Generalized theory for numerical instability of the Gaussian-filtered Navier-Stokes equations as a model system for large eddy simulation of turbulence

Masato Ida

Center of Computational Science and E-systems, Japan Atomic Energy Agency, 6-9-3 Higashi-Ueno, Taito-ku, Tokyo 110-0015, Japan

Nobuyuki Oshima

Division of Mechanical and Space Engineering, Graduate School of Engineering, Hokkaido University, Kita 13 Nishi 8, Kita-ku, Sapporo 060-8628, Japan

Abstract

The Gaussian-filtered Navier-Stokes equations are examined theoretically and a generalized theory of their numerical stability is proposed. Using the exact expansion series of subfilter-scale stresses or integration by parts, the terms describing the interaction between the mean and fluctuation portions in a statistically steady state are theoretically rewritten into a closed form in terms of the known filtered quantities. This process involves high-order derivatives with time-independent coefficients. Detailed stability analyses of the closed formulas are presented for determining whether a filtered system is numerically stable when finite difference schemes or others are used to solve it. It is shown that by the Gaussian filtering operation, second and higher even-order derivatives are derived that always exhibit numerical instability in a fixed range of directions; hence, if the filter widths are unsuitably large, the filtered Navier-Stokes equations can in certain cases be unconditionally unstable even though there is no error in modeling the subfilter-scale stress terms. As is proved by a simple example, the essence of the present discussion can be applied to any other smooth filters; that is, such a numerical instability problem can arise whenever the dependent variables are smoothed out by a filter.

PACS numbers: 47.27.E-, 47.10.ad, 47.11.-j, 47.10.-g
I. INTRODUCTION

Large eddy simulation (LES) \[1, 2\] is one of the typical numerical approaches to turbulent flows, in which large-scale structures in fluid motion are solved directly while the effects of the small-scale eddies are modeled based on a filtering operation that separates the high- and low-wavenumber modes in turbulent flow fields. Because LES enables us to treat time-dependent, high-Reynolds-number turbulence with substantially smaller computational effort and storage than direct numerical simulation (DNS) resolving all scales of motion, it has been used in many applications in a variety of research fields, including fluid machinery [3], combustion engineering [4, 5], atmospheric science [6, 7], geophysics [8, 9, 10], and astrophysics [11, 12].

For the past few years, however, several reports have been published that point out the incompleteness of current LES modeling. In those reports it has been implied that even a completely accurate LES model could be numerically unstable. In Ref. [13], Leonard showed that the tensor-diffusivity model, re-derived by truncating an exact expansion series of subfilter-scale forces [14, 15, 16], works as a negative-diffusion term in the stretching directions of fluid motion and hence, that it could lead to numerical instability when used for finite difference schemes. Since that model is exact for first-order velocity fields where the velocity components can be described by linear polynomials, the model’s negative diffusivity can be considered to exhibit the nature of the exact model under a particular condition. Also, Winckelmans et al. [17] and Kobayashi and Shimomura [18, 19, 20] pointed out that the tensor-diffusivity model behaves unstably in a plane channel flow, also due to the model’s negative diffusivity. In a comparative study of LES models (the tensor-diffusivity and rational LES models) [21], Iliescu et al. showed that the tensor-diffusivity model can be unstable in a high-Reynolds-number driven cavity flow, as well. In Ref. [22], Ida and Taniguchi derived a closed form of the Gaussian-filtered Navier-Stokes (GFNS) equations under a simple assumption about the instantaneous velocity profile and showed theoretically that the shears in time-averaged flow fields can also be the seed of the numerical instability of the filtered system, because a cross derivative of the filtered velocity component, being unconditionally unstable in numerical simulation, appears in the closed formula. The authors stressed that the unstable portions in the closed formula must be solved accurately without using artificial techniques (e.g., clipping or damping), since those portions derive naturally from the filtering operation and are thus a part of the governing equations for LES. In the sequel to that paper [23], Ida and Taniguchi further ascertained that the shears in the time-averaged fields can, through the filtering operation, cause the appearance of a numerically unstable term that always exhibits a negative diffusivity in a fixed direction, a conclusion that is able to explain the problematic instability that has frequently been confronted in wall-bounded turbulent flow computations (e.g., Refs. [17, 18]), where a strong shear appears in the time-averaged streamwise velocity. The theoretical and numerical findings listed above appear to suggest that the filtering operation itself is the underlying cause of the numerical instability in LES, raising the question whether a numerically stable LES model can be ideally accurate or not.

A similar scenario can be found in simulation strategies for collisionless plasma kinetics that use the Vlasov-Poisson or Vlasov-Maxwell system as a governing equation. In Refs. [24, 25], Klimas has attempted to apply a Gaussian filter to the Vlasov equations in order to mollify the filamentation of the distribution function (an infinitely fine structure in the phase space), and found that the filtered Vlasov equations can be rewritten into a closed
form in terms of the filtered distribution function and are thus solvable without any empirical modeling. (We note here that in Klimas’s study the filtering operation was only applied in the velocity space, which allows for relatively easy derivation of closed formulas and results in only a few additional terms.) In that closed formula, a cross derivative of the filtered distribution function appears, which, as Figuza et al. suggested [26] (see also Refs. [18, 22]), makes the filtered system ill-conditioned and unsuitable for numerical simulations using finite difference methods or others excluding the spectral method. As with the Navier-Stokes cases mentioned above, that finding implies that the Gaussian filtering operation itself, and not the modeling or approximations, destabilizes the governing equations.

The present paper extends the numerical stability analysis of the GFNS equations performed by Ida and Taniguchi [23] to construct a generalized theory for the numerical instability of the system. The present discussion assumes that the flow fields are, as in Ref. [23], in a statistically steady state (an assumption allowing us to decompose the velocity components into time-independent mean and time-dependent fluctuation portions), but the mean velocities may be described by high-order polynomials in terms of the spatial coordinates, while in Ref. [23] first-order velocity fields have mainly been considered. Under these assumptions and using the exact expansion series or integration by parts, we rewrite the terms that represent the interaction between the mean and fluctuation portions (referred to below as “mean-fluctuation terms”), filtered by a Gaussian function, into closed forms involving high-order cross derivatives, and show that through Gaussian filtering, various kinds of unconditionally unstable terms having time-independent coefficients are derived which numerically destabilize the modes in a fixed range of directions. Also, detailed stability analyses of the resulting closed formulas are presented to derive a stability criterion for the choice of filter widths. In the present paper, for simplicity we only discuss cases in which the mean velocity field has one-dimensional (1D) or two-dimensional (2D) structures. Moreover, we are not concerned with the commutation error between differentiation and filtering (see e.g. Refs. [27, 28, 29, 30] for recent efforts to resolve the commutation error), assuming each filter width to be constant in the corresponding spatial direction. This treatment warrants that the numerically unstable terms that we discuss are not those originating from the commutation error, which is a modeling failure.

The present theoretical investigation has been performed assuming the use of finite difference schemes. However, most of the results will be true for other numerical methods (e.g., finite volume, finite element, compact differencing) as well. Also, in order to accomplish the theoretical investigation without the aid of numerical analysis, the present study neglects the cutoff of high-wavenumber modes originating from the use of finite grid spacing. The Gaussian filter considered in the present study is, therefore, assumed to approximately represent the numerical damping of high-wavenumber modes due to numerical viscosity (also originating from the use of finite grid spacing), and also to be an explicit filter applied independently of numerical discretization [17, 31]. Because of these assumptions, we use the term “subfilter scale” in stead of “subgrid scale” throughout this paper.

The present paper is organized as follows. In Sec. II the governing equations and definitions useful for the present investigation are introduced. In Sec. III the numerical stability of arbitrary-order partial differential equations involving high-order cross derivatives is theoretically discussed to derive a stability criterion for them, which is essential for our study. Combining the result of this stability analysis with an exact expansion series or integration by parts allows us to construct a generalized theory for the filtering instability under statistically steady-state conditions. In Sec. IV several specific examples are investigated to
II. GOVERNING EQUATIONS, FILTERING OPERATIONS, AND DEFINITIONS

Incompressible viscous fluid flows are described by the Navier-Stokes equations:

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad \text{for } i = 1, 2, 3, \tag{1}
\]

\[
\frac{\partial u_i}{\partial x_i} = 0, \tag{2}
\]

where the summation convention is assumed, and \( u_i \) \( (i = 1, 2, 3) \) are the velocity components, \( p \) is the pressure divided by the constant fluid density, and \( \nu \) is the kinematic viscosity. The subfilter-scale terms, resulting from a low-pass filtering operation, are derived from the convection terms (i.e., the second term of Eq. (1)). In what follows, we assume that the velocity components can be decomposed into time-averaged and fluctuation portions as

\[
u(x, t) = U(x) + \nu'(x, t), \tag{3}
\]

where \( \nu = (u_1, u_2, u_3) \), \( U = (U_1, U_2, U_3) \), and \( \nu' = (\nu'_1, \nu'_2, \nu'_3) \). We also assume that the mean velocity \( U \) is time-independent; i.e., that the flow is in a statistically steady state. From Eqs. (2) and (3), one can derive

\[
\frac{\partial U_i}{\partial x_i} = \frac{\partial u'_i}{\partial x_i} = 0. \tag{4}
\]

Using Eqs. (3) and (4), the convection term in Eq. (1) is rewritten as follows:

\[
\frac{\partial u_j u_i}{\partial x_j} = h_i + u'_j \frac{\partial u'_i}{\partial x_j} + U_j \frac{\partial U_i}{\partial x_j}, \tag{5}
\]

\[
h_i \equiv U_j \frac{\partial u'_i}{\partial x_j} + U_i \frac{\partial u'_j}{\partial x_j} \quad \text{for } i = 1, 2, 3, \tag{6}
\]

where \( h_i \) represents the interaction between the mean and fluctuation portions, on which we focus our attention.

The filter function is assumed to be Gaussian:

\[
G(X; \Delta) = \sqrt{\frac{\gamma}{\pi \Delta^2}} \exp \left( -\frac{\gamma X^2}{\Delta^2} \right),
\]
which satisfies \( \int_{X=-\infty}^{X=\infty} G(X; \Delta) dX = 1 \), where \( \gamma \) is commonly set to 6 in LES and \( \Delta \) is the filter width. Using this, the filtering operation in the \( x_i \) direction is performed as a convolution integral:

\[
\tilde{f}(x_i, \ldots, t) = \int_{X=-\infty}^{X=\infty} G(x_i - X; \Delta_i) f(X, \ldots, t) dX = G_i \ast f,
\]

where the overbar denotes the filtered quantities. Three-dimensional (3D) filtering is achieved by successively performing this convolution as follows:

\[
\tilde{f}(x_i, \ldots, t) = \prod_{i=1}^{3} \int_{X=-\infty}^{X=\infty} G(x_i - X_i; \Delta_i) f(X, \ldots, t) dX = G_1 \ast [G_2 \ast (G_3 \ast f)]
\]

\[\equiv G_{123} \ast f,\]

where \( \Delta_i (i = 1, 2, 3) \) is the filter width in the \( x_i \) direction. As stated in Sec. I, we assume throughout this paper that each filter width is a constant, and thus

\[
G_i \ast \frac{\partial f}{\partial x_j} = \frac{\partial (G_i \ast f)}{\partial x_j},
\]

\[
G_i \ast (G_j \ast f) = G_j \ast (G_i \ast f) \quad \text{for } i, j = 1, 2, 3.
\]

For the convenience of the following discussion, we introduce the residual stress function defined as

\[
R_a[F(U_1, u_1', \ldots)] = G_a \ast F(U_1, u_1', \ldots) - F(G_a \ast U_1, G_a \ast u_1', \ldots), \quad (7)
\]

which yields, for example,

\[
R_1 \left[ U_j \frac{\partial u_i'}{\partial x_j} \right] = G_1 \ast \left( U_j \frac{\partial u_i'}{\partial x_j} \right) - (G_1 \ast U_j) \frac{\partial (G_i \ast u_i')}{\partial x_j}, \quad (8)
\]

\[
R_{123} \left[ u_1' u_2' \right] = G_{123} \ast (u_1' u_2') - (G_{123} \ast u_1') (G_{123} \ast u_2'). \quad (9)
\]

Based on the above assumptions and definitions, the Navier-Stokes equations filtered using a 3D Gaussian filter are written as

\[
\frac{\partial \tilde{u}_i'}{\partial t} + \frac{\partial \tilde{u}_j \tilde{u}_i}{\partial x_j} = - \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - R_{123} \left[ \frac{\partial u_j u_i}{\partial x_j} \right], \quad (10)
\]

or

\[
\frac{\partial \tilde{u}_i'}{\partial t} + \frac{\partial \tilde{u}_j \tilde{u}_i}{\partial x_j} = - \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - R_{123} [h_i] - R_{123} \left[ u_j' \frac{\partial u_i'}{\partial x_j} \right] + \left( \nu \frac{\partial^2 \tilde{U}_i}{\partial x_j \partial x_j} - R_{123} \left[ U_j \frac{\partial \tilde{U}_i}{\partial x_j} \right] \right), \quad (11)
\]

which can be considered an equation for both \( \tilde{u}_i' \) and \( \tilde{u}_i \) because \( \partial \tilde{u}_i'/\partial t = \partial \tilde{u}_i/\partial t \). The terms in the last parentheses of Eq. (11) can be considered time-independent source terms, which may have no influence on the numerical stability. The next to last term represents
the residual stress forces due to the nonlinear interaction between the fluctuation portions, the stability analysis of which is difficult to complete theoretically and thus requires numerical experiments. Although it has been pointed out that terms having the same form as \( R_{123} [u_j' \partial u_i' / \partial x_j] \) can instantaneously be numerically unstable [13, 22], such terms should not necessarily lead to numerical instability in actual computation, because their time-averaged nature can be dissipative. In what follows, we only consider the numerical stability of

\[
\nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - R_{123} [h_i],
\]

i.e., the difference between the molecular viscosity and the residual stress forces due to the mean-fluctuation interaction, and do not take into consideration the numerical effects of the nonlinear term. In this respect, our theoretical investigation is incomplete. Comments on potential approaches to resolving this incompleteness are given in Sec. V. As shown in what follows, the closed form of Eq. (12) has time-independent coefficients, meaning that the numerical stability of this portion is time-independent.

We introduce here some mathematical tools that allow us to rewrite the filtered mean-fluctuation term \( R_{123} [h_i] \) into a closed form. Yeo [14] and others [13, 15, 16] have derived a very interesting identity, which is applicable to all differentiable and continuous functions \( f(x) \) and \( g(x) \),

\[
(f g) - \bar{f} \bar{g} = \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{\Delta^2}{2\gamma} \right)^n \frac{\partial^n \bar{f}}{\partial x^n} \frac{\partial^n \bar{g}}{\partial x^n}.
\]

Here, the overbar indicates \( x \)-directional Gaussian filtering. It is worth noting that the right-hand side of this identity only involves the known filtered quantities \( \bar{f} \) and \( \bar{g} \). This outstanding feature of the series allows us to rewrite the residual \( R[f g] = (f g) - \bar{f} \bar{g} \) into a closed form. For 2D Gaussian filtering in the \((x_1, x_2)\) plane, this series becomes

\[
(f g) - \bar{f} \bar{g} = \sum_{k=1}^{2} \left( \frac{\Delta_k^2}{2\gamma} \right) \frac{\partial \bar{f}}{\partial x_k} \frac{\partial \bar{g}}{\partial x_k} + \sum_{k,l=1}^{2} \frac{1}{2!} \left( \frac{\Delta_k^2}{2\gamma} \right) \left( \frac{\Delta_l^2}{2\gamma} \right) \frac{\partial^2 \bar{f}}{\partial x_k \partial x_l} \frac{\partial^2 \bar{g}}{\partial x_k \partial x_l} + \sum_{k,l,m=1}^{2} \frac{1}{3!} \left( \frac{\Delta_k^2}{2\gamma} \right) \left( \frac{\Delta_l^2}{2\gamma} \right) \left( \frac{\Delta_m^2}{2\gamma} \right) \frac{\partial^3 \bar{f}}{\partial x_k \partial x_l \partial x_m} \frac{\partial^3 \bar{g}}{\partial x_k \partial x_l \partial x_m} + \cdots.
\]

The following identity is also useful:

\[
\mathcal{G}_i \ast (x_i f) = \left( x_i + \frac{\Delta_i^2}{2\gamma} \frac{\partial}{\partial x_i} \right) (\mathcal{G}_i \ast f), \quad i = 1, 2, 3,
\]

which can be derived using integration by parts (e.g., Refs. [22, 24, 26, 32]). This yields, for example,

\[
\mathcal{G}_i \ast x_i = x_i,
\]

\[
\mathcal{G}_i \ast x_i^2 = x_i^2 + \frac{\Delta_i^2}{2\gamma},
\]

\[
\mathcal{G}_i \ast x_i^3 = x_i^3 + \frac{3\Delta_i^2}{2\gamma} x_i,
\]
where the summation convention is not adopted. Using Eq. (10), Eq. (15) can be rewritten into
\[ R_i[x_i f] = \frac{\Delta^2}{2 \gamma} \frac{\partial (G_i \ast f)}{\partial x_i}, \quad i = 1, 2, 3. \] (19)

The expansion series (13) and (14) enable us to derive a closed form of Eq. (12). As can be seen from these series, the closed form has high-order derivatives including high-order cross derivatives, and the coefficients of these derivatives are time-independent, such as \( U_j \) and \( \partial U_i / \partial x_j \) in \( h_i \). The numerical stability of such high-order derivatives are examined below.

III. NUMERICAL STABILITY OF ARBITRARY-ORDER PARTIAL DIFFERENTIAL EQUATIONS

We derive and examine in this section a numerical-stability criterion to determine whether an arbitrary-order partial differential equation (PDE) can be solved stably (and accurately) by a finite difference scheme. Although the numerical stability of PDEs is known to depend on the discretization scheme applied, we do not discuss a certain form of finite differencing. We instead consider the exact amplification factor of the PDEs, which is essential and may be sufficient for our aim. It is well known that a diffusion equation, for example, is numerically stable (numerically unstable) when the coefficient of the diffusion term is positive (negative), i.e., when the exact amplification factor is less than (greater than) unity. We assume here that such is also the case for other types of PDEs including high-order ones, and use their amplification factors to judge whether a stable finite difference scheme can exist for the corresponding PDE.

Let us consider the exact solution of a 2D arbitrary-order PDE,
\[ \frac{\partial f}{\partial t} = \mu \left( \frac{\partial}{\partial x} \right)^m \left( \frac{\partial}{\partial y} \right)^n f, \] (20)
\[ f = f(x, y, t) \]
where \( \mu \) is a real constant and \( m, n \geq 0 \) are integers. The initial condition is
\[ f(x, y, 0) = \exp(i(k_x x + k_y y)), \] (21)
where \( k_x \) and \( k_y \) are real constants, \( i \) is the imaginary unit, and the boundary conditions are periodic. Suppose that the exact solution of this PDE has the form of
\[ f(x, y, t) = \exp(\omega t)f(x, y, 0), \] (22)
where \( \omega \) is a complex constant. Substituting this into Eq. (20) yields
\[ \omega = \mu^{m+n} \mu k_x^m k_y^n. \] (23)

The characteristic of this exact solution can roughly be categorized into the following two solutions:

For \( m + n = 2M \):
\[ f = \exp((-1)^M \mu k_x^m k_y^n t) \exp(i(k_x x + k_y y)), \] (24)
For \( m + n = 2M + 1 \):

\[
f = \exp(i(-1)^M \mu k_x^m k_y^n t) \exp(i(k_x x + k_y y)),
\]

where \( M = 0, 1, 2, \cdots \). The former represents exponential decay or growth of the solution, whereas the latter represents phase shift without changing amplitude.

Equation (24) suggests that in order for a stable finite difference scheme for \( m + n = 2M \) to exist, the amplification exponent of solution (24),

\[
\alpha(m, n; \mu) = (-1)^M \mu k_x^m k_y^n,
\]

must be zero or less for any value of wavenumbers. Furthermore, if \( m \) and \( n \) are even numbers, \( k_x^m k_y^n \) in this exponent is always positive and the stability is thus determined by the sign of \((-1)^M \mu\). (If, for example, \( m = 2 \) and \( n = 0 \), which results in \( M = 1 \), the PDEs with \( \mu \geq 0 \) are numerically stable, while those with \( \mu < 0 \) are unconditionally unstable, a conclusion that is consistent with the well-known fact that a positive diffusion equation can be solved stably but a negative one cannot.) Otherwise, i.e., if \( m \) and \( n \) are odd numbers, \( k_x^m k_y^n \) can be either positive or negative, meaning that the PDEs in this case are always unconditionally unstable because modes in any direction can appear in turbulent flows. (This conclusion is consistent with the known fact that the PDE for \( m = n = 1 \) is unconditionally unstable; see, e.g., Refs. [18, 22, 26]). For \((-1)^M \mu < 0\), for example, the modes of \( k_x k_y < 0 \) must be unstable, implying that if the sign of \( \mu \) is constant, the PDEs in this case always exhibit numerical instability in a fixed range of directions. This finding plays an important role in our main subject discussed in the next section.

On the other hand, Eq. (25) suggests that if \( m + n \) is an odd number, a stable finite difference scheme should always exist because the amplification exponent

\[
\alpha(m, n; \mu) = i(-1)^M \mu k_x^m k_y^n
\]

has an imaginary value and hence the absolute value of the amplification factor, \(|\exp(i(-1)^M \mu k_x^m k_y^n t)|\), is unity. Indeed, the advection equations (corresponding to the case of, e.g., \( m = 1 \) with \( n = 0 \)) and the Korteweg-de Vries (KdV) equations involving third- and/or fifth-order dispersion terms (e.g., for \( m = 1, 3, 5 \) with \( n = 0 \)) have been solved stably and accurately by finite difference schemes; see, e.g., Refs. [33, 34, 35] for recent progress in finite difference schemes for KdV equations.

The present theoretical results can be summarized as follows: A stable finite difference solver must exist for odd-order PDEs (i.e., when \( m + n \) is an odd number). For even-order PDEs, a stable solver exists only if both \( m \) and \( n \) are even numbers and \((-1)^{(m+n)/2} \mu \) is negative; otherwise, the PDE is unconditionally unstable by any finite difference scheme, since the numerical perturbations grow exponentially in numerical simulations. This conclusion may also be true for the finite volume, finite element, and compact difference schemes.

The total amplification exponent \( \alpha_T \) of a complicated PDE,

\[
\frac{\partial f}{\partial t} = \sum_i \mu_i \left( \frac{\partial}{\partial x} \right)^{m_i} \left( \frac{\partial}{\partial y} \right)^{n_i} f,
\]

can be determined by

\[
\alpha_T = \sum_i \text{Re}[\alpha(m_i, n_i; \mu_i)].
\]

Though this is, for variable \( \mu_i \), only an approximation, it should work sufficiently in many situations.
IV. STABILITY ANALYSIS OF THE FILTERED SYSTEM

We present several analytical results for the numerical stability of a filtered system determined by combining the stability analysis described in the previous section with the exact expansion series (13) and (14) or the identity given using integration by parts, (15). As stated in Sec. III, we consider up to 2D cases for the sake of simplicity, and only analyze the stability of Eq. (12).

A. 1D mean velocity cases

Suppose that

\[ U_1 = U_1(x_2) \quad \text{and} \quad U_2 = U_3 = 0, \]

(this means that the velocity satisfies the divergence-free condition), which leads to

\[ h_1 = U_1 \frac{\partial u'_1}{\partial x_1} + \frac{\partial U_1}{\partial x_2} u'_2, \]  
\[ h_2 = U_1 \frac{\partial u'_2}{\partial x_1}, \]  
\[ h_3 = U_1 \frac{\partial u'_3}{\partial x_1}. \]  

Because \( U_1 \) depends only on \( x_2 \), filtering in the \( x_1 \) and \( x_3 \) directions (i.e., in the homogeneous directions) results in

\[ \mathcal{R}_{13}[h_i] = 0 \quad \text{for} \quad i = 1, 2, 3, \]  

When the Gaussian filter in the \( x_2 \) direction is applied to Eqs. (30)-(32), some mathematical manipulations are needed to obtain a closed formula because \( U_1 \) and \( \partial U_1 / \partial x_2 \) cannot simply be put outside the convolution operation. We consider here the case where \( U_1 \) is described by a finite-order polynomial:

\[ U_1(x_2) = \sum_{n=0}^{N} a_n x_2^n, \]  

where \( a_n \) \((n = 0, 1, \ldots, N)\) are real constants and \( N \) is the order of this polynomial. Using the 1D expansion series (13), we have

\[ \mathcal{R}_2[h_1] = \mathcal{L}_{[1]} \bar{u}'_1 + \mathcal{L}_{[2]} \bar{u}'_2, \]  
\[ \mathcal{R}_2[h_2] = \mathcal{L}_{[1]} \bar{u}'_2, \]  
\[ \mathcal{R}_2[h_3] = \mathcal{L}_{[1]} \bar{u}'_3, \]  

where

\[ \mathcal{L}_{[1]} \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{\Delta \gamma}{2} \right)^n \frac{\partial^n \bar{U}_1}{\partial x_2^n} \frac{\partial^{n+1}}{\partial x_1 \partial x_2^n}. \]
\[ L_{[2]} \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{\Delta^2}{2\gamma} \right)^n \frac{\partial^{n+1} \bar{U}_1}{\partial x^{n+1}_2} \frac{\partial^n}{\partial x^n_2}. \] (39)

In the following, we examine some special cases for deriving the stability conditions for the 1D flows.

If \( N = 1 \), operators (38) and (39), respectively, reduce to

\[ L_{[1]} = \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial \bar{U}_1}{\partial x_2} \frac{\partial^2}{\partial x_1 \partial x_2}, \] (40)

\[ L_{[2]} = 0, \] (41)

and Eq. (12) then becomes

\[ \left( \nu \frac{\partial^2}{\partial x_1^2} + \nu \frac{\partial^2}{\partial x_2^2} - L_{[1]} \right) \bar{u}_i', \quad i = 1, 2, 3. \] (42)

Here the diffusion operator in the \( x_3 \) direction is neglected because it does not alter the resulting stability condition that is applicable to any wavenumber; note that the neglected operator does not stabilize the modes in the \((x_1, x_2)\) plane but that \( L_{[1]} \), being unstable, only has derivatives with respect to \( x_1 \) and \( x_2 \). Based on Eqs. (26) and (29), we have

\[ \alpha_T \simeq -\nu (k_x^2 + k_y^2) + \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial \bar{U}_1}{\partial x_2} k_x k_y. \] (43)

Substituting \((k_x, k_y) = |k| (\cos \theta, \sin \theta)\) with \( \theta \in [-\pi, \pi]\) into \( \alpha_T \leq 0 \) yields

\[ 1 \geq \max \left( \frac{\Delta^2}{4\gamma \nu} \left| \frac{\partial \bar{U}_1}{\partial x_2} \sin 2\theta \right| \right) = \frac{\Delta^2}{4\gamma \nu} \left| \frac{\partial \bar{U}_1}{\partial x_2} \right|. \] (44)

This stability condition is equivalent to that for linear shears determined in Ref. [23] by a different approach, which imposed a strong restriction on the choice of the wall-normal filter width for use in the viscous sublayer in plane channel flows.

For \( N = 2 \), \( L_{[1]} \) and \( L_{[2]} \) become

\[ L_{[1]} = \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial \bar{U}_1}{\partial x_2} \frac{\partial^2}{\partial x_1 \partial x_2} + \frac{1}{2} \left( \frac{\Delta^2}{2\gamma} \right)^2 \frac{\partial^2 \bar{U}_1}{\partial x_2^2} \frac{\partial^3}{\partial x_1 \partial x_2^2}, \] (45)

\[ L_{[2]} = \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial^2 \bar{U}_1}{\partial x_2^2} \frac{\partial}{\partial x_2}. \] (46)

As proven in Sec. III, the third-order operator in Eq. (45) can be ignored in stability analysis. Moreover, \( L_{[2]} \bar{u}_2' \) in Eq. (35) can also be neglected, because the numerical stability of \( \bar{u}_2' \) is determined independently of Eq. (35), by Eq. (36), and furthermore, if Eq. (36) is unstable, then Eq. (35) should be unstable. Therefore, the stability condition in the present example is the same as that in the previous case, Eq. (44).

For \( N = 3 \), the total amplification exponent for \( \nu (\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2) - L_{[1]} \) is

\[ \alpha_T \simeq -\nu (k_x^2 + k_y^2) + \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial \bar{U}_1}{\partial x_2} k_x k_y - \frac{1}{6} \left( \frac{\Delta^2}{2\gamma} \right)^3 \frac{\partial^3 \bar{U}_1}{\partial x_2^3} k_x k_y^3. \] (47)
Using this and \((k_x, k_y) = |\mathbf{k}|(\cos \theta, \sin \theta)\), we obtain the following stability condition:

\[
1 \geq \frac{1}{2\nu} \left( \frac{\Delta^2}{2\gamma} \right) \frac{\partial \bar{U}_1}{\partial x_2} \nu - \frac{1}{24\nu} \left( \frac{\Delta^2}{2\gamma} \right)^3 \frac{\partial^3 \bar{U}_1}{\partial x_2^3} |\mathbf{k}|^2 \nu \left( 1 \pm \sqrt{1 - s^2} \right), \tag{48}
\]

\[
s \equiv \sin 2\theta \in [-1, 1].
\]

This has to be fulfilled for any choice of \(|\mathbf{k}|\) and \(\theta\).

To show how the restriction (48) works in a realistic situation, we consider here the inertial sublayer forming in a plane channel flow. Following Dean [36], the streamwise mean velocity in the inertial sublayer is approximately described by

\[
\frac{U_1(x_2^+)}{u_\tau} = 2.44 \ln(x_2^+) + 5.17, \tag{49}
\]

where \(u_\tau\) is the wall-friction velocity and \(x_2^+ = x_2 u_\tau / \nu\) is the distance from the plane wall in wall units. For \(30 \leq x_2^+ \leq 80\), Eq. (49) can be well approximated by a cubic polynomial:

\[
\frac{U_1(x_2^+)}{u_\tau} = \sum_{n=0}^{3} a_n x_2^{+n}. \tag{50}
\]

\[
\begin{cases}
  a_0 = 10.5, & a_1 = 0.134, \\
  a_2 = -1.23 \times 10^{-3}, & a_3 = 5 \times 10^{-6}.
\end{cases}
\]

Using this and Eqs. (16) and (17), the filtered derivatives in Eq. (48) are determined as

\[
\frac{\partial \bar{U}_1}{\partial x_2} = u_\tau \frac{u_\tau}{\nu} \left[ a_1 + 2a_2 x_2^+ + 3a_3 \left( x_2^+ + \frac{\Delta_2^+}{2\gamma} \right) \right], \tag{51}
\]

\[
\frac{\partial^3 \bar{U}_1}{\partial x_2^3} = u_\tau \left( \frac{u_\tau}{\nu} \right)^3 6a_3, \tag{52}
\]

where \(\Delta_2^+ = \Delta_2 u_\tau / \nu\). Substituting them and \(\gamma = 6\) into Eq. (48) yields

\[
1 \geq \left( \frac{A_{[1]} \Delta_2^+}{24} + \frac{a_3 \Delta_2^+}{96} \right) \nu \left( \frac{u_\tau}{\nu} \right)^{-2} |\mathbf{k}|^2 s \left( 1 \pm \sqrt{1 - s^2} \right), \tag{53}
\]

where

\[
A_{[1]} = a_1 + 2a_2 x_2^+ + 3a_3 x_2^+.
\]

Assuming that \(\max(|\mathbf{k}|) \Delta_2 = \pi\), i.e., the maximum resolved wavenumber is determined by the Nyquist wavenumber based on the wall-normal filter width, Eq. (53) can be further rewritten as

\[
1 \geq \left( \frac{A_{[1]} \Delta_2^+}{24} + \frac{a_3 \Delta_2^+}{96} \right) \nu \left( \frac{u_\tau}{\nu} \right)^{-2} \left( 1 \pm \sqrt{1 - s^2} \right) \nu \left( \frac{u_\tau}{\nu} \right)^{-2} |\mathbf{k}|^2 s \left( 1 \pm \sqrt{1 - s^2} \right), \tag{54}
\]

At \(x_2^+ = 55\), for instance, this becomes

\[
1 \geq \left( 1.85 \times 10^{-3} \Delta^2 + 5.21 \times 10^{-8} \Delta^4 \right) s - 7.14 \times 10^{-9} \Delta^4 s \left( 1 \pm \sqrt{1 - s^2} \right). \tag{55}
\]

From this, for \(\Delta^+ = 10, 20, \) and \(25\), respectively, we have

\[
1 \geq 0.185 s - 7.14 \times 10^{-5} s \left( 1 \pm \sqrt{1 - s^2} \right), \tag{56}
\]
\[
1 \geq 0.748s - 0.00114s(1 \pm \sqrt{1 - s^2}),
\]
(57)

\[
1 \geq 1.18s - 0.00279s(1 \pm \sqrt{1 - s^2}).
\]
(58)

The first two are true for any \( s \in [-1, 1] \), but the last is not. (Note that \( \max_s[s(1 \pm \sqrt{1 - s^2})] = -\min_s[s(1 \pm \sqrt{1 - s^2})] = 3\sqrt{3}/4 \simeq 1.30 \). The filter width suggested here for stability is comparable to that used in actual channel flow computations.

Based on the stability analysis described in Sec. III, it is found that for larger \( N \), all of the even-order differential operators in Eq. (58) are unstable, whereas the odd-order ones have no influence on the numerical stability. That is, the high-order terms do not help stability. This result suggests that in most cases of 1D shear, the subfilter-scale stress terms would be unstable, thus leading to a divergence of numerical solution, if an unsuitably large filter width is used.

B. 2D mean velocity cases

Next, we consider 2D problems. Suppose that

\[ U_1 = U_1(x_1, x_2), \quad U_2 = U_2(x_1, x_2), \quad \text{and} \quad U_3 = 0, \]
resulting in

\[
h_1 = Du'_1 + \frac{\partial U_1}{\partial x_1} u'_1 + \frac{\partial U_1}{\partial x_2} u'_2, \quad (59)
\]

\[
h_2 = Du'_2 + \frac{\partial U_2}{\partial x_1} u'_1 + \frac{\partial U_2}{\partial x_2} u'_2, \quad (60)
\]

\[
h_3 = Du'_3, \quad (61)
\]

and

\[
\frac{\partial U_i}{\partial x_i} = \frac{\partial U_1}{\partial x_1} + \frac{\partial U_2}{\partial x_2} = 0. \quad (62)
\]

Here we introduced an advection operator,

\[
D = U_1 \frac{\partial}{\partial x_1} + U_2 \frac{\partial}{\partial x_2}.
\]

Because the mean velocity is independent of \( x_3 \), we know that

\[
\mathcal{R}_3[h_i] = 0 \quad \text{for} \quad i = 1, 2, 3, \quad (63)
\]

and consequently the resulting formulas of the residual stresses for \( \mathcal{G}_{123}^\star \) and for \( \mathcal{G}_{12}^\star \) are the same, allowing for the consideration based on 2D filtering. However, even in 2D, the complete set of the closed residual forces derived using Eq. (14) is intricate and inconvenient for theoretical analysis, and hence we only consider some simple cases.

The first example assumes that the mean velocities are described locally by

\[
U_1 = bx_1 \quad \text{and} \quad U_2 = -bx_2, \quad (64)
\]
where \( b \) is a positive constant, that is, stretches uniformly in the \( x_1 \) direction. Here, the term “locally” means “in a region sufficiently larger than the filter widths.” These assumptions reduce Eqs. (59)-(61) to

\[
 h_1 = D u'_1 + b u'_1, \\
 h_2 = D u'_2 - b u'_2, \\
 h_3 = D u'_3. 
\]

Since, in this case,

\[
 G_j \ast \left( U_k \frac{\partial u'_i}{\partial x_k} \right) = U_k \frac{\partial (G_j \ast u'_i)}{\partial x_k} \quad \text{for } j \neq k, \quad \text{no summation over } k
\]

and

\[
 R_{12}[bu'_1] = R_{12}[bu'_2] = 0
\]

are true, the residual forces are expressed as

\[
 R_{12}[h_i] = R_1 \left[ bx_1 \frac{\partial (G_2 \ast u'_i)}{\partial x_1} \right] - R_2 \left[ bx_2 \frac{\partial (G_1 \ast u'_i)}{\partial x_2} \right], \quad i = 1, 2, 3. 
\]

Using the 1D expansion series (13) or integration by parts (15), Eq. (68) is rewritten into the closed form,

\[
 R_{12}[h_i] = \frac{b \Delta^2 \partial^2 \bar{u}'_i}{2\gamma \partial x^2_1} - \frac{b \Delta^2 \partial^2 \bar{u}'_i}{2\gamma \partial x^2_2}. 
\]

This acts as negative diffusion in the \( x_1 \) direction (i.e., in the stretching direction) but as positive diffusion in the \( x_2 \) direction, a result that is consistent with Leonard’s finding shown in the studies on tensor-diffusivity models [13, 16]. The amplification exponent of the difference between the viscosity term and \( R_{12}[h_i] \) is

\[
 \alpha_T \simeq - \left( \nu - b \frac{\Delta^2}{2\gamma} \right) k^2_x - \left( \nu + b \frac{\Delta^2}{2\gamma} \right) k^2_y, 
\]

which expression leads to the stability condition

\[
 \Delta_1 \leq \frac{\sqrt{2\gamma \nu}}{\sqrt{b}}. 
\]

Equation (71) indicates that a smaller filter width is needed for stronger stretching, and the largest filter width usable in the stretching direction is inversely proportional to the square root of the velocity gradient.

The next example is complicated; not only the normal stresses but also a shear stress appear in the mean field. Suppose that \( U_1 \) is described locally by

\[
 U_1(x_1, x_2) = bx_1 x_2, 
\]

which involves both normal and shear stresses. Then one has, from the divergence-free condition,

\[
 U_2(x_2) = -\frac{b}{2} x^2_2, 
\]

13
where \( U_2(0) = 0 \) is assumed without loss of generality, and \( b \) denotes a positive constant as in the previous example; see Fig. 1I showing the vector plot of this velocity field around the origin \((x_1, x_2) = (0, 0)\). The upper side \((x_2 \geq 0)\) of this figure seems to represent a flow impinging on the wall located at \(x_2 = 0\). Substituting Eqs. (72) and (73), Eqs. (59)-(61) become

\[
\begin{align*}
  h_1 &= D u'_1 + bx_2 u'_1 + bx_1 u'_2, \\
  h_2 &= D u'_2 - bx_2 u'_2, \\
  h_3 &= D u'_3.
\end{align*}
\]

Since

\[
G_{12} \star \left( U_1 \frac{\partial u'_i}{\partial x_1} \right) = b G_{12} \star \left[ x_1 G_{22} \star \left( x_2 \frac{\partial u'_i}{\partial x_1} \right) \right],
\]

Eq. (15) (and also (13)) can be used to obtain

\[
\begin{align*}
  \mathcal{R}_{12} \left[ U_1 \frac{\partial u'_i}{\partial x_1} \right] &= \frac{\Delta_1^2}{2 \gamma} b x_2 \frac{\partial^2 \tilde{u}'_i}{\partial x_2^2} + \frac{\Delta_2^2}{2 \gamma} b x_1 \frac{\partial^2 \tilde{u}'_i}{\partial x_1 \partial x_2} + \frac{\Delta_2^2}{2 \gamma} b x_1 \frac{\partial^3 \tilde{u}'_i}{\partial x_1^3} + \frac{\Delta_1^2}{2 \gamma} b x_2 \frac{\partial^3 \tilde{u}'_i}{\partial x_2^3},
\end{align*}
\]

where we used \( G_{12} \star U_1 = U_1 \). Furthermore, using Eq. (13) yields

\[
\begin{align*}
  \mathcal{R}_{12} \left[ U_2 \frac{\partial u'_i}{\partial x_2} \right] &= \frac{\Delta_2^2}{2 \gamma} b x_2 \frac{\partial^2 \tilde{u}'_i}{\partial x_2^2} - \frac{1}{2} \left( \frac{\Delta_2^2}{2 \gamma} \right)^2 b \frac{\partial^3 \tilde{u}'_i}{\partial x_2^3},
\end{align*}
\]

where we used

\[
\frac{\partial U_2}{\partial x_2} = -bx_2 \quad \text{and} \quad \frac{\partial^2 U_2}{\partial x_2^2} = \frac{\partial^2 U_2}{\partial x_2^2} = -b.
\]

The remaining terms can also be rewritten into a closed form using Eq. (15) or (13). Finally, we obtain the closed residual stresses:

\[
\begin{align*}
  \mathcal{R}_{12}[h_1] &= \mathcal{L}_{[3]} \tilde{u}'_1 + b \frac{\Delta_2^2}{2 \gamma} \frac{\partial \tilde{u}'_1}{\partial x_2} + b \frac{\Delta_2^2}{2 \gamma} \frac{\partial \tilde{u}'_2}{\partial x_1}, \\
  \mathcal{R}_{12}[h_2] &= \mathcal{L}_{[3]} \tilde{u}'_2 - b \frac{\Delta_2^2}{2 \gamma} \frac{\partial \tilde{u}'_2}{\partial x_2}, \\
  \mathcal{R}_{12}[h_3] &= \mathcal{L}_{[3]} \tilde{u}'_3,
\end{align*}
\]

where

\[
\mathcal{L}_{[3]} \equiv bx_2 \left( \frac{\Delta_1^2}{2 \gamma} \frac{\partial^2}{\partial x_1^2} - \frac{\Delta_2^2}{2 \gamma} \frac{\partial^2}{\partial x_2^2} \right) + \frac{\Delta_2^2}{2 \gamma} b x_1 \frac{\partial^2}{\partial x_1 \partial x_2}
\]

\[
+ \frac{\Delta_2^2}{2 \gamma} b \left( \frac{\Delta_1^2}{2 \gamma} \frac{\partial^3}{\partial x_1^2 \partial x_2} - \frac{1}{2} \frac{\Delta_2^2}{2 \gamma} \frac{\partial^3}{\partial x_2^3} \right).
\]

In \( \mathcal{L}_{[3]} \) we can see various kinds of operators: negative and positive diffusions, second- and third-order cross derivatives, and third-order dispersion, among which third-order terms do
not alter the amplification exponent $\alpha_T$. Also, the last two terms of Eq. (80) and the last of Eq. (81), first-order derivatives, may not concern the numerical stability. That is, the differential operators responsible for stability are

$$
\nu \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) - bx_2 \left( \frac{\Delta_1^2}{2\gamma} \frac{\partial^2}{\partial x_1^2} - \frac{\Delta_2^2}{2\gamma} \frac{\partial^2}{\partial x_2^2} \right) - \frac{\Delta_2^2}{2\gamma} \frac{bx_1}{\partial x_1} \frac{\partial^2}{\partial x_1 \partial x_2},
$$

(84)

whose amplification exponent is

$$
\alpha_T \simeq -\nu (k_x^2 + k_y^2) + bx_2 \left( \frac{\Delta_1^2}{2\gamma} k_x^2 - \frac{\Delta_2^2}{2\gamma} k_y^2 \right) + \frac{\Delta_2^2}{2\gamma} bx_1 k_x k_y.
$$

(85)

From this, the stability condition of the present example is determined as

$$
1 \geq \frac{b}{4\gamma \nu} [(\Delta_1^2 - \Delta_2^2) x_2 + (\Delta_1^2 + \Delta_2^2) x_2 \cos 2\theta + \Delta_2^2 x_1 \sin 2\theta],
$$

(86)

which should be fulfilled for any choice of $\theta$.

Let us consider some particular cases to show how Eq. (86) works. The 2D formula can be used to discover the stability conditions for 1D filtering as well, because $\lim_{\Delta_i \to 0} (G_i * f) = f$.

For $\Delta_2 \to 0$ and $\Delta_1 \to 0$, respectively, Eq. (86) reduces to

$$
1 \geq \frac{b}{4\gamma \nu} (x_2 + x_2 \cos 2\theta) \Delta_1^2,
$$

(87)

$$
1 \geq \frac{b}{4\gamma \nu} (-x_2 + x_2 \cos 2\theta + x_1 \sin 2\theta) \Delta_2^2.
$$

(88)

On the other hand, if the condition $\Delta_1 = \Delta_2 = \Delta$ needs to be satisfied for some factor, then Eq. (86) becomes

$$
1 \geq \frac{b}{4\gamma \nu} (2x_2 \cos 2\theta + x_1 \sin 2\theta) \Delta^2.
$$

(89)

Below we briefly discuss these three cases.

For $x_1 = x_2 > 0$, Eqs. (87)-(89) reduce to

$$
1 \geq \max \left[ \frac{bx_2}{4\gamma \nu} (1 + \cos 2\theta) \Delta_1^2 \right] = \left( \frac{bx_2}{4\gamma \nu} \right)^2 2\Delta_1^2,
$$

(90)

$$
1 \geq \max \left[ \frac{bx_2}{4\gamma \nu} (-1 + \cos 2\theta + \sin 2\theta)\Delta_2^2 \right] = \left( \frac{bx_2}{4\gamma \nu} \right) (\sqrt{2} - 1) \Delta_2^2,
$$

(91)

and

$$
1 \geq \max \left[ \frac{bx_2}{4\gamma \nu} (2 \cos 2\theta + \sin 2\theta) \Delta^2 \right] = \left( \frac{bx_2}{4\gamma \nu} \right)^2 \sqrt{5} \Delta^2,
$$

(92)

and the respective influential differential operators are

$$
\nu \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) - bx_2 \frac{\Delta_1^2}{2\gamma} \frac{\partial^2}{\partial x_1^2},
$$

(93)

15
\[
\nu \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + bx_2 \frac{\Delta^2}{2\gamma} \frac{\partial^2}{\partial x_2^2} - bx_2 \frac{\Delta^2}{2\gamma} \frac{\partial^2}{\partial x_1 \partial x_2}, \tag{94}
\]

and

\[
\nu \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) - bx_2 \left( \frac{\Delta^2}{2\gamma} \frac{\partial^2}{\partial x_1^2} - \frac{\Delta^2}{2\gamma} \frac{\partial^2}{\partial x_2^2} \right) - bx_2 \frac{\Delta^2}{2\gamma} \frac{\partial^2}{\partial x_1 \partial x_2}. \tag{95}
\]

Among the stability conditions, Eq. (91) gives the weakest restriction on the filter width; the second-to-last term of Eq. (94), being a positive diffusion term resulting from compression in the \(x_2\) direction, mitigates the instability of the last term, the cross derivative resulting from the shear in the same direction. In contrast, Eq. (92) is the most restrictive condition, resulting from the coexistence of a negative-diffusion term and a cross derivative term.

For \(x_1 = x_2 < 0\), on the other hand, Eqs. (87)-(89) become

\[
1 \geq 0 \times \Delta^2_1, \tag{96}
\]

\[
1 \geq \left( \frac{-bx_2}{4\gamma\nu} \right) (1 + \sqrt{2}) \Delta^2_2, \tag{97}
\]

\[
1 \geq \left( \frac{-bx_2}{4\gamma\nu} \right) \sqrt{5} \Delta^2. \tag{98}
\]

In this case, Eqs. (97) and (98), whose respective influential derivatives have both negative-diffusion and cross-derivative terms, give restrictions of almost equal strength, while Eq. (96), involving positive-diffusion terms only, imposes no restriction. The results provided here denote that the numerical stability of the filtered system and the possible choice of filter widths depend on how the filtering operations are applied; this conclusion confirms the same assertion presented in Ref. [23].

V. DISCUSSION OF THE NEGATIVE-DIFFUSION TERM

As has been shown in the previous sections, many kinds of numerically unstable terms are derived by the Gaussian filtering operation. In this section we would like to remark on the negative-diffusion term appearing in the stretching direction to clarify why such unstable terms appear and how the terms work. The discussion also clarifies that the present suggestions are basically true even for other smooth filters.

In Ref. [13], Leonard considered the pure advection of a sinusoidal wave in a stretching velocity field where the amplitude of the (unfiltered) sinusoidal wave remains constant, and provided an interpretation of the negative diffusivity of the tensor-diffusivity model as follows: As a sinusoidal wave propagates into a stretching velocity field, its wavenumber gradually decreases, resulting in the increase of the Gaussian-filtered value of the amplitude because of the larger value of the Gaussian filter function for a lower wavenumber. The negative-diffusion term represents this amplification of the filtered value resulting from the wavenumber shift. We introduce here a different interpretation of the negative diffusivity, using Fig. 2. Let us consider the 1D pure advection of a step function,

\[
f(x, t = 0) = \begin{cases} 
1 & \text{for } x < x_0, \\
0 & \text{otherwise},
\end{cases}
\]
in a stretching velocity field $u = ax$, where $x_0 (> 0)$ is the initial position of the discontinuity in the step function and $a$ is a positive constant. The exact solution of $\partial f / \partial t + u \partial f / \partial x = 0$ under this condition is

$$f(x, t) = \begin{cases} 
1 & \text{for } x < x_0 \exp(\alpha t), \\
0 & \text{otherwise},
\end{cases}$$

which indicates that the discontinuous step will change its position without changing its height and profile; that is, the wavenumber shift does not occur in the unfiltered true solution of the present example. Applying the Gaussian filter to this solution smoothes out the discontinuity to yield a mollified step whose characteristic width is about $2\Delta$, where $\Delta$ is the characteristic length of the applied Gaussian filter. Obviously the characteristic width of the mollified step is time-independent if $\Delta$ is constant. If, however, the pure advection equation in terms of the filtered value, $\partial \bar{f} / \partial t + u \partial \bar{f} / \partial x = 0$, is used to advance the filtered profile (corresponding to the case where the residual stress term is clipped), the width of the mollified step, unlike that in the true solution, increases gradually as time goes by due to the stretching velocity field where a downstream fluid particle moves faster than an upstream particle. To counteract this artificial expansion of the mollified step, a modification by negative, not positive, diffusion is necessary, which sharpens $\bar{f}$. In the case of a compression velocity field, a similar but opposite treatment, i.e., the addition of a positive diffusion term, is needed because an artificial compression of the mollified step arises if only the pure advection equation is assumed.

The present physical picture may allow us to conclude that the subfilter-scale terms should have an analogous negative diffusivity also for any other filter functions that smooth the profile of dependent variables. In the above discussion, there is no reason that the filter shape must be Gaussian. The artificial expansion of the step discussed above must occur whenever the step is smoothed out by a smooth filter but the pure advection equation is solved. The above discussion also suggests that a numerically unstable term can appear by filtering even if the true solution (both filtered and unfiltered) is physically bounded.

VI. TOWARDS A FURTHER GENERALIZATION

The present theory has several limitations in its applicability resulting from the assumptions and simplifications made. In this section we remark on some significant issues that must be resolved for further generalization.

To construct a more general theory for the numerical stability of the GFNS equations in statistically steady states, one has to elucidate the numerical stability of, not only Eq. (28), but also

$$\frac{\partial f_i}{\partial t} = \mathcal{L}_{[ij]} f_j \quad \text{for } i = 1, 2, 3,$$

where $\mathcal{L}_{[ij]}$ ($i, j = 1, 2, 3$) are infinite sums of differential operators with position-dependent coefficients, determined by the expansion series, and in general

$$\mathcal{L}_{[ab]} \mathcal{L}_{[cd]} \neq \mathcal{L}_{[cd]} \mathcal{L}_{[ab]} \quad \text{for } (a, b) \neq (c, d);$$

that is, these operators do not commute with each other. Equation (99) represents a complicated coupling between the equations of different velocity components. In the present study, having assumed 1D or 2D mean velocity fields, some of the mean-fluctuation terms were uncoupled as Eqs. (31), (32), (61), and (76), and hence the determined stability conditions are accurate only for the corresponding uncoupled portions. In fully 3D cases where
high-order velocity fields must be assumed, however, we may well have to treat the fully coupled system (99).

The strongest assumption among those made in this paper may be the omission of the nonlinear fluctuation term $R_{123}[u'_i \partial u'_j/\partial x_i]$ in Eq. (11). We could not take into consideration the effects of this term since the theoretical investigation of it is quite difficult to perform accurately, and the present theory is thus only valid when the fluctuation is small. Terms of this type, as is well known, have a dissipative character in many turbulent flows, and hence when the dissipation of the omitted term is strong enough, the instability of the mean-fluctuation terms can be eliminated completely. One possible way to gain detailed knowledge of the nonlinear term is an \textit{a priori} test using DNS, which enables us to determine the values of all terms in the GFNS equations. Observing and examining the numerically determined terms should allow us to obtain a more accurate prediction of the numerical instability. When, for example, the absolute value of the nonlinear term (plus the molecular viscosity) is smaller than that of the sum of the unstable terms, the instability can not be eliminated irrespective of the specific characteristic of the nonlinear term. Also, comparing the amounts of the energy dissipations due to the unstable terms and the nonlinear terms should provide a useful insight. This issue will be addressed in a future paper.

Lastly, we make a brief comment on cases with a nonuniform filter width. Consider again pure advection of a step function being smoothed by a smooth filter. When the filter width is spatially nonuniform, in the advection process the width of the mollified step varies according to its position even for a constant velocity, and hence a negative diffusion must take place at least in the period where the width decreases. Such an effect of nonuniform filtering must be discussed carefully in the near future.

VII. CONCLUSION

We have presented a generalized theory for the numerical instability of the Gaussian-filtered Navier-Stokes equations. The theory allows for high-order mean velocity fields and high-order derivatives resulting from the Gaussian filtering operation. Also, we have described stability conditions regarding the choice of the filter widths in several situations, the violation of which should lead to unconditional numerical instability of the filtered system even when a completely accurate subfilter-scale model exists and is used. It is worth noting again that the closed formulas of the filtered mean-fluctuation terms determined under statistically steady-state conditions involve various kinds of unstable derivatives that, because their coefficients are time-independent, always exhibit numerical instability in a fixed range of directions. As has been proven by a simple example, the essential part of the present results can be true even if a non-Gaussian smooth filter is assumed.

We stress that if one skirts this numerical instability problem, the accuracy of the LES results will plateau. It is hard to imagine that ideally accurate solutions can be achieved by incorporating an artificial damping or clipping technique to avoid this numerical difficulty, because when the subfilter-scale terms act unstably, the absolute values of their unstable portions must be greater than that of the molecular and turbulent viscosities, and the adoption of such artificial techniques thus corresponds to the disregard of a term whose dominance is greater than that of a term involved \textit{ab initio} in the Navier-Stokes equations. Recently, Moeleker and Leonard [16] have tackled this numerical instability problem and proposed an approach to potentially resolve it, based on an anisotropic particle method incorporating a remeshing technique. Their method has provided excellent results for a
A 2D scalar advection-diffusion equation with a known velocity field. However, the extension of that approach to the 3D Navier-Stokes equations has to the author’s knowledge not yet been achieved. Because finite difference schemes have been used widely in turbulence computations, constructing a stable and accurate solver in the finite difference framework would be preferable, though it will be an exceedingly difficult task and might even be an unsolvable problem, such as the gravitational three-body problem and the algebraic solution of general fifth-order polynomial equations of one variable. We do not know so far whether this instability problem is resolvable or not, but we can say that this problem is not something that can be avoided when an accurate solution is desired.

Acknowledgments

One of the authors (M.I.) thanks F. Hamba for helpful and valuable discussions. Thanks are extended to A. Yoshizawa and Y. Morinshii for encouragement and comments. This work was supported by the Ministry of Education, Culture, Sports, Science, and Technology of Japan through the Grant-in-Aid for Young Scientists (B) (No. 17760151) and also under an IT research program “Frontier Simulation Software for Industrial Science.”

APPENDIX: ALTERNATIVE DERIVATION OF THE EXACT EXPANSION SERIES FOR GAUSSIAN FILTERS

The exact expansion series for Gaussian filters has served as a powerful tool in our study. We present here a derivation of the series to improve the self-consistency of the present paper. This derivation seems to be rather intricate and drawn out compared to those by Moeleker and Leonard [16] and by Carati et al. [15], but it only consists of elementary mathematics: the Taylor expansion, integration by parts, and some simple algebraic operations. Some readers may prefer the present derivation.

Let \( a(x) \), \( b(x) \), \( f(x) \), and \( g(x) \) be arbitrary, differentiable and continuous functions of \( x \). For the Gaussian filter with \( \gamma = 1/2 \) and the characteristic width of \( \Delta \), the exact expansion series in 1D reads

\[
(ab) = \sum_{n=0}^{\infty} \frac{\Delta^{2n}}{n!} \frac{\partial^n a}{\partial x^n} \frac{\partial^n b}{\partial x^n}. \tag{A.1}
\]

In what follows, we derive the right-hand side of this equation from the left-hand side.

Taylor expanding \( a \) with respect to \( x \) results in

\[
a = \sum_{m=0}^{\infty} A_m x^m \quad \text{with} \quad A_m = \frac{1}{m!} \left. \frac{\partial^m a}{\partial x^m} \right|_{x=0}. \tag{A.2}
\]

Substituting this into \((ab)\) yields

\[
(ab) = \left( \sum_{m=0}^{\infty} A_m x^m b \right) = \sum_{m=0}^{\infty} A_m (x^m b). \tag{A.3}
\]

Successively using

\[
(xf) = \mathcal{L} \bar{f} \quad \text{with} \quad \mathcal{L} = x + \Delta^2 \frac{\partial}{\partial x}. \tag{A.4}
\]
which corresponds to Eq. (15) derived using integration by parts, we obtain the identity

$$\frac{\partial}{\partial x} (x^m f) = \mathcal{L}^m f.$$  

(A.5)

This rewrites Eq. (A.3) as

$$\langle ab \rangle = \sum_{m=0}^{\infty} [A_m(\mathcal{L}^m \bar{b})].$$

(A.6)

The component $\mathcal{L}^m \bar{b}$ in Eq. (A.6) can further be rewritten as follows: Operating $\mathcal{L}$ once on $\bar{b}$ yields

$$\mathcal{L} \bar{b} = x \bar{b} + \Delta^2 \frac{\partial}{\partial x} \bar{b}$$

$$= (\mathcal{L}^1 \cdot 1) \left( \Delta^2 \frac{\partial}{\partial x} \right)^0 \bar{b} + (\mathcal{L}^0 \cdot 1) \left( \Delta^2 \frac{\partial}{\partial x} \right)^1 \bar{b},$$  

(A.7)

where

$$\mathcal{L}^1 \cdot 1 \equiv \left( x + \Delta^2 \frac{\partial}{\partial x} \right) 1 = x \quad \text{and} \quad \mathcal{L}^0 \cdot 1 = 1.$$  

(A.8)

We introduce here

$$B_{N,M} \equiv (\mathcal{L}^N \cdot 1) \left( \Delta^2 \frac{\partial}{\partial x} \right)^M \bar{b}.$$  

(A.9)

Based on Eq. (A.7), definition (A.9), and

$$\mathcal{L}(gf) = (\mathcal{L}g)f + g \left( \Delta^2 \frac{\partial}{\partial x} \right)f,$$

the following identities are derived:

$$\mathcal{L} \bar{b} = \mathcal{L}B_{0,0}$$

$$= B_{1,0} + B_{0,1},$$

(A.10)

$$\mathcal{L}B_{N,M} = (\mathcal{L}^{N+1} \cdot 1) \left( \Delta^2 \frac{\partial}{\partial x} \right)^M \bar{b} + (\mathcal{L}^N \cdot 1) \left( \Delta^2 \frac{\partial}{\partial x} \right)^{M+1} \bar{b}$$

$$= B_{N+1,M} + B_{N,M+1},$$

(A.11)

which allow us to obtain

$$\mathcal{L}^2 \bar{b} = \mathcal{L}^2 B_{0,0} = \mathcal{L}B_{1,0} + \mathcal{L}B_{0,1}$$

$$= B_{2,0} + 2B_{1,1} + B_{0,2},$$

$$\mathcal{L}^3 \bar{b} = \mathcal{L}^3 B_{0,0} = \mathcal{L}B_{2,0} + 2\mathcal{L}B_{1,1} + \mathcal{L}B_{0,2}$$

$$= B_{3,0} + 3B_{2,1} + 3B_{1,2} + B_{0,3},$$

$$\ldots$$

$$\mathcal{L}^m \bar{b} = \sum_{n=0}^{m} s_{m-n,n} B_{m-n,n}.$$
Here, the coefficients $s_{m-n,n}$ ($m = 0, 1, 2 \ldots$ and $n = 0, 1, \ldots, m$) form a so-called Pascal’s triangle, and thus

$$s_{m-n,n} = \frac{m!}{n!(m-n)!}. \quad (A.13)$$

From Eqs. (A.9), (A.12), and (A.13), we have

$$\mathcal{L}^m \tilde{b} = \sum_{n=0}^{m} \frac{\Delta^2 n \cdot m! \cdot (\mathcal{L}^{m-n} \cdot 1) \partial^n \tilde{b}}{n! \cdot (m-n)! \cdot \partial x^n}. \quad (A.14)$$

Substituting Eq. (A.14) into Eq. (A.6) yields

$$\overline{ab} = \sum_{m=0}^{\infty} \left[ A_m \sum_{n=0}^{m} \frac{\Delta^2 n \cdot m! \cdot (\mathcal{L}^{m-n} \cdot 1) \partial^n \tilde{b}}{n! \cdot (m-n)! \cdot \partial x^n} \right]. \quad (A.15)$$

Using Eq. (A.5), $(\mathcal{L}^{m-n} \cdot 1)$ in this equation can easily be rewritten into $(x^{m-n})$, which can further be rewritten as

$$\overline{(x^{m-n})} = \frac{(m-n)!}{m!} \left( \frac{\partial^n x^m}{\partial x^n} \right). \quad (A.16)$$

Substituting this into Eq. (A.15) yields

$$\overline{ab} = \sum_{m=0}^{\infty} \left[ A_m \sum_{n=0}^{m} \frac{\Delta^2 n \cdot \overline{(x^{m-n})} \partial^n \tilde{b}}{n! \cdot \partial x^n} \right]. \quad (A.17)$$

Moreover, because

$$\frac{\partial^n x^m}{\partial x^n} = 0 \quad \text{for } n > m, \quad (A.18)$$

the summation over $n = 1, 2, \ldots, m$ in Eq. (A.17) can be extended to that over $n = 1, 2, \ldots, \infty$ to obtain

$$\overline{ab} = \sum_{m=0}^{\infty} \left[ \sum_{n=0}^{\infty} \frac{\Delta^2 n \cdot A_m \overline{(x^{m-n})} \partial^n \tilde{b}}{n! \cdot \partial x^n} \right]. \quad (A.19)$$

Based on the commutativity between differentiations and filtering, after some mathematical operations we finally obtain Eq. (A.1).
[1] C. Meneveau and J. Katz, Annu. Rev. Fluid Mech. 32, 1 (2000).
[2] P. Sagaut, Large Eddy Simulation for Incompressible Flows, 2nd edition (Springer-Verlag, Berlin, New York, Heidelberg, 2002).
[3] C. Kato, M. Kaiho, and A. Manabe, J. Appl. Mech. Trans. ASME 70, 32 (2003).
[4] C. Stone and S. Menon, J. Supercomput. 22, 7 (2002).
[5] Y. Huang, H.-G. Sung, S.-Y. Hsieh, and V. Yang, J. Propul. Power 19, 782 (2003).
[6] P. J. Mason, J. Atmos. Sci. 46, 1492 (1989).
[7] C. H. Moeng and P. P. Sullivan, J. Atmos. Sci. 51, 999 (1994).
[8] T. Dürbeck and T. Gerz, Geophys. Res. Lett. 22, 3203 (1995).
[9] D. W. Denbo and E. D. Skyllingstad, J. Geophys. Res. 101, 1095 (1996).
[10] N. Cantin, A. P. Vincent, and D. A. Yuen, Geophys. J. Int. 140, 163 (2000).
[11] X. Xie and J. Toomre, Astrophys. J. 405, 747 (1993).
[12] V. M. Canuto, Astrophys. J. 428, 729 (1994).
[13] A. Leonard, AIAA Pap. No. 97-0204 (1997).
[14] W. Yeo, A generalized high pass/low pass filtering procedure for deriving and solving turbulent flow equations, Ph.D. thesis, Ohio State University, 1987 (unpublished).
[15] D. Carati, G. S. Winckelmanns, and H. Jeanmart, J. Fluid Mech. 441, 119 (2001).
[16] P. Moeleker and A. Leonard, J. Comput. Phys. 167, 1 (2001).
[17] G. S. Winckelmanns, A. A. Wray, O. V. Vasilyev, and H. Jeanmart, Phys. Fluids 13, 1385 (2001).
[18] H. Kobayashi and Y. Shimomura, Phys. Fluids 15, L29 (2003).
[19] A. W. Vreman, Phys. Fluids 16, 490 (2004).
[20] H. Kobayashi and Y. Shimomura, Phys. Fluids 16, 492 (2004).
[21] T. Iliescu, V. John, W. J. Layton, G. Matthies, and L. Tobiska, Int. J. Comput. Fluid Dyn. 17, 75 (2003).
[22] M. Ida and N. Taniguchi, Phys. Rev. E 68, 036705 (2003).
[23] M. Ida and N. Taniguchi, Phys. Rev. E 69, 046701 (2004).
[24] A. J. Klimas, J. Comput. Phys. 68, 202 (1987).
[25] A. J. Klimas and W. M. Farrell, J. Comput. Phys. 110, 150 (1994).
[26] H. Figua, F. Bouchut, M. R. Feix, and E. Fijalkow, J. Comput. Phys. 159, 440 (2000).
[27] S. Ghosal and P. Moin, J. Comput. Phys. 118, 24 (1995).
[28] H. van der Ven, Phys. Fluids 7, 1171 (1995).
[29] O. V. Vasilyev, T. S. Lund, and P. Moin, J. Comput. Phys. 146, 82 (1998).
[30] A. L. Marsden, O. V. Vasilyev, and P. Moin, J. Comput. Phys. 175, 584 (2002).
[31] J. Gullbrand, Annual Research Briefs, Center for Turbulence Research, 167 (2002).
[32] Y. Shimomura, J. Phys. Soc. Jpn. 68, 2483 (1999).
[33] K. Djidjeli, W. G. Price, E. H. Twizell, and Y. Wang, J. Comput. Appl. Math 58, 307 (1995).
[34] B.-F. Feng and T. Mitsui, J. Comput. Appl. Math 90, 95 (1998).
[35] M. S. Ismail and T. R. Taha, Math. Comput. Simul. 47, 519 (1998).
[36] R. B. Dean, Trans. ASME, J. Fluids Eng. 100, 215 (1978).
FIG. 1: Vector plot of the flow field described by Eqs. (72) and (73) in arbitrary units; note that this flow field is self-similar with respect to constant multiplication of the coordinates, \((x_1, x_2) \rightarrow (cx_1, cx_2)\), where \(c\) is a real constant. The center point of the coordinate system shows the origin \((x_1, x_2) = (0, 0)\).
FIG. 2: Physical meaning of the negative diffusivity in the pure advection of a discontinuous step function in a stretching field. The solid lines in the upper figure denote $f(t = 0)$ and $f(t = t_1 > 0)$, and the dashed curves denote $\bar{f}(t = 0)$ and $\bar{f}(t = t_1 > 0)$. If $\bar{f}$ is advanced using a pure advection equation, its characteristic width gradually expands, as shown by the dots. A negative diffusion term must appear in the filtered advection equation to counteract this artificial expansion.