

Developing a subgrid scale noise model for use with large-eddy simulation

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1. Motivation and objectives

In the aeroacoustic calculation of turbulent flows using large-eddy simulation (LES), the temporal frequency range of the predicted sound is a direct function of the available resolution; a more resolved simulation will have a wider range of acoustic frequencies. In the prediction of jet noise, for example, Bodony & Lele (2005) found their acoustic spectra to be limited to Strouhal numbers of $St = fU_j/D_j \leq 1.2$ due to the resolution. Such limitations are unacceptable for engineering predictions as the ‘missing noise’ may be important. Again using the example of jet noise, when scaled to realistic dimensions the missing noise with $St > 1.2$ corresponds to those frequencies which are most sensitive to the human ear (Pierce 1994) and which are weighted most heavily during the noise certification process (Huff 2001). Therefore, a need exists to develop techniques for recovery or for estimation of this missing noise.

The needs of a subgrid scale noise model are different from those of usual subgrid scale stress closures. Typical subgrid scale models used in LES, for example in the Smagorinsky model (Smagorinsky 1963), in its dynamic variant (Germano *et al.* 1991), or in the scale similarity model (Bardina *et al.* 1980), give an expression for the unclosed stress

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j \quad (1.1)$$

in terms of the resolved velocity field \bar{u}_i and its gradient. Here, the LES-defining filter is denoted by an overbar, in lieu of a more precise definition, which will be given later. The tensor τ_{ij} is needed point-wise in the calculations and, except in a few situations such as the Approximate Deconvolution Model (ADM) by Stolz & Adams (1999), the implied subgrid velocity u'_i , is not resolvable by definition and is therefore not available.

For analogy-based aeroacoustic predictions one needs not just τ_{ij} but also u'_i (and ρ' and p' for compressible calculations), as the space-time statistics of the noise source are key. For example, in the Lighthill acoustic analogy (Lighthill 1952) context, the far-field pressure spectrum is directly related to the space-time correlation (with averaging denoted by $\langle \cdot \rangle$)

$$\langle T_{ij}(\mathbf{x}_1, t_1) T_{k\ell}(\mathbf{x}_2, t_2) \rangle$$

with

$$T_{ij}(\mathbf{x}, t) = (\bar{\rho} + \rho')(\bar{u}_i + u'_i)(\bar{u}_j + u'_j) + [(\bar{p} + p') - p_\infty - a_\infty^2((\bar{\rho} + \rho') - \rho_\infty)]\delta_{ij}$$

for which the \mathbf{x} - t dependence of the subgrid scale field is needed. However, by definition, these quantities are not resolvable on the provided grid, and alternative representations must be found. Thus a first step in deriving a subgrid scale noise model is finding a suitable model for the subgrid fluctuations.

One such alternative is the development of a subgrid scale model that estimates the subgrid fields directly and that permits direct calculation of terms such as $\overline{u'_i u'_j}$, which are

needed in the expression for the subgrid scale stress τ_{ij} in (1.1). This stress reconstruction argument implies an interest in a decomposition of the subgrid scale fields that efficiently characterizes the high wavenumber fluctuations. The WKB (Wentzel-Kramers-Brillouin) approximation is one form in which the highly oscillatory phase is represented by a slowly varying function. In the context of three-dimensional turbulent flows, the WKB-RDT approach of Nazarenko *et al.* (1999) was effective.

Following the work of Laval *et al.* (2004) on two-dimensional, incompressible turbulence, a numerical method is formulated which will be used to model the subgrid scale fluctuations and will ultimately lead to SGS noise predictions. It is to be noted that the present work does not attempt to prescribe a relation between the subgrid scale fluctuations and the resolved field, as is done in typical LES subgrid scale stress closures. Rather, the Gabor transform, which is defined in the following section, will be used to perform a scale separation in spatial-wavenumber space. Then for the subgrid scale quantities with a wavenumber $|\mathbf{k}|$ greater than a cut-off, for example the grid Nyquist wavenumber k_N , approximate equations will be derived that describe their evolution. The subgrid fluctuations will then be used to reconstruct the unclosed stresses such as τ_{ij} . Of more importance to the missing noise problem, the subgrid scale contribution to noise source terms can be estimated as for $\langle T_{ij}(\mathbf{x}_1, t_1) T_{k\ell}(\mathbf{x}_2, t_2) \rangle$, discussed above.

2. The Gabor transform and definitions

Let the function $\hat{q}(\mathbf{x}, \mathbf{k}, t)$, with $\mathbf{x}, \mathbf{k} \in \mathbb{R}^3$, be the *Gabor transform* (Gabor 1946) of the function $q(\mathbf{x}, t)$ defined by

$$\hat{q}(\mathbf{x}, \mathbf{k}, t) = \int_{\mathbb{R}^3} f(\epsilon^*|\mathbf{x} - \mathbf{x}_0|) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}_0)} q(\mathbf{x}_0, t) d\mathbf{x}_0 \quad (2.1)$$

where $f(\mathbf{x})$ is a ‘smooth’ function with maximum at $\mathbf{x} = \mathbf{0}$ and compact support, or effectively compact as with $f(x) = \exp(-x^2)$. The parameter ϵ^* is related to the separation of scales and will be discussed in detail below. By integrating both sides of (2.1) with respect to the wavenumber \mathbf{k} the inverse transform is found as

$$q(\mathbf{x}, t) = \frac{1}{f(0)(2\pi)^3} \int_{\mathbb{R}^3} \hat{q}(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}. \quad (2.2)$$

Also, a *low-pass filter* in physical space is defined as the convolution between f^2 and the quantity to be filtered, and the filtered variable is denoted with an overbar, as in

$$\bar{q}(\mathbf{x}, t) = \int_{\mathbb{R}^3} f^2(\epsilon^*|\mathbf{x} - \mathbf{x}_0|) q(\mathbf{x}_0, t) d\mathbf{x}_0. \quad (2.3)$$

The difference $q'(\mathbf{x}, t) = q(\mathbf{x}, t) - \bar{q}(\mathbf{x}, t)$ will be referred to as the *subfilter fluctuation*, or subgrid scale fluctuation, where the definition of ‘small’ is tied to ϵ^* .

2.1. Defining ‘small’ through ϵ^*

Dimensionally ϵ^* used in (2.1) has dimensions of (1/length) and is to be interpreted as that lengthscale $\ell^* = 1/\epsilon^*$ for which the large scale field has characteristic length $L \gg \ell^*$ and the subfilter field has length $\ell \ll \ell^*$. When applied in a LES the grid *induces* a lengthscale $\ell^* = \Delta$, with, for example, $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$, so that the filter (2.3) retains those motions with characteristic lengthscale greater than Δ . If we further assume that

the most energetic wavenumbers of turbulence are resolved in the LES, their associated lengthscales L will satisfy $L \gg \Delta$.

Suppose we nondimensionalize the equations by the lengthscale of the subfilter fluctuations ℓ . By (2.1), q' can be represented as the sum of complex-valued amplitude and phase functions, i.e. wavepackets, with the phase function varying much faster in space than does the amplitude. This is analogous to the WKB ansatz. Thus we can write (with $\mathbf{X} = \mathbf{x}/\ell$, $\epsilon = \epsilon^* \ell \ll 1$ and $\mathbf{K} = \mathbf{k}\ell \sim \mathcal{O}(1)$)

$$\overline{q'}(\mathbf{X}, t) = \int_{\mathbb{R}^3} f^2(\epsilon|\mathbf{X} - \mathbf{X}_0|) (\hat{A}(\mathbf{X}, t) e^{i\mathbf{K} \cdot \mathbf{X}_0} + \mathcal{O}(\epsilon)) d\mathbf{X}_0, \quad (2.4)$$

where $\hat{A}(\mathbf{X}_0, t) = \hat{A}(\mathbf{X}, t) + \mathcal{O}(\epsilon)$ is the wavepacket amplitude expanded in a Taylor series about the point \mathbf{X} . Equation (2.4) is now the integral of the windowed complex exponential where periodicity of $\exp\{i\mathbf{K} \cdot \mathbf{X}_0\}$ ensures that most of the integral cancels. In fact, if f is Gaussian then the integral is $\mathcal{O}(\epsilon^{-3} e^{-1/\epsilon^2})$, which tends to zero much faster than $\mathcal{O}(\epsilon)$. The result that $\overline{q'} \sim \mathcal{O}(\epsilon)$ immediately follows.

To obtain an asymptotically convergent expansion in the case of scale separation we require $\epsilon = \epsilon^*/|\mathbf{k}| \ll 1$ for a wavepacket of wavenumber \mathbf{k} . In a LES in which a distinct scale separation does not exist, the approximations made ‘to order ϵ^* ’ constitute the model; that is, WKB-like assumptions are made and a simplified set of equations is derived. Only in the aforementioned scale separated limit are they rigorous.

2.2. Properties of the Gabor transform

With these definitions the following properties are found:

(a) Filter of a subgrid scale fluctuation:

$$\overline{\overline{q'}} = 0 + \mathcal{O}(\epsilon^*) \quad (2.5)$$

(b) Filter of a filtered quantity:

$$\overline{\overline{q}} = \overline{q} + \mathcal{O}(\epsilon^*) \quad (2.6)$$

(c) Commutation of filtering and differentiation away from solid boundaries:

$$\overline{\partial_{x_j} q} = \partial_{x_j} \overline{q}. \quad (2.7)$$

(d) Gabor transform of the gradient of a small scale fluctuation:

$$\widehat{\frac{\partial q'}{\partial x_j}} = ik_j \hat{q} + \mathcal{O}(\epsilon^*) \quad (2.8)$$

(e) Gabor transform of the bilinear product of \overline{q} and q' :

$$\widehat{q' \overline{q}} = \overline{q} \hat{q} + i \nabla_{\mathbf{x}} \overline{q} \cdot \nabla_{\mathbf{k}} \hat{q} + \mathcal{O}(\epsilon^*) \quad (2.9)$$

(f) Gabor transform of the mean velocity \overline{u}_j and a small scale gradient

$$\overline{u}_j \widehat{\frac{\partial q'}{\partial x_j}} = ik_j \overline{u}_j \hat{q} - \hat{q} \partial_{x_j} \overline{u}_j - \nabla_{\mathbf{x}}(k_j \overline{u}_j) \cdot \nabla_{\mathbf{k}} \hat{q} \quad (2.10)$$

3. Subgrid scale equations

Using the above definitions and properties, the filtered equations may be constructed in the usual sense of the Navier-Stokes equations for the variables of specific volume $\overline{\vartheta}$,

velocity $\bar{\mathbf{u}}$, and entropy \bar{s} . Subtracting the filtered equations from the original, unfiltered equations yields the *subfiltered* equations for the specific volume ϑ' , velocity u'_i , and entropy s'

$$\frac{\partial \vartheta'}{\partial t} + u_j \frac{\partial \vartheta'}{\partial x_j} - \overline{u_j \frac{\partial \vartheta'}{\partial x_j}} = \vartheta' \nabla \cdot \mathbf{u} - \overline{\vartheta' \nabla \cdot \mathbf{u}} \quad (3.1)$$

$$\frac{\partial u'_i}{\partial t} + u_j \frac{\partial u'_i}{\partial x_j} - \overline{u_j \frac{\partial u'_i}{\partial x_j}} + \vartheta' \frac{\partial p}{\partial x_i} - \overline{\vartheta' \frac{\partial p}{\partial x_i}} = \vartheta' \frac{\partial \sigma_{ji}}{\partial x_j} - \overline{\vartheta' \frac{\partial \sigma_{ji}}{\partial x_j}} \quad (3.2)$$

$$\begin{aligned} \frac{\partial s'}{\partial t} + u_j \frac{\partial s'}{\partial x_j} - \overline{u_j \frac{\partial s'}{\partial x_j}} = & -\gamma \left[\frac{\vartheta'}{T} \nabla \cdot \mathbf{q} - \overline{\frac{\vartheta'}{T} \nabla \cdot \mathbf{q}} \right. \\ & \left. - \left(\frac{\vartheta' \sigma_{ji}}{T} \frac{\partial u'_i}{\partial x_j} - \overline{\frac{\vartheta' \sigma_{ji}}{T} \frac{\partial u'_i}{\partial x_j}} \right) \right] \end{aligned} \quad (3.3)$$

Here, $\sigma_{ij} = \mu(\partial_j u_i + \partial_i u_j) + \lambda \partial_k u_k \delta_{ij}$ is the viscous stress tensor and $q_i = -\kappa \partial_i T$ is the heat flux vector.

If the decomposition $(\cdot) = \overline{(\cdot)} + (\cdot)'$ is employed then the subfilter equations take the more familiar form of

$$\begin{aligned} \frac{\partial \vartheta'}{\partial t} + \bar{u}_j \frac{\partial \vartheta'}{\partial x_j} + u'_j \frac{\partial \bar{\vartheta}}{\partial x_j} + u'_j \frac{\partial \vartheta'}{\partial x_j} - \vartheta' \nabla \cdot \bar{\mathbf{u}} - \bar{\vartheta} \nabla \cdot \mathbf{u}' - \vartheta' \nabla \cdot \mathbf{u}' \\ = \left(\overline{u_j \frac{\partial \vartheta'}{\partial x_j}} - \bar{u}_j \frac{\partial \bar{\vartheta}}{\partial x_j} \right) - \left(\overline{\vartheta' \nabla \cdot \mathbf{u}} - \bar{\vartheta} \nabla \cdot \bar{\mathbf{u}} \right) \end{aligned} \quad (3.4)$$

$$\begin{aligned} \frac{\partial u'_i}{\partial t} + u'_j \frac{\partial \bar{u}_i}{\partial x_j} + \bar{u}_j \frac{\partial u'_i}{\partial x_j} + u'_j \frac{\partial u'_i}{\partial x_j} + \vartheta' \frac{\partial \bar{p}}{\partial x_i} + \bar{\vartheta} \frac{\partial p'}{\partial x_i} + \vartheta' \frac{\partial p'}{\partial x_i} - \vartheta' \frac{\partial \bar{\sigma}_{ji}}{\partial x_j} - \bar{\vartheta} \frac{\partial \sigma'_{ji}}{\partial x_j} - \vartheta' \frac{\partial \sigma'_{ji}}{\partial x_j} \\ = \left(\overline{u_j \frac{\partial u'_i}{\partial x_j}} - \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} \right) + \left(\overline{\vartheta' \frac{\partial p'}{\partial x_i}} - \bar{\vartheta} \frac{\partial \bar{p}}{\partial x_i} \right) - \left(\overline{\vartheta' \frac{\partial \sigma_{ji}}{\partial x_j}} - \bar{\vartheta} \frac{\partial \bar{\sigma}_{ji}}{\partial x_j} \right) \end{aligned} \quad (3.5)$$

$$\begin{aligned} \frac{\partial s'}{\partial t} + u'_j \frac{\partial \bar{s}}{\partial x_j} + \bar{u}_j \frac{\partial s'}{\partial x_j} + u'_j \frac{\partial s'}{\partial x_j} + \gamma \left[\left(\frac{\vartheta'}{T} \right)' \nabla \cdot \bar{\mathbf{q}} + \overline{\left(\frac{\vartheta'}{T} \right) \nabla \cdot \mathbf{q}'} + \left(\frac{\vartheta'}{T} \right)' \nabla \cdot \mathbf{q}' \right] \\ - \gamma \left[\left(\frac{\vartheta' \sigma_{ji}}{T} \right)' \frac{\partial \bar{u}_i}{\partial x_j} + \overline{\left(\frac{\vartheta' \sigma_{ji}}{T} \right) \frac{\partial u'_i}{\partial x_j}} + \left(\frac{\vartheta' \sigma_{ji}}{T} \right)' \frac{\partial u'_i}{\partial x_j} \right] \\ = \left(\overline{u_j \frac{\partial s'}{\partial x_j}} - \bar{u}_j \frac{\partial \bar{s}}{\partial x_j} \right) + \gamma \left[\left(\overline{\frac{\vartheta'}{T} \nabla \cdot \mathbf{q}} - \left(\frac{\vartheta'}{T} \right) \nabla \cdot \bar{\mathbf{q}} \right) \right] - \gamma \left[\overline{\frac{\vartheta' \sigma_{ji}}{T} \frac{\partial u'_i}{\partial x_j}} - \left(\frac{\vartheta'}{T} \right) \frac{\partial \bar{u}_i}{\partial x_j} \right] \end{aligned} \quad (3.6)$$

Equations (3.4)–(3.6) are of the general form of $N(q') = R(q)$ where N is a nonlinear operator and R is a ‘forcing’ term. Under the assumption that $\overline{(\cdot)} \gg (\cdot)'$ products of subfilter scale fluctuations may be neglected relative to the bilinear products of the filtered and subfilter quantities. In the wavenumber space \mathbf{k} this assumption may be called ‘nonlocal,’ as the wavenumbers describing a filtered quantity are (assumed to be) much smaller than those describing a subfiltered quantity, and products that are local in \mathbf{k} are neglected.

Applying the Gabor transform (2.1) and utilizing the properties enumerated in Section

1 the linear equations for the Gabor coefficients $\{\hat{\vartheta}, \hat{u}_i, \hat{s}\}$ may be derived as

$$\frac{D\hat{\vartheta}}{Dt} - 2\bar{\theta}\hat{\vartheta} + \hat{u}_j \frac{\partial \bar{\vartheta}}{\partial x_j} + i \left[\frac{\partial^2 \bar{\vartheta}}{\partial x_i \partial x_j} + \frac{\partial \bar{\theta}}{\partial x_j} \frac{\partial \hat{\vartheta}}{\partial k_j} - k_j \hat{u}_j \bar{\vartheta} \right] + \frac{\partial}{\partial x_\ell} (\bar{\vartheta} k_j) \frac{\partial \hat{u}_j}{\partial k_\ell} = \hat{Q} \quad (3.7)$$

$$\begin{aligned} \frac{D\hat{u}_i}{Dt} - \bar{\theta}\hat{u}_i + \hat{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + i \left[\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_\ell} \frac{\partial \hat{u}_j}{\partial k_\ell} + k_i \hat{p} \bar{\vartheta} + \frac{\partial^2 \bar{p}}{\partial x_i \partial x_\ell} \frac{\partial \hat{\vartheta}}{\partial k_\ell} \right] \\ - \frac{\partial \bar{\vartheta}}{\partial x_i} \hat{p} - \frac{\partial}{\partial x_\ell} (k_i \bar{\vartheta}) \frac{\partial \hat{p}}{\partial k_\ell} + \hat{\vartheta} \frac{\partial \bar{p}}{\partial x_i} - \bar{\vartheta} \frac{\partial \sigma'_{ji}}{\partial x_j} - \widehat{\vartheta' \sigma'_{ji}} = \hat{F}_i \end{aligned} \quad (3.8)$$

$$\frac{D\hat{s}}{Dt} - \bar{\theta}\hat{s} + i \frac{\partial^2 \bar{s}}{\partial x_j \partial x_\ell} \frac{\partial \hat{u}_j}{\partial k_\ell} + \hat{u}_j \frac{\partial \bar{s}}{\partial x_j} + \hat{V} = \hat{S} \quad (3.9)$$

where $\bar{\theta} = \partial_{x_j} \bar{u}_j$ is the filtered dilatation and \hat{Q} , \hat{F}_i , and \hat{S} are the components of the Gabor transformed ‘force’ R . Lastly, \hat{V} is the Gabor transform of the viscous terms in the subfilter entropy in (3.6). The derivative D/Dt is given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_\ell} (k_j \bar{u}_j) \frac{\partial}{\partial k_\ell} \quad (3.10)$$

and represents differentiation along the characteristic in $\mathbf{x}\text{-}\mathbf{k}$ space with trajectory

$$\dot{\mathbf{x}} = \mathbf{u} \quad (3.11)$$

$$\dot{\mathbf{k}} = -\nabla_{\mathbf{x}} (k_\ell \bar{u}_\ell). \quad (3.12)$$

Fluctuations in the pressure p' and temperature T' are related to those of the primary variables s' and ϑ' by the linearized equations of state:

$$p'/\bar{p} = s' - \gamma \vartheta'/\bar{\vartheta} \quad (3.13)$$

$$T'/\bar{T} = s' - (\gamma - 1) \vartheta'/\bar{\vartheta}. \quad (3.14)$$

Substitution of these relations into (3.7)–(3.9) closes the system. As an aside, it is possible to use the Gabor-transformed equations of state directly to determine \hat{p} and \hat{T} through an implicit relation between \hat{p} and its \mathbf{k} -derivative.

4. Numerical discretization of the subfilter equations

An approximate form of (3.7)–(3.9) is implemented numerically as Lagrangian particles that follow trajectories in the $\mathbf{x}\text{-}\mathbf{k}$ space. The discretization of the subfilter equations proceeds by writing the subfiltered fields as (Laval *et al.* 2004)

$$\hat{\vartheta}(\mathbf{x}, \mathbf{k}, t) = \sum_{\alpha=1}^{N_p} \sigma_\alpha^{\hat{\vartheta}}(t) S_{\mathbf{x}}(\mathbf{x} - \mathbf{x}_\alpha) S_{\mathbf{k}}(\mathbf{k} - \mathbf{k}_\alpha) \quad (4.1)$$

$$\hat{u}_i(\mathbf{x}, \mathbf{k}, t) = \sum_{\alpha=1}^{N_p} \sigma_\alpha^{\hat{u}_i}(t) S_{\mathbf{x}}(\mathbf{x} - \mathbf{x}_\alpha) S_{\mathbf{k}}(\mathbf{k} - \mathbf{k}_\alpha) \quad (4.2)$$

$$\hat{s}(\mathbf{x}, \mathbf{k}, t) = \sum_{\alpha=1}^{N_p} \sigma_\alpha^{\hat{s}}(t) S_{\mathbf{x}}(\mathbf{x} - \mathbf{x}_\alpha) S_{\mathbf{k}}(\mathbf{k} - \mathbf{k}_\alpha), \quad (4.3)$$

where α enumerates the N_p particles with location $\mathbf{x}_\alpha(t)$ and wavenumber $\mathbf{k}_\alpha(t)$. The particle amplitudes are given by $\{\sigma_\alpha^{\hat{v}}(t), \sigma_\alpha^{\hat{u}_i}(t), \sigma_\alpha^{\hat{s}}(t)\}$. The functions $S_{\mathbf{x}}$ and $S_{\mathbf{k}}$ are the support for each particle in the \mathbf{x} and \mathbf{k} spaces. In general,

$$S_{\mathbf{x}}(\mathbf{x}) = \zeta_{\epsilon_x}(\mathbf{x}) \quad (4.4)$$

$$S_{\mathbf{k}}(\mathbf{k}) = \zeta_{\epsilon_k}(\mathbf{k}) \quad (4.5)$$

where $\zeta_\epsilon(\mathbf{x}) := \epsilon^{-3}\zeta(\mathbf{x}/\epsilon)$ (with ϵ representing either ϵ_k or ϵ_x) is the so-called ‘blob function,’ which approaches the Dirac distribution in the limit as $\epsilon \rightarrow 0$. This choice of functions $S_{\mathbf{x}}$ and $S_{\mathbf{k}}$ makes the Lagrangian method similar to that outlined by Eldredge *et al.* (2002) and to vortex particle methods (Cottet & Koumoutsakos 2000). The order of accuracy is determined once the function ζ is chosen. For this application we choose the second order representation

$$\zeta(\mathbf{x}) = \pi^{-3/2} \exp\{-|\mathbf{x}|^2\}. \quad (4.6)$$

4.1. Calculation of \hat{Q} , \hat{F}_i and \hat{S}

The ‘forcing’ terms Q , F_i and S must be Gabor transformed before use in (3.7)–(3.9). A fast, three-dimensional algorithm for computing the Gabor transform does not seem to exist but in the case of periodic functions the fast Fourier transform may be used. Consider the Fourier series representation of Q ,

$$Q(\mathbf{x}) = \sum_{\ell, m, n = -N/2}^{N/2-1} c_{\ell, m, n} e^{i(\ell x + m y + n z)}, \quad (4.7)$$

where $c_{\ell, m, n}$ are the Fourier coefficients of Q . Applying the Gabor transform (2.1) then yields

$$\hat{Q}(\mathbf{x}, \mathbf{k}) = (\pi^{1/2}/\epsilon^*)^3 \sum_{\ell, m, n} c_{\ell, m, n} e^{i(\ell x + m y + n z)} e^{-(2\epsilon^*)^{-2}[(\ell + k_1)^2 + (m + k_2)^2 + (n + k_3)^2]} \quad (4.8)$$

where $\mathbf{k} = (k_1, k_2, k_3)$. Thus (4.8) is the Gabor transform of Q . The particle representation follows by writing $\sigma_\alpha^{\hat{Q}} = \hat{Q}(\mathbf{x}_\alpha, \mathbf{k}_\alpha)$ for particle α . Precisely the same argument follows for F_i and S .

4.2. Final form of the equations

Using the particle expansions of (4.1)–(4.3) the final form of the subfiltered equations for each particle is arrived upon:

$$\dot{\mathbf{x}} = \mathbf{u} \quad (4.9)$$

$$\dot{\mathbf{k}} = -\nabla_{\mathbf{x}}(k_\ell \bar{u}_\ell) \quad (4.10)$$

for the trajectories and

$$\frac{D\hat{\vartheta}}{Dt} = 2\bar{\theta}\hat{\vartheta} - \hat{u}_j \frac{\partial \bar{\vartheta}}{\partial x_j} - i \left[\frac{\partial^2 \bar{\vartheta}}{\partial x_i \partial x_j} + \frac{\partial \bar{\theta}}{\partial x_j} \frac{\partial \hat{\vartheta}}{\partial k_j} - k_j \hat{u}_j \bar{\vartheta} \right] - \frac{\partial}{\partial x_\ell} (\bar{\vartheta} k_j) \frac{\partial \hat{u}_j}{\partial k_\ell} + \hat{Q} \quad (4.11)$$

$$\begin{aligned} \frac{D\hat{u}_i}{Dt} = & \bar{\theta}\hat{u}_i - \hat{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - \left(ik_i \bar{p} \bar{\vartheta} - \frac{\partial}{\partial x_i} (\bar{p} \bar{\vartheta}) \right) \hat{s} + \frac{\partial}{\partial x_\ell} (k_i \bar{p} \bar{\vartheta}) \frac{\partial \hat{s}}{\partial k_\ell} - \bar{\vartheta} \frac{\partial \bar{p}}{\partial x_i} \hat{s} - i \frac{\partial \bar{\vartheta}}{\partial x_\ell} \frac{\partial \bar{p}}{\partial x_i} \frac{\partial \hat{s}}{\partial k_\ell} \\ & - i \left[\frac{\partial^2 \bar{\vartheta}}{\partial x_i \partial x_j} + \frac{\partial \bar{\theta}}{\partial x_j} \frac{\partial \hat{\vartheta}}{\partial k_j} \right] + \gamma \left(ik_i \bar{p} - \frac{\partial \bar{p}}{\partial x_i} \right) \hat{\vartheta} - \gamma \frac{\partial}{\partial x_\ell} (k_i \bar{p}) \frac{\partial \hat{\vartheta}}{\partial k_\ell} \\ & + \left(\frac{1}{\bar{\vartheta}} \frac{\partial \bar{p}}{\partial x_i} - \frac{\bar{p}}{\bar{\vartheta}^2} \frac{\partial \bar{\vartheta}}{\partial x_i} \right) \left(\bar{\vartheta} \hat{\vartheta} + i \frac{\partial \bar{\vartheta}}{\partial x_\ell} \frac{\partial \hat{\vartheta}}{\partial k_\ell} \right) + \hat{\vartheta} \frac{\partial \bar{p}}{\partial x_i} \\ & - \frac{\bar{\vartheta} \bar{\mu} |\mathbf{k}|^2 \hat{u}_i + \bar{\vartheta} (\bar{\mu} + \bar{\lambda}) k_i k_j \hat{u}_j}{Re} + \hat{F}_i \end{aligned} \quad (4.12)$$

$$\frac{D\hat{s}}{Dt} = \bar{\theta}\hat{s} - \hat{u}_j \frac{\partial \bar{s}}{\partial x_j} - i \frac{\partial^2 \bar{s}}{\partial x_j \partial x_\ell} \frac{\partial \hat{u}_j}{\partial k_\ell} - \frac{\bar{\mu}}{RePr} \left\{ \frac{(\gamma - 1) \bar{T}}{\bar{p}} |\mathbf{k}|^2 \hat{s} - \gamma (\gamma - 1) |\mathbf{k}|^2 \hat{\vartheta} \right\} + \hat{S} \quad (4.13)$$

for the particle amplitudes. Note that it is assumed that viscous dissipation of subgrid-scale velocity is not strongly dependent on the subfilter fluctuations of the viscosities μ and λ , and $\mathcal{O}(\epsilon^*)$ approximations are made for the remaining viscous terms. It has been noted (Laval *et al.* 2004) that some terms may be negligible for a wide variety of frequently encountered flows; these terms are retained at present until this claim can be verified.

4.3. Reconstruction of the subgrid scale stress

Before the approximate Gabor transform of §4.1 can be applied, the large scale/small scale interaction terms such as

$$u'_j \frac{\partial \bar{u}_i}{\partial x_j},$$

must be expressed in terms of known and resolvable quantities. Consequently, the Gabor transform is chosen, for, by definition, u'_j cannot be resolved on the LES grid and, therefore, the stress cannot be computed. Using the definitions of the Gabor transform (2.1), its associated filter (2.3) and the discretization of (4.1)–(4.3), it is straightforward to show that

$$\overline{u'_j \frac{\partial \bar{u}_i}{\partial x_j}} = \frac{\partial \bar{u}_i}{\partial x_j} \frac{1}{(2\pi)^3} \Re \left\{ \sum_{\alpha=1}^{N_p} \sigma_{\alpha}^{\hat{u}_j}(t) S_{\mathbf{x}}(\mathbf{x} - \mathbf{x}_{\alpha}(t)) \int_{\mathbb{R}^3} S_{\mathbf{k}}(\mathbf{k} - \mathbf{k}_{\alpha}(t)) \hat{f}(-\mathbf{k}) d\mathbf{k} \right\} + \mathcal{O}(\epsilon^*) \quad (4.14)$$

where $\Re(\cdot)$ denotes the real part. Note that the integration over \mathbf{k} can be done analytically and obviates the need to resolve directly any subgrid scale quantity. The Gabor basis function transform \hat{f} is given by

$$\hat{f}(\mathbf{k}) = \int_{\mathbb{R}^3} f(\epsilon^* |\mathbf{x} - \mathbf{x}_0|) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}_0)} d\mathbf{x}_0 \quad (4.15)$$

and may also be computed analytically. Similar manipulations yield the necessary reconstructions for the remaining terms of \hat{Q} , \hat{F}_i , and \hat{S} . The very same argument allows

the reconstruction of the subgrid scale *noise* source terms involving products with the subgrid scale variables, such as $\overline{\rho u_i u_j'}$ in Lighthill's analogy.

5. Conclusions and future work

Using the Gabor transform, a consistent set of large- and small-scale equations are derived for the compressible Navier-Stokes equations. Following a scale separation argument, simplified versions of these equations are proposed that may be easily implemented in a Lagrangian particle framework. When coupled with the particle approach, the equations permit direct calculation of the subgrid scale stress and subgrid scale noise source terms without the necessity of resolving the subgrid scale fluctuations. Equations (4.9)–(4.13) have been implemented in a Message Passing Interface (MPI) code used to simulate compressible homogeneous, isotropic turbulence. Initial results are encouraging but additional verification is needed. Once complete a term-by-term analysis will examine which terms—if any—can be reasonably neglected. Comparisons of the present method with the dynamic Smagorinsky model are expected.

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