A dynamic approximate deconvolution model for unfiltered scalars in LES

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Large-Eddy Simulations (LES) of turbulent flows require closure models for the subgrid-scale (SGS) fluxes of momentum, energy and scalars. However, those do not provide SGS models for unfiltered scalar flow variables, which may be necessary in evaluating, for instance, chemical reaction rates, gas constants, or the carrier-phase temperature near a point particle. Instead, the question addressed here is how to obtain a model for the full-scale version of a scalar field Y, given only its LES resolved version $\overline{Y}$ computed from integration of its corresponding filtered conservation equation. In the absence of spectral information from the real subgrid scales, a possible low-cost alternative is to approximately deconvolve $\overline{Y}$ using a model. This report proposes one such model that does not require tuning of parameters.

The model proposed here makes use of an elliptic differential filter (Germano 1986) to express the deconvolved scalar Y as

$$Y = \overline{Y} - b^2 \frac{\partial^2 \overline{Y}}{\partial x_j \partial x_j}, \tag{1}$$

where b represents a characteristic filter width. If b is uniform in space and the domain of integration is unbounded, the solution of Eq. (1) is $\overline{Y}(\mathbf{x},t) = \int_{\mathbf{x}'} Y(\mathbf{x}',t) G(\mathbf{x},\mathbf{x}') d^3\mathbf{x}'$, where $G(\mathbf{x},\mathbf{x}') = \exp[-|\mathbf{x}-\mathbf{x}'|/b]/[4\pi b^2 |\mathbf{x}-\mathbf{x}'|]$ is a filter kernel that represents the Green's function of Eq. (1). Comparing Eq. (1) with $Y = \overline{Y} + Y'$, the SGS portion of the scalar field Y can be simply modeled as $Y' = -b^2 \partial^2 \overline{Y}/\partial x_j \partial x_j$. However, the problem now becomes how to determine the parameter b. Several criteria may be proposed for modeling b, including fitting its numerical value to filtered DNS results. A more predictive alternative consists of imposing a dynamic constraint on Eq. (1) that leads to consistency with SGS quantities predicted by the transport models used in the main LES calculation. For instance, consider the SGS scalar variance

$$\overline{Y'^2} = \overline{Y^2} - \overline{Y}^2. \tag{2}$$

An estimate of $\overline{Y'^2}$ in LES is typically obtained from simple models such as

$$\overline{Y'^2}_{\text{LES}} = C\Delta^2 \frac{\partial \overline{Y}}{\partial x_i} \frac{\partial \overline{Y}}{\partial x_i}, \tag{3}$$

where Δ is the grid spacing and C is a dynamic constant computed as in Eq. (7) of Pierce & Moin (1998), or by integrating the corresponding transport equation for the SGS variance subjected to additional second-order closures. These models provide the estimate $\overline{Y'^2}_{\text{LES}}$, but their details are irrelevant for the purposes of the present study. The constraint that the prediction of $\overline{Y'^2}$ made by any these models matches the one made by Eq. (1) leads to a dynamic determination of the coefficient b as follows. A separate expression for $\overline{Y'^2}$ can be obtained from the model (1) by subtracting

$$Y^2 = \left(\overline{Y} - b^2 \frac{\partial^2 \overline{Y}}{\partial x_j \partial x_j}\right)\left(\overline{Y} - b^2 \frac{\partial^2 \overline{Y}}{\partial x_k \partial x_k}\right) \tag{4}$$

from

$$Y^2 = \overline{Y^2} - b^2 \frac{\partial^2 \overline{Y^2}}{\partial x_j \partial x_j}, \tag{5}$$

which are trivially obtained by applying Eq. (1) to Y and Y^2, respectively. This leads to the expression

$$\overline{Y'^2} = b^2 \frac{\partial^2 \overline{Y'^2}}{\partial x_j \partial x_j} + 2b^2 \frac{\partial \overline{Y}}{\partial x_j} \frac{\partial \overline{Y}}{\partial x_j} + b^4 \frac{\partial^2 \overline{Y}}{\partial x_j \partial x_j} \frac{\partial^2 \overline{Y}}{\partial x_k \partial x_k}, \tag{6}$$

where $\overline{Y}$ is computed from the LES. Upon space averaging and imposing that $\overline{Y'^2}$ is equal to $\overline{Y'^2}_{\mathrm{LES}}$ computed from Eq. (3) or any other LES model, the bi-quadratic equation

$$\langle \alpha \rangle \, b^4 + \langle \beta \rangle \, b^2 - \langle \gamma \rangle = 0 \tag{7}$$

is obtained, where b is the only unknown. The coefficients

$$\alpha = \frac{\partial^2 \overline{Y}}{\partial x_j \partial x_j} \frac{\partial^2 \overline{Y}}{\partial x_k \partial x_k}, \quad \beta = 2 \frac{\partial \overline{Y}}{\partial x_j} \frac{\partial \overline{Y}}{\partial x_j} + \frac{\partial^2 \overline{Y'^2}_{\mathrm{LES}}}{\partial x_j \partial x_j}, \quad \gamma = \overline{Y'^2}_{\mathrm{LES}} \tag{8}$$

are sole functions of the LES resolved values $\overline{Y}$ and of the estimated SGS scalar variance $\overline{Y'^2}_{\mathrm{LES}}$. Since $\gamma \geq 0$ in practical LES models such as the one of Pierce & Moin (1998) (note that this does not necessarily have to be the general case when DNS results are *a-priori* filtered), Eq. (7) has only one positive root given by

$$b = \sqrt{\left[-\beta + \sqrt{\beta^2 + 4\alpha\gamma} \right] / (2\alpha)}, \tag{9}$$

which corresponds to the instantaneous value of the dynamic coefficient b. Upon substituting Eq. (9) into Eq. (1), the deconvolved scalar Y can be straightforwardly computed from its resolved value $\overline{Y}$.

Some additional aspects merit discussion regarding the model described above. For instance, the coefficients α, β and γ can be locally filtered or globally averaged along homogeneous directions in order to regularize the spatial distribution of the dynamic constant b. Additionally, the model can easily be implemented in structured or unstructured computational setups. Similarly, in the limit when the filter width goes to zero, the SGS variance vanishes and $\gamma = 0$. As a result, $b = 0$ and the model does not yield any contribution. This limit may be of some relevance for LES modeling of scalars in wall-bounded flows. Furthermore, this model can easily be employed in variable-density flows by using the Favre-filtered scalar $\widetilde{Y}$ in Eq. (1) in place of $\overline{Y}$ and the Favre variance $\widetilde{Y''^2}$ in place of $\overline{Y'^2}$. Lastly, note that similar ideas can be used as SGS models for carrier-phase velocities in LES of particle-laden turbulent flows, as shown in our previous work (Park *et al.* 2015).

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