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Mathematical Constraints in Multiscale Subgrid-Scale Modeling of Nonlinear Systems *

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To shed light on the subgrid-scale (SGS) modeling methodology of nonlinear systems such as the Navier–Stokes turbulence, we define the concepts of assumption and restriction in the modeling procedure, which are shown by generalized derivation of three general mathematical constraints for different combinations of restrictions. These constraints are verified numerically in a one-dimensional nonlinear advection equation. This study is expected to inspire future research on the SGS modeling methodology of nonlinear systems.

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In physics, nonlinearity is the origin of many complicated multiscale phenomena. To quantitatively investigate the mechanisms, numerical simulations usually require a certain type of multiscale model, such as the subgrid-scale (SGS) model. The SGS modeling technique has been developed in the last half-century, which assumes a similarity between the SGS quantities and the grid-scale (GS) quantities, then translates the nonlinear equations to GS linear equations for numerical simulations.[1] As an example, in the community of turbulence research, the SGS modeling spirit has led to the many related investigations on the large-eddy simulation and detached-eddy simulation methods, which have been applied in practical engineering projects. However, there are also some confusions involved in these distinctive SGS models: (i) in the engineering community, researchers are not able to select an appropriate SGS model for a typical problem, and (ii) in the turbulence community, researchers may also be confused on the (necessary) criteria of constructing an SGS model. Park *et al.*[2] obtained three basic requirements for evaluating a good SGS model, which are helpful for clarifying the first confusion. However, the second point is still unclear, which indeed calls for better understanding of the SGS modeling procedure. Specifically, how should researchers 'correctly' involve physical and mathematical restrictions to model the SGS quantities?

In recent years, along with developing the SGS modeling technique,[3–5] we have also been curious about clarifying the methodology of SGS modeling. In fact, we found that when employing these SGS models, if the model coefficient is calculated dynamically, the LES calculations will usually diverge. Instead, a constant model coefficient leads to better performance in many applications. This fact has been discussed in Refs. [1,4,6], but we did not manage to give a convincing theoretical explanation. In Ref. [1], we summarized various attempts of this modeling methodology, and phenomenally guessed that there are conflicts among the assumptions and restrictions in SGS modeling. In Ref. [7] we found a typical criterion of orthogonality with one assumption and multiple restrictions of stationarity. However, these discussions have not touched the spirit of multiscale modeling, i.e., the multiscale law among scales such as the scaling law. An example of the multiscale law can be the famous Richardson–Komogorov 4/5 scaling law,[8] which has been widely used in SGS modeling, but presently there is no related theoretical investigation for clarifying the necessary mathematical constraints.

In this Letter, we discuss a more general situation by considering the multiscale law, and show the corresponding mathematical constraints. The results are expected to inspire future research of SGS modeling methodology.

To better explain the research context and to define the terms, here we review our previous analyses on the procedure of SGS modeling methodology. In general, by reviewing the existing SGS models, we describe the procedure of SGS modeling as the following two steps:[1,9] (1) Any SGS model should be based on a certain assumption on the SGS motion, that is, a formulation for SGS quantities (in particular, the SGS stress tensor). However, there are always undetermined factors in this assumption. (2) A complete SGS model should employ a certain closure method to determine the unknown factors mentioned in step (1). 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 concepts in the above two-step description. There are various assumptions such as the eddy-viscosity assumption,[10] the scale-similarity assumption,[11] the gradient diffusion assumption,[12] and the velocity increment

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assumption.[4,13] We conclude that an assumption assumes a (local) similarity between GS and SGS quantities. Usually there cannot 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 modeling closure. There are various types of restrictions, for example the inviscid simplification,[14] the scaling laws,[6,15] the filter similarity,[16] the velocity profile restriction.[17] We remark that there can be multiple restrictions in one SGS model, for example in Ref. [14], four restrictions are employed: the inviscid simplification, the scaling law, the stationarity simplification of structure function, and the subgrid feasibility for the Taylor expansion. In general, the reason for choosing multiple restrictions is that we hope the generated turbulence can satisfy more physical or mathematical laws. However, sometimes multiple restrictions lead to non-negligible error, and we do not understand the underlying reason.

To provide mathematical descriptions of the present problem, we consider a general formulation of a nonlinear partial differential equation

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

where t is the time, u is a continuous physical field, and f is defined as a nonlinear vector function. Defining $\bar{\bullet}$ as the GS filter operator, Eq. (1) can be rewritten as

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

where τ is the SGS quantity which needs to be modelled. Under this framework, we define three conceptual terms in the following mathematically. An assumption is to assume a direct linear similarity between GS and SGS quantities, which can be written as

$$\tau = c \cdot s(\bar{u}), \tag{3}$$

where c is a constant model coefficient, and s is a specified function. A restriction of the multiscale law is a physical statistical law concerning multiple scales including the GS and SGS parts, which can be written as

$$\langle p(\bar{u})\rangle = \langle q(\tau)\rangle, \tag{4}$$

where p and q are two scalar functions, and $\langle\rangle$ is the ensemble average. Compared with the assumption (3), the restriction of the multiscale law does not assume similarity on fluctuations, but only provides a physical statistical constraint. A restriction of stationarity is a physical statistical law concerning a stationary GS quantity,

$$\frac{d\langle h(\bar{u})\rangle}{dt} = 0, \tag{5}$$

with h being a scalar function. This usually corresponds to a conservation law of GS energy, enstrophy, helicity or other statistical quantities in practice.

In the following we show mathematical constraints on the conceptual terms defined above, by analyzing three typical situations. As there is always only one assumption in an SGS modeling, these three possible situations are multiple restrictions of stationarity, multiple restrictions of the multiscale law, and restrictions of both stationarity and the multiscale law.

We consider n restrictions of stationarity, corresponding to the definition (5) with $h = h_k$, $k = 1, 2, \ldots, n$. Multiplying both sides of Eq. (2) with $\frac{dh_i(\bar{u})}{d\bar{u}}$ and by noting that $\frac{\partial h_i(\bar{u})}{\partial t} = \frac{dh_i(\bar{u})}{d\bar{u}}\frac{\partial \bar{u}}{\partial t}$, we can obtain

$$\frac{\partial h_i(\bar{u})}{\partial t} = \frac{dh_i(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_i(\bar{u})}{d\bar{u}}\tau. \tag{6}$$

Taking ensemble average on Eq. (6) and noting the restriction (5), we have

$$\frac{d\langle h_i(\bar{u})\rangle}{dt} = \left\langle \frac{dh_i(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_i(\bar{u})}{d\bar{u}}\tau \right\rangle = 0. \tag{7}$$

From Eqs. (3) and (7) the model coefficient c can be solved as

$$c = -\left\langle \frac{dh_i(\bar{u})}{d\bar{u}} f(\bar{u}) \right\rangle \Big/ \left\langle \frac{dh_i(\bar{u})}{d\bar{u}} s(\bar{u}) \right\rangle. \tag{8}$$

Therefore, for any j there is

$$\begin{aligned} \frac{d\langle h_j(\bar{u})\rangle}{dt} &= \left\langle \frac{dh_j(\bar{u})}{d\bar{u}} f(\bar{u}) + \frac{dh_j(\bar{u})}{d\bar{u}}\tau \right\rangle \\ &= \left\langle \frac{dh_j(\bar{u})}{d\bar{u}} f(\bar{u}) \right\rangle \\ &\quad - \frac{\left\langle \frac{dh_i(\bar{u})}{d\bar{u}} f(\bar{u}) \right\rangle \left\langle \frac{dh_j(\bar{u})}{d\bar{u}} s(\bar{u}) \right\rangle}{\left\langle \frac{dh_i(\bar{u})}{d\bar{u}} s(\bar{u}) \right\rangle}. \end{aligned} \tag{9}$$

From the restrictions of stationarity $\frac{d\langle h_j(\bar{u})\rangle}{dt} = 0$ we finally obtain

$$\begin{aligned} &\left\langle \frac{dh_j(\bar{u})}{d\bar{u}} f(\bar{u}) \right\rangle \left\langle \frac{dh_i(\bar{u})}{d\bar{u}} s(\bar{u}) \right\rangle \\ &- \left\langle \frac{dh_i(\bar{u})}{d\bar{u}} f(\bar{u}) \right\rangle \left\langle \frac{dh_j(\bar{u})}{d\bar{u}} s(\bar{u}) \right\rangle = 0, \end{aligned} \tag{10}$$

for any possible combination of i and j. This mathematical constraint should be satisfied under the situation of multiple restrictions of stationarity.

We then consider n restrictions of the multiscale law, corresponding to the definition (4) with $p = p_k$, $q = q_k$, $k = 1, 2, \ldots, n$. Considering the ith restriction, substituting Eq. (3) into Eq. (4) yields

$$\langle p_i(\bar{u})\rangle = \langle q_i(c \cdot s(\bar{u}))\rangle. \tag{11}$$

If q_i is a linear function, we will have

$$c = \langle p_i(\bar{u})\rangle / \langle q_i \circ s(\bar{u})\rangle. \tag{12}$$

Substituting Eq. (12) to the jth restriction, we finally obtain the following mathematical constraints to the situation of multiple restrictions of the multiscale law

$$\langle p_j(\bar{u})\rangle\langle q_i \circ s(\bar{u})\rangle - \langle p_i(\bar{u})\rangle\langle q_j \circ s(\bar{u})\rangle = 0, \tag{13}$$

for any possible combination of i and j.

We here consider m restrictions of stationarity, corresponding to the definition (5) with $h = h_k$, $k = 1, 2, \ldots, m$ and n restrictions of the multiscale law, corresponding to the definition (4) with $p = p_k$, $q = q_k$, $k = 1, 2, \ldots, n$. Clearly, the mathematical constraints (10) and (13) should be satisfied. Moreover, additional constraints exist by mixing these two types of restrictions together. Considering the ith restriction of the multiscale law and the jth restriction of stationarity, by using Eqs. (5) and (12) we have

$$\langle h_j \circ f(\bar{u})\rangle\langle q_i \circ s(\bar{u})\rangle - \langle h_j \circ s(\bar{u})\rangle\langle p_i(\bar{u})\rangle = 0, \quad (14)$$

for any possible combination of i and j.

In the following we select the simplest nonlinear partial differential equation, i.e., the one-dimensional nonlinear advection equation, or 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 in other physical problems, such as the high-dimensional KdV-Burgers equation and the KdV equation, but the analytical analysis will be more difficult. In the present contribution the governing equation can be simply written as (the factor $1/2$ on the right hand side is omitted for simplicity)

$$\frac{\partial \bar{u}}{\partial t} = \frac{\partial \bar{u}^2}{\partial x} + \tau, \quad (15)$$

with the resolved-scale initial condition

$$\bar{u}(x)|_{t=0} = \sin x. \quad (16)$$

This implies that $\bar{u}$ is always periodic with a period 2π. It is also evident that at initial time we have $\bar{u} \in [-1, 1]$. Note that the governing Eq. (15) does not indicate that the full-scale equation is $\partial_t u = \partial_x u^2$, while indeed, this only shows that the large-scale motion is advected nonlinearly, and the SGS term τ is undetermined. Here we assume that the SGS term τ is appropriate, thus the resolved-scale quantity $\bar{u}$ is always in the interval $[-1, 1]$ at any time, and changing the variable of integral leads to

$$\langle g(\bar{u})\rangle = \int_{-\pi}^{\pi} g(\bar{u}(x))dx = \int_{-1}^{1} g(\bar{u})\frac{1}{\sqrt{1-\bar{u}^2}}d\bar{u}. \quad (17)$$

Note that to derive this weight function, for the first equal sign of Eq. (17) we use the spatial average (i.e., the integral over x) to replace the ensemble average, which implies that the spatial direction is considered to be statistically homogeneous to satisfy the SGS modeling 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 $\bar{u}_s(x) = \bar{u}(x - \alpha)$, with α being a uniformly distributed random variable. If we assume other types of statistical samples, this procedure will accordingly change. The second equal sign of Eq. (17) implies the translation from sample-space integral to probability-space integral, and leads to the probability distribution $\rho(s) = (1 - s^2)^{-1/2}$.

Numerical tests are then performed to validate the mathematical constraints, respectively. For all tests the assumption is always selected as $s(\bar{u}) = \bar{u}^2$, which is similar to the velocity increment assumptions in practical SGS modeling.[4,13] Three different restrictions of stationarity are listed as

$$h_1(\bar{u}) = \bar{u},\ h_2(\bar{u}) = \bar{u}^2,\ h_3(\bar{u}) = \bar{u}^4, \quad (18)$$

which correspond to the conservation of mean velocity, resolved kinetic energy and the fourth-order moment of resolved velocity (which is related to the flatness of resolved velocity distribution), respectively. Four different restrictions of the multiscale law are also listed as

$$\begin{aligned} p_1(\bar{u}) &= \frac{4}{3}\bar{u}^2,\ q_1(\tau) = \tau, \\ p_2(\bar{u}) &= \bar{u}^2(4\bar{u}^2 - 2),\ q_2(\tau) = \tau^2, \\ p_3(\bar{u}) &= \bar{u}^2(4 - 4\bar{u}^2),\ q_3(\tau) = \tau^2, \\ p_4(\bar{u}) &= \frac{16}{3}\bar{u}^2,\ q_4(\tau) = \tau, \end{aligned} \quad (19)$$

where both (p_1, q_1) and (p_4, q_4) correspond to the restriction $\langle \bar{u}^2\rangle \sim \langle \tau\rangle$, which means that the mean value of SGS variable is determined by the resolved energy, and (p_2, q_2) corresponds to the restriction $\langle -\bar{u}^2\partial^2\bar{u}^2/\partial x^2\rangle = \langle \tau^2\rangle$ at $t = 0$ because $\partial^2\bar{u}^2/\partial x^2 = 2 - 4\bar{u}^2$, and represents a statistical balance between the GS velocity-gradient correlation and the SGS energy. Similarly, (p_3, q_3) corresponds to the restriction $\langle(\partial\bar{u}^2/\partial x)^2\rangle = \langle \tau^2\rangle$ at $t = 0$, which implies a statistical balance between the energy of the GS nonlinear advection term and the SGS energy.

We then perform three groups of test cases to validate the three different mathematical constraints, respectively. The first group uses only restrictions of stationarity: case C_1 uses h_1 and h_2 which satisfy constraint Eq. (10), while case C_2 uses h_1 and h_3 which do not satisfy this constraint. The second group uses only restrictions of the multiscale law: case C_3 uses (p_1, q_1) and (p_2, q_2) which satisfy constraint (13), while case C_4 uses (p_1, q_1) and (p_3, q_3) which do not satisfy this constraint. The third group uses restrictions of both stationarity and the multiscale law: case C_5 uses h_2 and (p_4, q_4) which satisfy constraint Eq. (14), while case C_6 uses h_2 and (p_1, q_1) which do not satisfy this constraint.

Figure 1 shows the error evolution of these test cases. The solid symbols correspond to the cases that satisfy the specific mathematical constraints, while the empty symbols otherwise. Clearly, in each group when the constraints are satisfied, errors are always reduced compared with those cases that break the constraints. We then obtain that all constraints (10), (13) and (14) are important in practice and should not be ignored. Another fact is that compared with different restrictions, the restrictions of stationarity lead to greater

errors even if it is already satisfied (see the solid symbols in Fig. 1, as the restrictions of stationarity lead to errors of order 10^{-5}, while the restrictions of the multiscale law lead to errors of order 10^{-8}). This might be explained by the fact that the restrictions of stationarity are time-dependent while the multiscale laws are not, hence the former one would possibly accumulate errors compared with the latter one.

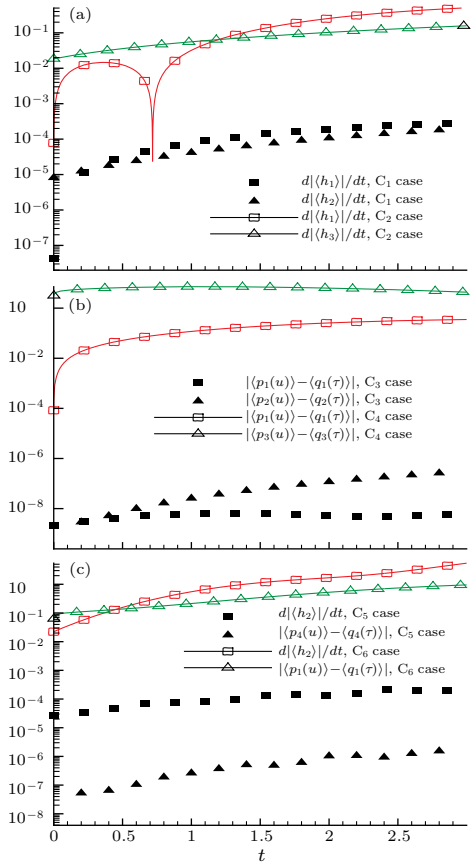

Fig. 1. Error evolution in different numerical test cases. (a) Cases C_1 and C_2 using only restrictions of stationarity, (b) cases C_3 and C_4 using only restrictions of the multiscale law, and (c) cases C_5 and C_6 using restrictions of both stationarity and the multiscale law.

In summary, we have mathematically defined the assumption and two types of restrictions in SGS modeling, and then have shown by general derivations that multiple restrictions must satisfy specific mathematical constraints among them. These constraints can be classified into three situations, denoted by Eqs. (10), (13) and (14). In practice, if some of these constraints are not satisfied, mathematical systematical errors rather than numerical errors will be inevitable. In addition, it is also observed that the restrictions of stationarity yield more accumulated errors compared with the restrictions of the multiscale law. These mathematical constraints then provide theoretical supports for analyzing the existing SGS modeling methods, and for designing new SGS models.

Although many conceptual explanations in the present study come from the research of turbulence, the present work will not be limited in it. Indeed, the theoretical analysis here provides a general SGS modeling methodology and the corresponding general mathematical constraints to all nonlinear problems.

We remark that in the present work a linear function q is assumed to allow analytical expressions for the model coefficient c. Indeed, in practical cases the function q is usually nonlinear, and an explicit formula of c will be difficult. In that case, however, implicit formulations can also be obtained using the present method, although the results of mathematical constraints will be very complicated.

Finally we remark that the present study is a preliminary step in understanding the SGS modeling methodology. As there are many types of restrictions in the modeling process, we cannot provide a general criterion on them. However, the contribution of the present study is to strictly illustrate that there are general mathematical constraints for the two types of restrictions, i.e., the restrictions of stationarity and restrictions of the multiscale law. We admit that the present idea is still ideal to be validated and employed in real SGS modeling, since in real SGS models the restrictions are usually more complicated. However, the method in the present work will also be consistent to other types of restrictions. This also naturally raises a question whether existing SGS modeling methods have similar mathematical conflicts. We believe that the answer should be positive. We therefore expect to clarify this question and to guide the SGS modeling methodologies of nonlinear systems in future studies.

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