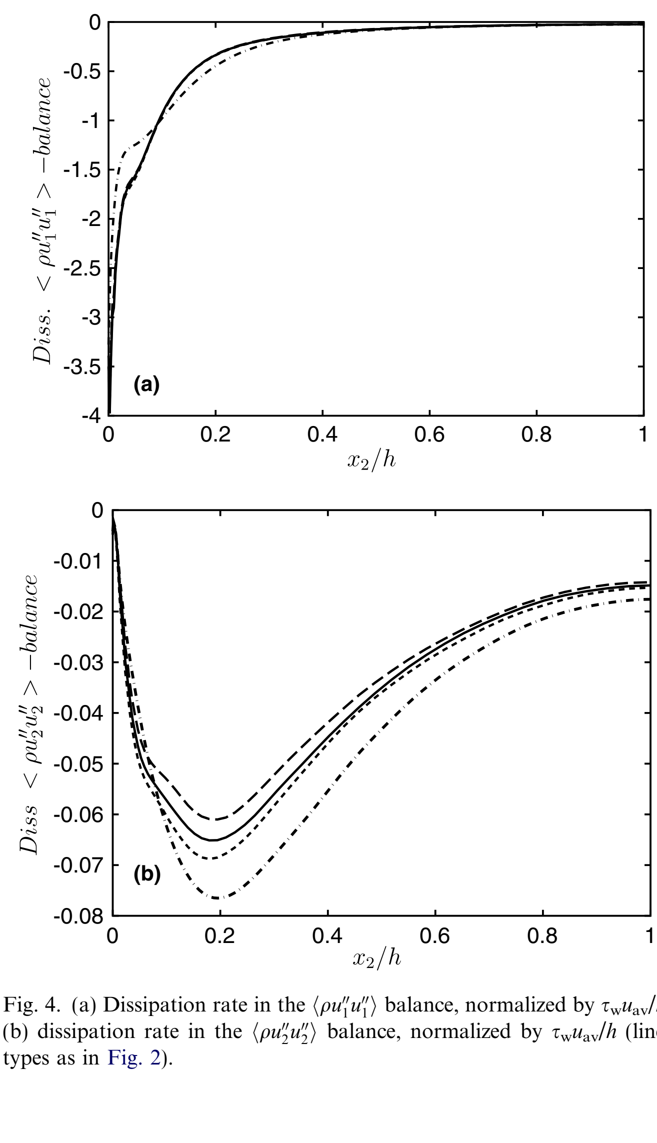

Fig. 4. (a) Dissipation rate in the $\langle \rho u_1'' u_1'' \rangle$ balance, normalized by $\tau_w u_{av}/h$; (b) dissipation rate in the $\langle \rho u_2'' u_2'' \rangle$ balance, normalized by $\tau_w u_{av}/h$ (line-types as in Fig. 2).

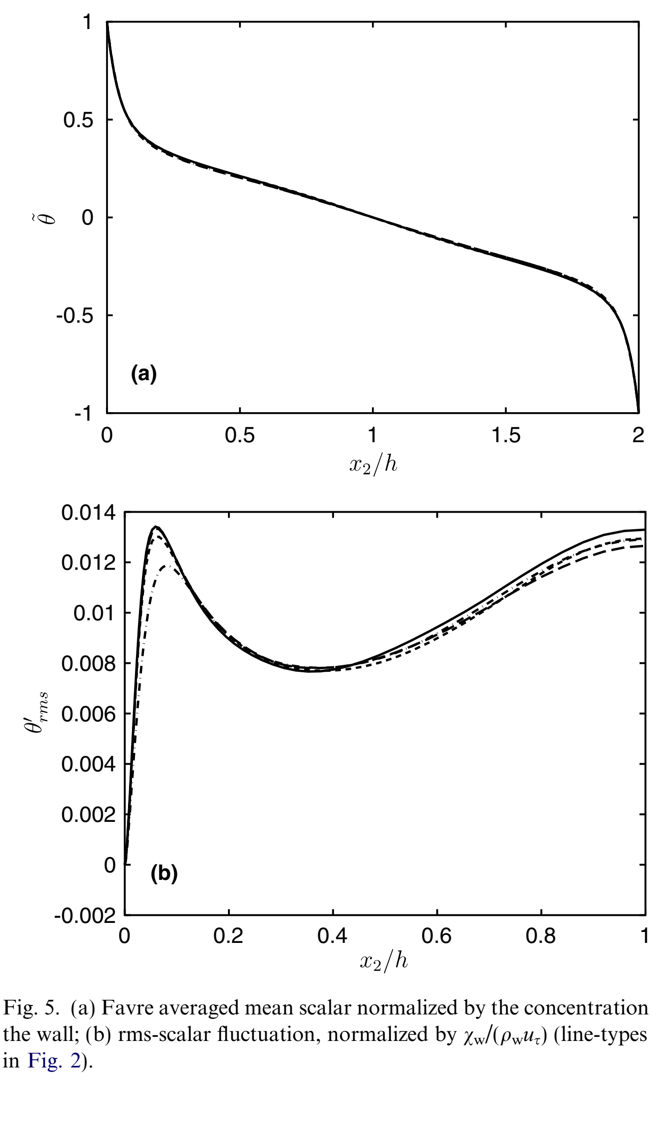

Fig. 5. (a) Favre averaged mean scalar normalized by the concentration at the wall; (b) rms-scalar fluctuation, normalized by $\chi_w/(\rho_w u_\tau)$ (line-types as in Fig. 2).

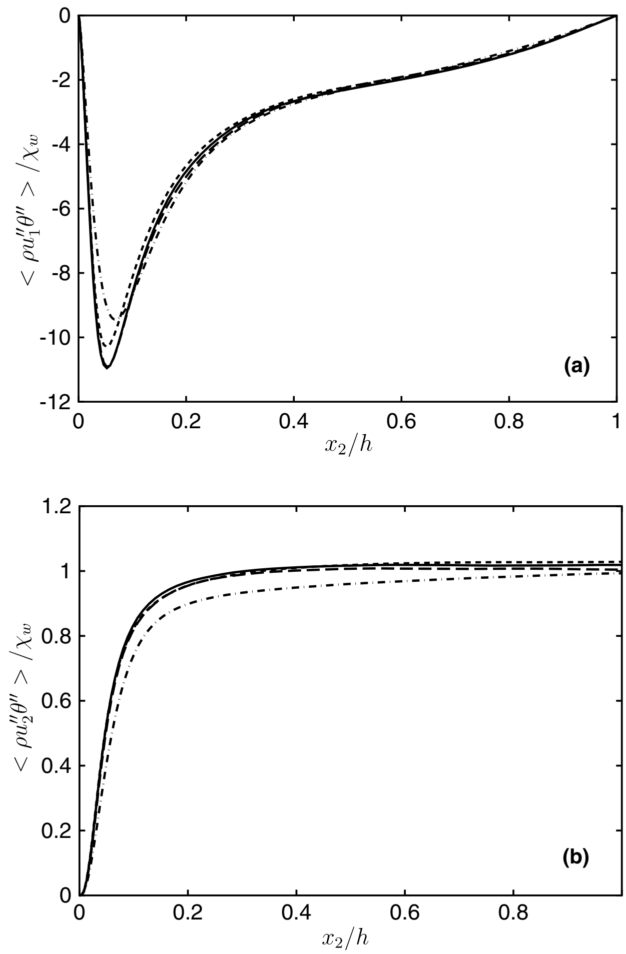

Fig. 6. Turbulent scalar flux, normalized by the scalar diffusion flux at the wall (a) $\langle \rho u_1''\theta'' \rangle$; (b) $\langle \rho u_2''\theta'' \rangle$ (line-types as in Fig. 2).

5. Conclusions

A new approach to LES has been proposed and tested in supersonic channel flow with passive scalar transport. The model is derived directly from the governing equations of the flow without any heuristic modeling. In the basic model presented before, the unclosed terms which appear on filtering were estimated using an approximate deconvolution of the filtered field and resulted in simple explicit filtering procedure for LES. In the refinement presented here, new terms appear which can also be estimated by an additional filtering. In the test flow, the new method was shown to give accurate results. In the past, LES models which appeared to mimic the model terms, such as the scale similarity model, were not complete by themselves. Then, computations diverged unless some kind of regularization was added to take care of the net transfer of energy out of the field at the represented small scales. The Leray form, which provides automatic regularization, is an exception (Geurts and Holm, 2003). The present model, appears to offer a similar, built-in regularization. It remains to be determined whether the new terms provide just the right corrections so that solutions on a given grid are not very sensitive to the cut-off location of the filter $Q * G$.

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