Subgrid-scale modeling of shock-turbulence interaction for large-eddy simulations

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1. Motivation and objective

The study of the interaction of a shock passing through a turbulent velocity field has been the focus of considerable attention for several decades. Being a fundamental fluid mechanics problem, a wide range of fields and applications can benefit from an improved understanding of it, such as aeronautics (supersonic and hypersonic flight), astrophysics (supernovae explosions), and energy generation (inertial confinement fusion).

Theoretical studies based on the mode decomposition of turbulence in supersonic flows (Kovásznay 1953) were first developed in Ribner's linear analysis (Ribner 1953, 1954) and revisited by Lee *et al.* (1992). Lele (1992) combined rapid distortion theory (RDT) with gas dynamics to formulate the jump relations across a shock in a turbulent mean flow, whereas Jacquin *et al.* (1993) used RDT and Helmholtz's decomposition of the fluctuating field to obtain two regimes (solenoidal-acoustic and "pressure-released") thus limiting the amplification of turbulent kinetic energy that occurs when the fluid is processed by the shock. Rapid distortion theory incorporates more restrictive assumptions than does the broader linear interaction analysis, resulting in its more limited scope and agreement with experiments. By using recently developed analytical techniques, Wouchuk *et al.* (2009) constructed an exact analytical model of the shock-turbulence interaction obtaining closed-form expressions for several quantities of interest.

Experiments have been carried out in shock tubes and wind tunnels with different means of generating turbulence. Hesselink & Sturtevant (1988) considered the propagation of weak shocks in a random medium and explained the wave front distortion they encountered in terms of medium inhomogeneities that focus/defocus the front. Keller & Merzkirch (1990) used a shock tube with grid-generated turbulence and a shock wave reflecting at the end wall; they saw amplification of turbulence occurring at larger scales, but not at the small scale structures. Barre *et al.* (1996) studied, with hot-wire and laser Doppler velocimetry techniques, the interaction in a wind-tunnel of a normal shock and quasi-homogeneous isotropic turbulence generated using a multinozzle in a Mach 3 flow. They found close agreement with Ribner's linear theory for the amplification of velocity fluctuations, and some discrepancy with earlier experiments for the turbulent energy amplification present at low wave numbers. In an experiment by Agui *et al.* (2005), an incident shock generated an induced flow behind it that passed later through a grid to obtain a nearly homogeneous and isotropic flow field, that was then processed by the reflected shock. Intense-vorticity structures were suggested as the cause of high-amplitude events of time signals of enstrophy, dissipation-rate, and dilatational stretching; the dissipation seemed to have a more dominant effect on the flow motions than the enstrophy.

Direct numerical simulations (DNS) of the shock-turbulence interaction problem have emerged in the literature over the last couple of decades. Lee *et al.* (1993) found partial agreement with linear analysis, with some discrepancy arising as the turbulent Mach number, M_t, was increased, resulting in distorted shock waves lacking a well defined front. This work was later extended to stronger shocks (Lee *et al.* 1997). Hannappel & Friedrich (1995) related the amplification of turbulent kinetic energy to the ratio of compressible to incompressible kinetic energy, explaining the different behavior in terms of the pressure diffusion term of the turbulent kinetic energy equation. Mahesh *et al.* (1997) found that upstream correlations of vorticity-entropy and velocity-temperature fluctuations have a strong influence in the turbulence evolution across the shock. Jamme *et al.* (2002) studied the effect of different types of isotropic turbulence (by combining entropy, vortical, and acoustic fluctuations), and reported their influence in the amplification of kinetic energy and vorticity variance, as well as in the reduction of the transverse microscale. Their results agreed well with linear analysis. Sesterhenn *et al.* (2005) used a shock-fitting algorithm that provided good agreement with the more widely used shock-capturing methods. In the DNS of Larsson (2008), viscous dissipation (and therefore, turbulence) was fully resolved in the most restrictive region immediately downstream of the shock, as it was shown from grid-converged computed statistics. They observed that the Taylor microscale in the streamwise direction was larger than in the transverse direction, which differs from linear analysis and some previous numerical results. This fact was explained by the observed return to isotropy at the smallest scales for the vorticity components and the lack thereof at larger scales. The kinetic energy amplification, on the other hand, agreed well with linear theory. Grube *et al.* (2009) considered highly compressible turbulence and found general agreement with weakly compressible results. They determined that the distortion of the shock by the incoming turbulence resulted in enough movement of the shock upstream so that peak thermodynamic fluctuations occurred toward the upstream side of the interaction region.

The objective of the present research focuses on the modeling aspects of the problem applied to large-eddy simulations (LES). This brief is organized as follows. In section 2 the mathematical formulation of LES is exposed. Section 3 summarizes a set of existing compressible subgrid-scale turbulence models currently used in LES that are applicable to this problem. Section 4 comments on relevant physical aspects of the shock-turbulence interaction problem and their implications in modeling. We end with an outline of future developments in section 5. Because the present work is in an early stage, this brief is intended as a compilation of resources and considerations meant to guide the implementation of subgrid-scale models for LES of shock-turbulence interaction.

2. Mathematical formulation

In this section, the basic equations of compressible fluid motion are recalled, and then their filtered counterpart is developed keeping all terms in the formulation.

2.1. *Governing equations of compressible fluid motion*

Conservation laws of mass, linear momentum, and total energy for a compressible flow, in the absence of external forces, can be expressed, in differential form, as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0, \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2.2}$$

$$\frac{\partial \rho e_T}{\partial t} + \frac{\partial}{\partial x_j}(\rho e_T u_j) = \frac{\partial u_i \sigma_{ij}}{\partial x_j} - \frac{\partial q_j}{\partial x_j}, \tag{2.3}$$

where Einstein summation convention is implied: ρ is the density, u_i is the velocity, $e_T = e + \frac{1}{2}u_i u_i$ is the total energy per unit mass (e is the internal energy per unit mass), q_j is the heat flux given by Fourier's law as $q_j = -\kappa\,\partial T/\partial x_j$ (T is the temperature and κ is the thermal conductivity), and σ_{ij} is the stress tensor, defined as:

$$\sigma_{ij} = -p_m\delta_{ij} + d'_{ij} = -\left(p - \mu_v \frac{\partial u_k}{\partial x_k}\right)\delta_{ij} + d'_{ij} = -p\delta_{ij} + d_{ij}, \tag{2.4}$$

where p_m is the mechanical pressure, p is the thermodynamic (or equilibrium) pressure, μ_v is the bulk (or volume) viscosity, d'_{ij} is the deviatoric part of the stress tensor, which is, for a Newtonian fluid:

$$d'_{ij} = 2\mu\left(S_{ij} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right), \qquad \text{and} \qquad d_{ij} = 2\mu S_{ij} + \left(\mu_v - \frac{2}{3}\mu\right)\frac{\partial u_k}{\partial x_k}\delta_{ij}, \tag{2.5}$$

μ being the dynamic (or shear) viscosity, and $S_{ij} = (1/2)(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ the strain-rate tensor (symmetric part of the velocity gradient tensor).

In general, $\mu = \mu(T)$, $\kappa = \kappa(T)$. Thus $d_{ij} = d_{ij}(T, \mathbf{u})$, $q_j = q_j(T)$. An equation of state relates p to two other state variables of the fluid; for an ideal gas $p = R\rho T$, where $R = R_g/M$ is the ratio of the gas constant, R_g, and the molar mass, M.

Multiplying (2.2) by u_i and using (2.1), the kinetic energy equation is obtained. It can be subtracted from (2.3) to obtain the internal energy equation:

$$\frac{\partial \rho e}{\partial t} + \frac{\partial}{\partial x_j}(\rho e u_j) = \sigma_{ij}\frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \tag{2.6}$$

The enthalpy, h, is defined as $h = e + p/\rho$. Thus from (2.6), after developing the stress tensor on the right-hand side and canceling terms, it results:

$$\frac{\partial \rho h}{\partial t} + \frac{\partial}{\partial x_j}(\rho h u_j) = \frac{\partial p}{\partial t} + u_j\frac{\partial p}{\partial x_j} + d_{ij}\frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \tag{2.7}$$

For a thermally perfect gas, $\mathrm{d}e = c_v(T)\mathrm{d}T$, $\mathrm{d}h = c_p(T)\mathrm{d}T$, where c_p and c_v are the heat capacities at constant pressure and volume, respectively. The ratio of specific heat capacities, is defined as $\gamma \equiv c_p/c_v$, and the gas constant is related to the heat capacities by $R = c_p - c_v$. Therefore $c_v = R/(\gamma - 1)$ and $c_p = \gamma R/(\gamma - 1)$. For a calorically perfect gas c_p, c_v, and γ are constant so that $e = c_v T = p/[(\gamma - 1)\rho]$, $h = c_p T = \gamma e$.

2.2. *Filtered equations*

Define the filter operator, $\mathcal{F}$, [denoted by $\overline{(\cdot)}$] acting on a function f, by

$$\overline{f} \equiv \mathcal{F}[f] \equiv \int_D G(\vec{\xi} - \vec{\xi'}) f(\vec{\xi'})\mathrm{d}\vec{\xi'}, \tag{2.8}$$

where G is a kernel filter function and D is the filtering domain. In general, $\vec{\xi} = \{\mathbf{x}; t\}$. Define also the filter-α-derivative commutation operator, $\mathcal{C}_\alpha[f]$ as

$$\mathcal{C}_\alpha[f] \equiv \mathcal{F}\left[\frac{\partial f}{\partial \alpha}\right] - \frac{\partial \mathcal{F}[f]}{\partial \alpha} = \int_D G(\vec{\xi} - \vec{\xi'})\frac{\partial f(\vec{\xi'})}{\partial \alpha}\mathrm{d}\vec{\xi'} - \frac{\partial}{\partial \alpha}\int_D G(\vec{\xi} - \vec{\xi'}) f(\vec{\xi'})\mathrm{d}\vec{\xi'}, \tag{2.9}$$

which is zero for a filter that commutes with the α-derivative operator.

Using Favre (or density-averaged) quantities (Favre 1965), $\widetilde{f} \equiv \overline{\rho f}/\overline{\rho}$, application of the filter operator to the governing equations yields, after reordering terms:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j}{\partial x_j} = -\mathcal{C}_t[\rho] - \mathcal{C}_{x_j}[\rho u_j],$$

$$
\begin{aligned}
\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} &= -\frac{\partial \overline{p}}{\partial x_j} + \frac{\partial \check{d}_{ij}}{\partial x_j} \\
&\quad - \left[\frac{\partial \overline{\rho}\widetilde{u_i u_j}}{\partial x_j} - \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j}\right] + \left[\frac{\partial \overline{d_{ij}}}{\partial x_j} - \frac{\partial \check{d}_{ij}}{\partial x_j}\right] \\
&\quad - \mathcal{C}_t[\rho u_i] - \mathcal{C}_{x_j}[\rho u_i u_j] - \mathcal{C}_{x_j}[p] + \mathcal{C}_{x_j}[d_{ij}], \\
\frac{\partial \overline{\rho}\widetilde{e}_T}{\partial t} + \frac{\partial \overline{\rho}\widetilde{e}_T\widetilde{u}_j}{\partial x_j} &= -\frac{\partial \overline{p}\widetilde{u}_j}{\partial x_j} + \frac{\partial \check{d}_{ij}\widetilde{u}_i}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j} \\
&\quad - \left[\frac{\partial \overline{\rho}\widetilde{e_T u_j}}{\partial x_j} - \frac{\partial \overline{\rho}\widetilde{e}_T\widetilde{u}_j}{\partial x_j}\right] - \left[\frac{\partial \overline{p u_j}}{\partial x_j} - \frac{\partial \overline{p}\widetilde{u}_j}{\partial x_j}\right] \\
&\quad + \left[\frac{\partial \overline{d_{ij} u_i}}{\partial x_j} - \frac{\partial \check{d}_{ij}\widetilde{u}_i}{\partial x_j}\right] - \left[\frac{\partial \overline{q_j}}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j}\right] \\
&\quad - \mathcal{C}_t[\rho e_T] - \mathcal{C}_{x_j}[\rho e_T u_j] - \mathcal{C}_{x_j}[p u_j] + \mathcal{C}_{x_j}[d_{ij} u_i] - \mathcal{C}_{x_j}[q_j], \\
\frac{\partial \overline{\rho}\widetilde{e}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{e}\widetilde{u}_j}{\partial x_j} &= -\overline{p}\frac{\partial \widetilde{u}_j}{\partial x_j} + \check{d}_{ij}\frac{\partial \widetilde{u}_i}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j} \\
&\quad - \left[\frac{\partial \overline{\rho}\widetilde{e u_j}}{\partial x_j} - \frac{\partial \overline{\rho}\widetilde{e}\widetilde{u}_j}{\partial x_j}\right] - \left[\overline{p\frac{\partial u_j}{\partial x_j}} - \overline{p}\frac{\partial \widetilde{u}_j}{\partial x_j}\right] \\
&\quad + \left[\overline{d_{ij}\frac{\partial u_i}{\partial x_j}} - \check{d}_{ij}\frac{\partial \widetilde{u}_i}{\partial x_j}\right] - \left[\frac{\partial \overline{q_j}}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j}\right] \\
&\quad - \mathcal{C}_t[\rho e] - \mathcal{C}_{x_j}[\rho e u_j] - \mathcal{C}_{x_j}[q_j], \\
\frac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{h}\widetilde{u}_j}{\partial x_j} &= \frac{\partial \overline{p}}{\partial t} + \widetilde{u}_j\frac{\partial \overline{p}}{\partial x_j} + \check{d}_{ij}\frac{\partial \widetilde{u}_i}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j} \\
&\quad - \left[\frac{\partial \overline{\rho}\widetilde{h u_j}}{\partial x_j} - \frac{\partial \overline{\rho}\widetilde{h}\widetilde{u}_j}{\partial x_j}\right] + \left[\overline{u_j\frac{\partial p}{\partial x_j}} - \widetilde{u}_j\frac{\partial \overline{p}}{\partial x_j}\right] \\
&\quad + \left[\overline{d_{ij}\frac{\partial u_i}{\partial x_j}} - \check{d}_{ij}\frac{\partial \widetilde{u}_i}{\partial x_j}\right] - \left[\frac{\partial \overline{q_j}}{\partial x_j} - \frac{\partial \check{q}_j}{\partial x_j}\right] \\
&\quad - \mathcal{C}_t[\rho e] - \mathcal{C}_{x_j}[\rho e u_j] + \mathcal{C}_t[p] - \mathcal{C}_{x_j}[q_j],
\end{aligned}
\tag{2.10}
$$

where $\check{f}$ refers to the formal expression of f with all constituent variables replaced with their Favre-filtered counterparts, from which it differs (i.e., $\widetilde{f} \neq \check{f}$):

$$
\check{d}_{ij} \equiv d_{ij}(\widetilde{T}, \widetilde{\mathbf{u}}) = \mu(\widetilde{T})\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right) + \left[\mu_v(\widetilde{T}) - \frac{2}{3}\mu(\widetilde{T})\right]\frac{\partial \widetilde{u}_k}{\partial x_k}\delta_{ij} \neq \widetilde{d}_{ij}, \tag{2.11}
$$

$$
\check{q}_j \equiv -\check{\kappa}\partial\widetilde{T}/\partial x_j = -\kappa(\widetilde{T})\partial\widetilde{T}/\partial x_j = q_j(\widetilde{T}) \neq \widetilde{q}_j. \tag{2.12}
$$

Terms in square brackets on the right-hand side of the set of equations (2.10) are unsolvable in a LES simulation and require modeling. The filtered thermodynamic pressure can be obtained through the filtered equation of state; for an ideal gas: $\overline{p} = R\overline{\rho T} = R\overline{\rho}\,\widetilde{T} = (\gamma-1)\overline{\rho}\,\widetilde{e}$. If the total energy equation is used, this brings modeled quantities into the calculation of the filtered pressure (and temperature):

$$
\frac{\overline{p}}{\gamma - 1} = c_v\overline{\rho}\,\widetilde{T} = \overline{\rho e} = \overline{\rho e_T} - \frac{1}{2}\overline{\rho u_i u_i} = \overline{\rho}\,\widetilde{e_T} - \frac{1}{2}\overline{\rho}\,\widetilde{u}_i\widetilde{u}_i - \frac{1}{2}\overline{\rho}(\widetilde{u_i u_i} - \widetilde{u}_i\widetilde{u}_i). \tag{2.13}
$$

Some of the terms requiring modeling present in the set of equations (2.10) and (2.13) either coincide or can be related to the following common definitions (see, for example, Martín *et al.* 2000): subgrid-scale stress tensor, $\tau_{ij}^S = \overline{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j)$, subgrid-scale heat flux, $q_j^S = \overline{\rho}(\widetilde{T u_j} - \widetilde{T}\widetilde{u}_j)$, subgrid-scale pressure dilatation, $\Pi_{\text{dil}}^S = \overline{p S_{kk}} - \overline{p}\widetilde{S}_{kk}$, subgrid-scale viscous dissipation, $\epsilon_v^S = \overline{d_{ji} S_{ij}} - \check{d}_{ji}\widetilde{S}_{ij}$, subgrid-scale turbulent diffusion, $\partial \mathcal{J}_j^S/\partial x_j$ (where $\mathcal{J}_j^S = \overline{\rho}(\widetilde{u_k u_k u_j} - \widetilde{u_k u_k}\widetilde{u}_j)$), and subgrid-scale viscous diffusion, $\partial \mathcal{D}_j^S/\partial x_j$ (where $\mathcal{D}_j^S = \overline{d_{ij} u_i} - \check{d}_{ij}\widetilde{u}_i$). The turbulent diffusion term, present in the total energy equation, introduces triple correlations of the velocity field. Existing subgrid-scale models usually focus on the contribution of the first two (subgrid-scale stress tensor and heat flux), neglecting the the remaining terms, based on a priori assessment of their relative importance in simple flows (e.g., isotropic turbulence) through DNS. The applicability of those simplifications in the shock-turbulence interaction problem should be revisited. Nevertheless, models for some of the additional terms have also been proposed in the literature (see Martín *et al.* 2000, and the references therein).

Considerations about the particular discretization strategies used to translate each term of equations (2.10) into the computational domain (split conservative form, for instance) are not discussed here. Nonetheless, we remark that aliasing errors and stability issues are largely affected by those choices of discretization. For an in-depth study see, for example, Blaisdell *et al.* (1996); Honein & Moin (2004).

3. Existing subgrid-scale models considered for application to shock-turbulence interaction

This section briefly describes the main features of compressible LES models currently available in the literature that are being implemented in the context of this research for an evaluation and comparison of their performance in shock-turbulence interaction.

3.1. *Generalized dynamic eddy-viscosity model*

Proposed by Moin *et al.* (1991), this model uses the Germano procedure (Germano *et al.* 1991) to dynamically compute model coefficients for the subgrid-scale stress tensor and heat flux (treatment for scalar transport also exists) by means of an explicit test-filter operation and an implicit assumption of scale-similarity between both filters (test and grid levels).

Several extensions/modifications of this model have been proposed. Lilly (1992) utilized a least-squares error minimization technique to solve an indetermination in the calculation of the coefficients. This resulted in a less dissipative model for compressible isotropic homogeneous decaying turbulence (Spyropoulos 1996). Ghosal *et al.* (1995) introduced, for the incompressible case, a generalized variational error-minimization procedure that allowed the dynamic model to be applied when no homogeneous directions are present. With a similar objective, Meneveau *et al.* (1996) proposed a Lagrangian averaging procedure, that takes into account the history of the flow, incorporating two relaxation-transport equations. You & Moin (2008) considered global (instead of local) equilibrium, by solving additional transport equations, at the grid and test filter levels, for the trace of the subgrid-scale stress tensor and the temperature variance.

3.2. *Generalized mixed similarity/eddy-viscosity model*

Models that explicitly use the scale-similarity assumption by subtracting single- and twice-filtered velocity fields were proposed to be utilized in combination with dissipative (eddy-viscosity-like) models by Bardina *et al.* (1980) and later extended to compressible flows by Erlebacher *et al.* (1992). Two enhancements brought by the similarity part of the model are a higher correlation of modeled stresses with respect to experimental and DNS data and an intrinsic capability for backscatter (eddy-viscosity models alone require dynamic procedures to allow backscatter). Dynamic versions (Vreman *et al.* 1995) have also been proposed (see Meneveau & Katz 2000, for more details).

3.3. *Tensorial/anisotropic/non-linear eddy-viscosity model*

When the assumption of linear dependence between the subgrid-scale stress tensor and the strain-rate tensor is removed (as suggested by evidence), more general forms of the model can be considered. This comes at the expense of multiple model coefficients. For example, anisotropic tensorial models were proposed in Carati & Cabot (1996) for incompressible flows, and a non-linear compressible model was introduced in Kosovic *et al.* (2002). Dynamic procedures are also applicable (Gallerano & Napoli 1999).

3.4. *Approximate deconvolution procedure*

This modeling strategy uses invertible spatial filter kernels to approximate the unresolved flow quantities by deconvolving the solved (filtered) ones with an approximated inverse of the filter, obtained by truncated iteration (see Stolz & Adams 1999). It has been successfully applied in the presence of shocks (Adams *et al.* 1998) without the need of shock-capturing schemes.

3.5. *Stretched-vortex model*

This is a structure-based, phenomenological model that assumes a superposition of nearly axisymmetric, straight vortices to be responsible for subgrid-scale motion and estimates the subgrid-scale energy for closure (Misra & Pullin 1997). Different approaches for determining the orientation of those vortices are proposed. The compressible extension (Kosovic *et al.* 2002) uses the subgrid-scalar flux model (Pullin 2000) for treating the temperature when obtaining the subgrid-scale heat flux. This model has been used in LES of the converging shock-driven Richtmyer-Meshkov instability to study the turbulent mixing generated by the reshock, through hybrid methods combined with adaptive mesh refinement (Lombardini 2008).

3.6. *Artificial fluid properties LES (AFLES)*

The physical transport coefficients of the fluid (dynamic and bulk viscosities, and thermal conductivity) are modified by adding grid-dependent components that are modeled (Cook 2007). The design criterion for those models is to damp wavenumber modes near the resolution limit while minimizing corruption of lower modes. Multi-fluid flows are also addressed by modifying the species diffusion coefficients. Mani *et al.* (2009) proposed an alternative formulation that parametrizes the bulk viscosity with the dilatation-rate instead of the strain-rate, thus enhancing its performance in sound-prediction by reducing the dissipation of dilatational and thermodynamic fluctuations.

4. Considerations for application of LES models to shock-turbulence interaction

In this section, we highlight some features of the canonical shock-turbulence interaction and comment on how they can affect the development of specific subgrid-scale models. References to solutions to similar problems proposed in the literature are given.

4.1. *Shock presence, turbulence amplification, and inhomogeneity*

The presence of the shock, with a position known a priori in the computational domain, suggests a refinement of the grid in its vicinity. A direct reason has to do with minimizing the added dissipation and its spatial extent that results from application of shock-capturing schemes. This applies both to DNS and LES.

Besides, as the incoming isotropic turbulence is processed by the shock, turbulence amplification results in decreased Kolmogorov and Taylor microscales downstream of the shock. Thus, there are added benefits of using a refined grid immediately downstream of the shock in terms of making the subgrid-scale model operate in a similar range of relative length scales (e.g., in the energy spectrum) throughout the domain. In DNS, the different criterion of being able to resolve the viscous scales leads to the same outcome.

As the flow evolves downstream, those length-scales smoothly recover from their abrupt change through the shock, slowly increasing, so the use of a stretched grid in the streamwise direction with its minimum spacing located at the shock seems optimal to address the inhomogeneity in that direction.

We note that for the transverse directions, grid refinement would also be needed in the vicinity of the shock. For structured grids this is achievable through adaptive mesh refinement (that leaves the rest of the domain unaffected).

The use of stretched grids typically results in spatial filters with variable width so that extra terms appear in the LES filtered equations ($\mathcal{C}_{x_j}[f]$ terms in the set of equations (2.10)), because variable-width filtering and spatial derivation operations do not generally commute (see Ghosal & Moin 1995). Families of spatial high-order filters that commute with spatial derivatives up to a desired order of magnitude can been constructed (Vasilyev *et al.* 1998). They can be applied to this problem when explicit filtering operations are involved. Not only do they decrease the error of commutation but also the turbulent stresses, so explicit models for the commutation errors have also been proposed (van der Bos & Geurts 2005*a*,*b*). While not specific to this type of flow, it is pointed out that the definition of the filter width is not unique (see Bardina *et al.* 1980; Lund 1997), but its influence in the model results seems even more important than the choice of the filter shape.

Averaging operations needed, for example, to stabilize the computation of dynamic model coefficients, are also affected by flow inhomogeneities. Typically, these operations are performed in homogeneous directions. For the canonical shock-turbulence interaction flow, planes parallel to the ideal (laminar) normal shock could be approximately considered homogeneous for low intensities of the incoming turbulence. But as the turbulence intensity increases, corrugation of the shock could compromise the validity of such assumption, especially near the shock. This topic of corrugation is treated separately below. As explained in section 3, alternative treatments of inhomogeneities in the flow have been presented in the literature for averaging steps of subgrid-scale models.

4.2. *Anisotropy*

Turbulence amplification is observed to affect the streamwise and transverse directions with different intensities. This behavior depends on the Mach number. As a result, the flow immediately downstream of the shock is also anisotropic. Therefore, subgrid-scale models that do not rely on the assumption of local isotropy at the small scales, such as the tensorial models described in section 3.3, seem more suited for this type of flow.

The resulting anisotropy of turbulence is known to be of axisymmetric nature, as predicted by linear analysis and confirmed by experimental results and numerical simulations. This could be used as a design criterion implemented in improved models, for example, by using anisotropic/tensorial models simplified with axisymmetric assumptions (Carati & Cabot 1996).

4.3. *Applicability of subgrid-scale models in the shock-captured region*

Filtering enlarges the region where shock-capturing effects are present. This is an intrinsic handicap of LES when shock-capturing is used, since as discussed earlier, shock-capturing schemes necessarily introduce dissipation to smear out the shock and be able to capture it. Additional filter operations, such as those required in the test-filtering of dynamic models will further enlarge the region affected by the shock-capturing method. This enlarged region will have a negative effect on the physical fidelity of resolved field, in particular, immediately downstream of the shock, which, in turn, affects the computation of subgrid-scale terms, where the focus of the model development in the present work is. For a quantification and modeling approach to estimate the error resulting from the damping of turbulence introduced by shock-capturing schemes in DNS, plus some remarks on its influence in LES, see Larsson (2009) in this volume.

A careful treatment of those regions, perhaps turning off subgrid-scale models at grid points where shock-capturing is active (in a hybrid approach) and using skewed filters nearby might be required. Solutions have been proposed for related flows, such as the use of deconvolution (Adams *et al.* 1998) without shock-capturing schemes or adaptive shock-confining filters (Grube & Martín 2009).

4.4. *Non-equilibrium*

After being processed by the shock, the flow downstream is left in a state which is out of local equilibrium, meaning that there is an imbalance between energy production and dissipation. The relaxation time required for the flow to reach local equilibrium again translates, as the fluid is being convected downstream, into a relaxation region where the common picture of turbulent energy cascade does not hold. Therefore, subgrid-scale models based on arguments derived from that picture, such as the existence of an inertial range and the subsequent scale-similarity hypothesis, may yield inaccurate predictions. The presence and extent of backscatter immediately downstream of the shock derived from non-equilibrium have not been well established yet and should be investigated.

The incorporation of transport equations in the formulation of subgrid-scale models (Deardoff 1973) has been successfully applied in other flows exhibiting non-equilibrium states (e.g., Befeno & Schiestel 2007). Other alternatives, based on Padé and relaxation time approximations have also been proposed in the literature (Speziale 1999).

4.5. *Bulk viscosity in the shock region and immediately downstream*

Typically, the bulk viscosity of a fluid is not known very accurately, owing to exceptional difficulties in its measurement. Stokes' hypothesis is used to assume a nil value (el Hak 1995). For a fluid with non-zero bulk viscosity (generally true for polyatomic gases), the high compressibility effects occuring in and near the shock can result in non-negligible differences between the mechanical and thermodynamic pressures (see equation (2.4)).

Whereas this issue affects both DNS and LES, use of the latter to simulate more relevant flow conditions not yet achievable with DNS, including higher compressibility effects, may lead to deviations from comparable experiments in the vicinity of the shock, where strong "peaked" events are already observed in DNS (Larsson 2008; Grube *et al.* 2009) and experiments (Hesselink & Sturtevant 1988). Such events could also be amplified in LES.

4.6. *Corrugation of shock wave*

The interaction of turbulence and the shock is twofold. While most of the considerations discussed above focus on the effect of the shock on the incoming turbulent flow, there is also a counterpart in how the strength and shape of the shock is affected by the turbulence intensity of the incoming flow. As a consequence of this interaction, the shock becomes corrugated, with high variations in time of its spatial location. This results in a wider interval, in the coordinate normal to the ideal planar shock, affected by the shock capturing scheme, which will influence the determination of the scope of filtering and averaging operations used in subgrid-scale models.

If the intensity of the incoming turbulence is high enough, the shock might even become discontinuous, with "holes" in it that subject the incoming fluid to an isentropic compression, as opposed to the surrounding fluid which is processed by the shock. In this regard, subgrid-scale models that consider the Lagrangian trajectories of the fluid (such as the one proposed by Meneveau *et al.* (1996)) can be especially useful, because the history of the fluid elements is tracked, which allows a distinction of the different physical character of the compression to which neighboring elements have been subjected.

4.7. *Presence of shocklets*

Another effect related to the compressibility of the fluid that can have a considerable impact in the applicability of subgrid-scale models is the formation of shocklets that occurs in decaying turbulence (Lee *et al.* 1991). Samtaney *et al.* (2001) performed a statistical analysis of DNS databases of isotropic turbulence at moderate fluctuation Mach numbers, M_t, finding reasonable agreement when compared with a simple model that uses weak-shock theory. This model predicted a most probable shocklet strength proportional to $M_t/Re_\lambda^{1/2}$ (Re_λ being the Taylor Reynolds number) and a thickness somewhat larger than the Kolmogorov length (rather than the mean free path). As in the case of the shock itself, this scaling imposes (weaker) restrictions on the relation between the shock(let) detection/capturing algorithms and the grid spacing needed by LES, for flows with relevant combinations of M_t and Re_λ. Also, the dissipation added by shock capturing schemes, which act on a constant number of grid points, will affect a larger portion of the domain in LES than that actually occupied by the shocklets, which distorts the statistics. The use of shock-confining filters (Grube & Martín 2009) that avoid filtering across shocks and other discontinuities has shown favorable results in highly compressible isotropic turbulence.

4.8. *Coupling between temperature and velocity correlations*

As pointed out in section 1, Mahesh *et al.* (1997) found that downstream evolution of turbulence is largely affected by temperature and velocity correlations: negative/positive correlations enhance/suppress the turbulence amplification.

Although this coupling can be regarded as a validation criterion for a posteriori testing of developed subgrid-scale models, it can also be used as a design element for improved models, by incorporating it into a built-in feature for small scale turbulent amplification based on the upstream correlation of such quantities tracked in a Lagrangian sense.

5. Future work

The subgrid-scale models outlined in section 3 are being implemented in Larsson's DNS *Hybrid* code to establish a comparison of their performance when applied to the canonical shock-turbulence interaction problem. This will be done through a posteriori testing with the DNS databases obtained by Larsson (2008) and validation with experiments and theory. The incorporation into those models of the considerations discussed in section 4 affecting this specific type of flow is aimed at improving their performance.

An evaluation of the importance of traditionally neglected modeling terms (see section 2), needs to be done through DNS data of this flow (particularly for the region immediately downstream of the shock, where results may differ from previous studies).

After the development of improved models, they could be applied to more complex flows, such as Richtmyer-Meshkov mixing, turbulent boundary layers in the presence of shocks, etc. Their applicability to more complex geometric configurations will therefore be an important design factor when developing such models.

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