A criterion of orthogonality on the assumption and restrictions in subgrid-scale modelling of turbulence

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Abstract: In order to shed light on understanding the subgrid-scale (SGS) modelling methodology, we analyze and define the concepts of assumption and restriction in the modelling procedure, then show by a generalized derivation that if there are multiple stationary restrictions in a modelling, the corresponding assumption function must satisfy a criterion of orthogonality. Numerical tests using one-dimensional nonlinear advection equation are performed to validate this criterion. This study is expected to inspire future research on generally guiding the SGS modelling methodology.

Keywords: large-eddy simulation; subgrid-scale modelling; nonlinear differential equation

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I. INTRODUCTION

The large-eddy simulation (LES) technique has achieved great success in the last half-century in both academic community and industry applications[1–3]. Numerous SGS models have been introduced under various frameworks. The classification and comparison of these models can be found in literature [1, 4–8]. These subgrid-scale (SGS) models clearly show the variety of the turbulence community and illustrate the common interest of SGS modeling. However, confusions are also involved in these distinctive SGS models: (i) in the engineering community, researchers **are usually not able to *a-priori* suggest the best** SGS model for a typical problem and (ii) in the turbulence community, researchers may also be confused on the (necessary) criterion of constructing an SGS model. Reference [9] concluded three basic requirements for evaluating a good SGS model, which is helpful for clarifying the first confusion. However, the second point is still not clear, which indeed calls for better understanding on SGS modeling procedure. Specifically, as researchers on SGS modelling, how should we “correctly” involve physical and mathematical restrictions to model the SGS quantities?

In recent years, along with developing the SGS models using the Kolmogorov equation of filtered velocity (KEF)[10–14], we have also been curious on clarifying the high-level methodology of SGS modelling. In fact, we found that when employing these SGS models, if we calculate the model coefficient dynamically, the LES calculations are usually unstable. Instead, a constant model coefficient usually leads to better performance. This fact has been discussed in Refs. [3, 13, 15], but we did not manage to give a convincing theoretical explanation. In Ref. [3] we summarized the various attempts of this modelling methodology, and phenomenally guessed that there are some conflicts among the *assumptions* and *restrictions* in SGS modelling.

In order to better explain the research context and to define the terms, here we review our analysis on the procedure of SGS modelling methodology. In general, by reviewing the existing SGS models, we describe the procedure of SGS modeling as the following two steps [3, 16, 17]:

(i) Any SGS model should be based on a certain *assumption* on the SGS motion, that is, we need to assume a formulation for SGS quantities (in particular, the SGS stress tensor). However, there are always undetermined factors in this *assumption*.

(ii) A complete SGS model should employ a certain closure method to determine the unknown factors mentioned in step (i). This closure implies one or more *restrictions* in either physical or mathematical frameworks.

Let us comment on the definitions of *assumptions* and *restrictions*, which are abstract conceptions of the above two-step description. There are various *assumptions* such as the eddy-viscosity assumption[18], the scale-similarity assumption [19], the gradient diffusion assumption[20], the velocity increment assumption[13, 21], *etc.*. We conclude that *an assumption assumes a (local) similarity between GS and SGS quantities*. Usually there can not be two or more *assumptions* at the same time in one SGS model. By contrast, *a restriction is a physical or mathematical simplification which is employed in the SGS modelling closure*. There are various types of *restrictions*, for example the inviscid simplification[10], the scaling laws[15, 22, 23], the filter similarity[24], the velocity profile restriction[25], *etc.*. We remark that there can be multiple *restrictions* in one SGS model, for example in Ref. [10] four *restrictions* are employed: the inviscid simplification, the scaling law, the stationary simplification of structure function, and the subgrid feasibility for Taylor expansion. In general, the reason of choosing multiple *restrictions* is that we hope the generated turbulence can satisfy more physical or mathematical laws. Whereas, sometimes multiple *restrictions* lead to non-negligible error but we do not know the reason.

As introduced above, from previous numerical practices we intuitively feel that there are some conflicts among the *assumptions* and *restrictions* in SGS modelling. Aiming at demonstrating that, considering the complexity of different *restrictions*, in this contribution we choose a simple type of *restriction*, *i.e.*, the stationary *restriction* for a statistical quantity. We will show by a generalized derivation that if there are multiple stationary *restrictions* in a modelling, the corresponding *assumption* function must satisfy a criterion of orthogonality. Numerical tests in one-dimensional nonlinear advection equation are performed to support this criterion.

II. THEORETICAL ANALYSIS

We consider here the general formulation of a nonlinear partial differential equation

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

where t is time and u is a continuous physical quantity. For simplicity, here we consider u as a scalar function. $f(u)$ is a nonlinear function, which needs an SGS modelling in numerical applications. Defining $\bar{\bullet}$ the grid-scale filter operator, Eq. (1) can be rewritten as

$$\frac{\partial \bar{u}}{\partial t} = f(\bar{u}) + \tau, \quad (2)$$

with τ the SGS term which needs to be modelled. As introduced in the previous section, we should involve one *assumption* and some *restriction(s)*. In this contribution we only consider typical stationary *restrictions* for a **statistical** quantity, which can be written as

$$\frac{\partial \langle h_i(\bar{u}) \rangle}{\partial t} = 0, \quad (3)$$

with $i = 1, 2, \dots, n$ and n the number of *restrictions*, h_i a nonlinear function, and $\langle \bullet \rangle$ the ensemble average. We remark that, for example, this type of *restrictions* can refer to the stationary simplification of resolved longitudinal structure function $D_{ll}^<[10, 11]$, and the stationary simplification of Lagrangian velocity gradient correlation[26]. Here we consider that there are two *restrictions* h_1 and h_2 , and use the following methodology to involve an *assumption* to link the resolved and SGS quantities.

Multiplying both sides of Eq. (2) with $\frac{dh_1(\bar{u})}{d\bar{u}}$ and by noting that $\frac{\partial h_1(\bar{u})}{\partial t} = \frac{dh_1(\bar{u})}{d\bar{u}} \frac{\partial \bar{u}}{\partial t}$, we can obtain

$$\frac{\partial h_1(\bar{u})}{\partial t} = \frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_1(\bar{u})}{d\bar{u}} \tau. \quad (4)$$

Taking ensemble average on Eq. (4) and by noting the *restriction* (3), it is

$$\left\langle \frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_1(\bar{u})}{d\bar{u}} \tau \right\rangle = 0. \quad (5)$$

In order to satisfy the statistical property (5) by keeping the instantaneous scale-similarity, in SGS modelling we usually introduce an *assumption* here, which involves a function $Z(\bar{u})$ of the resolved quantities $\bar{u}$ with zero average and suppose that it is locally similar to the average-zero SGS expression $\frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_1(\bar{u})}{d\bar{u}} \tau$. This is an abstraction of practical assumptions, such as the viscosity assumption which assumes a local similarity between the trace-zero SGS tensor $\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}$ (which is analogy to $\frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_1(\bar{u})}{d\bar{u}} \tau$) and the resolved strain rate $\bar{S}_{ij}$ (which is analogy to $Z(\bar{u})$) with δ Kronecker delta. We therefore write this local similarity as

$$\frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_1(\bar{u})}{d\bar{u}} \tau = Z(\bar{u}), \quad (6)$$

which yields the expression of the SGS quantity

$$\tau = \frac{1}{\frac{dh_1(\bar{u})}{d\bar{u}}} \left(Z(\bar{u}) - \frac{dh_1(\bar{u})}{d\bar{u}} f(\bar{u}) \right). \quad (7)$$

The above procedure describes a generalized methodology for determining the SGS quantity with one *assumption* and one *restriction*. However, as introduced in the previous section, there are usually multiple *restrictions* in an SGS modelling. It is then interesting to see whether other *restrictions* are able to be satisfied under this procedure. Substituting Eq. (7) to (2) for $i \neq 1$, and multiplying both sides with $\frac{dh_i(\bar{u})}{d\bar{u}}$, we obtain

$$\frac{\partial h_i(\bar{u})}{\partial t} = Z(\bar{u}) \frac{dh_i(\bar{u})}{d\bar{u}} \bigg/ \frac{dh_1(\bar{u})}{d\bar{u}}. \quad (8)$$

Taking ensemble average, it is shown that the *restrictions* (3) lead to

$$\langle Z(\bar{u}) h'_i(\bar{u}) / h'_1(\bar{u}) \rangle = 0. \quad (9)$$

If we consider $\bar{u}$ as a random variable with probability density function (PDF) $\rho(\bar{u})$, Eq. (9) can be rewritten as

$$\int_{-\infty}^{+\infty} Z(s) H_i(s) \rho(s) ds = 0, \quad (10)$$

where H_i is defined as $H_i = h'_i / h'_1$, and s is the variable of integration in probability space for replacing $\bar{u}$ in Eq. (9). This can also be further rewritten as a formula of inner product

$$Z \cdot H_i := \int_{-\infty}^{+\infty} Z(s) H_i(s) \rho(s) ds = 0. \quad (11)$$

This inner product then defines an inner product space with a weight function ρ . The *restrictions* h_i correspond to a series of elements H_i in this space, while $Z(s)$ must be orthogonal to the linear subspace $\text{Vect}(H_1, H_2, \dots, H_n)$. This describes a criterion of orthogonality on the *assumption* and *restrictions*.

III. NUMERICAL TESTS

In this section we select the most simple nonlinear partial differential equation, *i.e.*, the one-dimensional nonlinear advection equation, or say, the one-dimensional *inviscid* Burgers equation, to validate the conclusions in the present contribution. We remark that the

analysis of the previous section might also be used to more physical examples, such as the high-dimensional KdV-Burgers equation and the KdV equation, however analytical analysis will be very difficult. In the present contribution the governing equation simply writes (the factor 1/2 in the right hand side is omitted for simplicity)

$$\frac{\partial \bar{u}}{\partial t} = \frac{\partial \bar{u}^2}{\partial x} + \tau, \quad (12)$$

with the resolved-scale initial condition

$$\bar{u}(x)|_{t=0} = \sin x. \quad (13)$$

This implies that $\bar{u}$ is always periodic with a period 2π . It is also evident that at initial time $\bar{u} \in [-1, 1]$. Note that the governing equation (12) does not indicate that the full-scale equation is $\partial_t u = \partial_x u^2$ — indeed, this only shows that the large-scale motion is advected nonlinearly, while the SGS term τ is underdetermined. Here we assume that the SGS term τ is appropriate so that the resolved-scale quantity $\bar{u}$ is always in the interval $[-1, 1]$ at any time, and consider two *arbitrary restrictions*

$$\begin{aligned} h_1(\bar{u}) &= \frac{2}{3}\bar{u}^3 + 2\bar{u} + 2, \\ h_2(\bar{u}) &= \cos \bar{u}. \end{aligned} \quad (14)$$

Note that these *restrictions* are only designed for validation, and do not have physical or mathematical meanings. Future investigations would focus on the physical *restrictions* such as the stationary velocity profile, kinetic energy, enstrophy or helicity. Following the conclusion (11), for the *assumption* function Z , our theoretical criterion of orthogonality writes

$$\begin{aligned} Z \cdot H_1 &= \int_{-1}^1 Z(s) \rho(s) ds = 0, \\ Z \cdot H_2 &= \int_{-1}^1 Z(s) \frac{-\sin s}{2s^2 + 2} \rho(s) ds = 0, \end{aligned} \quad (15)$$

with the weight function $\rho(s) = (1 - s^2)^{-1/2}$. This weight function can be derived from the initial condition (13) by using the following fact of changing variable on Eq. (3)

$$\frac{\partial \langle h_i(\bar{u}) \rangle}{\partial t} = \int_{-\pi}^{\pi} \frac{\partial h(\bar{u}(x))}{\partial t} dx = \int_{-1}^1 \frac{\partial h(\bar{u})}{\partial t} \frac{1}{\sqrt{1 - \bar{u}^2}} d\bar{u}, \quad (16)$$

and does not depend on time due to the property of advection equations. Note that in order to derive this weight function, for the first equal sign of Eq. (16) we use the spatial

average (*i.e.*, the integration over x) to replace the ensemble average, which implies that the spatial direction is considered to be statistically homogeneous to satisfy the SGS modelling spirit. The underlying assumption of using the spatial average is that every statistical sample is a phase shift of the present problem, *i.e.*, every statistical sample $\bar{u}_s(x)$ satisfies $\bar{u}_s(x) = \bar{u}(x - c)$, with c a uniformly distributed random variable. Similar concept has been employed in many theories of homogeneous isotropic turbulence. If we assume other types of statistical samples, this procedure will change. The second equal sign of Eq. (16) implies the translation from sample-space integration to probability-space integration, and leads to the probability distribution $\rho(s) = (1 - s^2)^{-1/2}$.

The subspace orthogonal to $\text{Vect}(H_1, H_2)$ can be analytically described by involving the Chebychev polynomials[27] $\{T_n(s)\}$ defined in the interval $[-1, 1]$:

$$\begin{aligned} T_0(s) &= 1, \\ T_1(s) &= s, \\ T_{n+1}(s) &= 2sT_n(s) - T_{n-1}(s), \quad n \geq 1, \end{aligned} \tag{17}$$

which are orthogonal between each other under the present weight function $\rho(s)$ and therefore constitute the orthogonal bases in functional space. Employing the classic Gram-Schmidt procedure, we can calculate the bases of the subspace orthogonal to $\text{Vect}(H_1, H_2)$. For example, a basis can write

$$\begin{aligned} Z_1(s) &= s - \frac{T_1 \cdot H_2}{H_2 \cdot H_2} H_2(s) \\ &= s + \frac{\int_{-1}^1 \frac{s \sin s}{(2s^2+2)\sqrt{1-s^2}} ds}{\int_{-1}^1 \frac{\sin^2 s}{(2s^2+2)^2\sqrt{1-s^2}} ds} \frac{-\sin s}{2s^2+2} \\ &\approx s + 3.5789 \frac{-\sin s}{2s^2+2}. \end{aligned} \tag{18}$$

As described above, Z_1 is an *assumption* function which is orthogonal to $\text{Vect}(H_1, H_2)$. For comparison, we also formulate three *assumption* functions which do not satisfy the criterion of orthogonality

$$\begin{aligned} Z_2(s) &= s, \\ Z_3(s) &= s^2, \\ Z_4(s) &= s + s^2, \end{aligned} \tag{19}$$

with the following property of orthogonality respectively

$$\begin{aligned}
Z_2 \cdot H_1 &= 0, & Z_2 \cdot H_2 &\neq 0, \\
Z_3 \cdot H_1 &\neq 0, & Z_3 \cdot H_2 &= 0, \\
Z_4 \cdot H_1 &\neq 0, & Z_4 \cdot H_2 &\neq 0.
\end{aligned} \tag{20}$$

Numerical simulations are then performed to validate the orthogonality criterion. The computational domain is taken as $[-\pi, \pi]$ with periodic condition and 100 grids. Second-order central difference scheme is employed in spatial discretization, while explicit Euler scheme is employed for time advance. Trapezoidal integration is used in the spatial average operator. The **reason** of not choosing high-order schemes is because although these simple schemes involve numerical error, results are satisfactorily illustrated. Figure 1 shows the time evolution of the *restrictions*, *i.e.*, $\partial\langle h_i \rangle / \partial t$ which are expected to be zero. Comparing the four different *assumptions*, it can be concluded that for an *assumption* Z , when $Z \cdot H_i = 0$, this simply leads to $\partial\langle h_i \rangle / \partial t \approx 0$ (see the filled symbols in the figure); otherwise, when $Z \cdot H_i \neq 0$, the corresponding *restriction* $\partial\langle h_i \rangle / \partial t = 0$ cannot be satisfied (see the empty symbols in the figure). Note that even when $Z \cdot H_i = 0$, the corresponding *restriction* $\partial\langle h_i \rangle / \partial t$ is not exactly null, which stems from the **numerical calculations: on one side, the numerical errors are generated due to spatial and temporal discretizations; on another side, the SGS models may destroy the distribution of $\bar{u}$ which is expected to be $(1 - \bar{u}^2)^{-1/2}$, and then involve errors of orthogonal relations.** Figure 2 shows the time evolution of the inner product between assumption and restrictions. As a result, for the second restriction $Z \cdot H_2 = 0$ is not exactly satisfied even for Z_1 and Z_3 . The solution to guarantee orthogonality would be to estimate the distribution of $\bar{u}$ and then calculate the restriction Z dynamically, but this will no longer yield analytical formulas, and is beyond the scope of the present **contribution**. For the *restriction* h_2 (see Fig. 1b and 2b) the error is more obvious, since the calculation of $Z \cdot H_2$ is approximate, while $Z \cdot H_1$ simply relies on symmetry and is easy to be satisfied. However, this does not affect the conclusion of comparison, since in each subfigure the values of filled symbols are always much smaller than those of empty symbols. In brief, these results agree well with the theoretical analysis in the previous section and support the criterion of orthogonality on the *assumption* and *restrictions*.

Fig. 1. Time evolution of restrictions. (a) $|\partial\langle h_1 \rangle / \partial t|$; (b) $|\partial\langle h_2 \rangle / \partial t|$. The filled symbols correspond to orthogonal relations, the empty symbols otherwise.

IV. CONCLUSION

Researchers have developed numerous SGS models in the last half-century. Many of these models do not perform well as expected in practice, but there are few methods to theoretically analyze the SGS modelling methodology. Presently we can only evaluate an SGS model via *a-priori* and *a-posteriori* tests, whereas mathematical and physical criterions are quite rare. Also, good *a-priori* results do not always lead to good *a-posteriori* results[9], which inspires us to think about the criterions on the modelling methodology. In the present contribution we first analyze and define the concepts of *assumption* and *restriction* in SGS modelling, then show by a generalized derivation that if there are multiple stationary *restrictions* in a modelling, the corresponding *assumption* function must satisfy a criterion of orthogonality. Numerical tests using one-dimensional nonlinear advection equation are performed **to provide some validations on this approach**.

We remark that the present study is a preliminary step on understanding the SGS modelling methodology. As there are quite a lot of types of *restrictions* in the modelling process, we cannot provide a general criterion on them. However, the contribution of the present study is to strictly illustrate that, at least for a typical type of *restrictions*, *i.e.*, the stationary *restrictions* for statistical quantities, they call for a criterion of orthogonality on

Fig. 2. Time evolution of the inner product between assumption and restrictions. (a) $Z \cdot H_1$; (b) $Z \cdot H_2$. The filled symbols correspond to orthogonal relations, the empty symbols otherwise.

the *assumption*, otherwise these *restrictions* cannot be mathematically satisfied. We admit that the present idea is too ideal to be validated and employed in real SGS modelling, since no real SGS model uses only stationary *restrictions*. Also, the present validation only aims to reproduce the situation that the assumption of the SGS scheme is orthogonal to the restrictions, but there is no demonstration on the fact that the LES/filtered balance equation is well solved, which is expected to be investigated in the future. For existing SGS modelling methods, it is still not clear whether their *assumption* conflicts with *restrictions*, while future investigations would be necessary. We therefore expect more studies to clarify this question and to guide the future SGS modelling methodologies.

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