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Building proper invariants for eddy-viscosity subgrid-scale models

F. X. Trias,^{1,a)} D. Folch,^{1,b)} A. Gorobets,^{1,2,c)} and A. Oliva^{1,d)}

¹Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/Colom 11, 08222 Terrassa, Spain

²Keldysh Institute of Applied Mathematics, Miusskaya Sq. 4A, Moscow 125047, Russia

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Direct simulations of the incompressible Navier-Stokes equations are limited to relatively low-Reynolds numbers. Hence, dynamically less complex mathematical formulations are necessary for coarse-grain simulations. Eddy-viscosity models for large-eddy simulation is probably the most popular example thereof: they rely on differential operators that should properly detect different flow configurations (laminar and 2D flows, near-wall behavior, transitional regime, etc.). Most of them are based on the combination of invariants of a symmetric tensor that depends on the gradient of the resolved velocity field, $\mathbf{G} = \nabla \bar{\mathbf{u}}$. In this work, models are presented within a framework consisting of a 5D phase space of invariants. In this way, new models can be constructed by imposing appropriate restrictions in this space. For instance, considering the three invariants P_{GGT} , Q_{GGT} , and R_{GGT} of the tensor $\mathbf{GG}^T$, and imposing the proper cubic near-wall behavior, i.e., $\nu_e = O(y^3)$, we deduce that the eddy-viscosity is given by $\nu_e = (C_{s3pqr}\Delta)^2 P_{GGT}^p Q_{GGT}^{-(p+1)} R_{GGT}^{(p+5/2)/3}$. Moreover, only R_{GGT} -dependent models, i.e., $p > -5/2$, switch off for 2D flows. Finally, the model constant may be related with the Vreman's model constant via $C_{s3pqr} = \sqrt{3}C_{Vr} \approx 0.458$; this guarantees both numerical stability and that the models have less or equal dissipation than Vreman's model, i.e., $0 \leq \nu_e \leq \nu_e^{Vr}$. The performance of the proposed models is successfully tested for decaying isotropic turbulence and a turbulent channel flow. The former test-case has revealed that the model constant, C_{s3pqr} , should be higher than 0.458 to obtain the right amount of subgrid-scale dissipation, i.e., $C_{s3pq} = 0.572$ ($p = -5/2$), $C_{s3pr} = 0.709$ ($p = -1$), and $C_{s3qr} = 0.762$ ($p = 0$). © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4921817>]

I. INTRODUCTION

We consider the numerical simulation of the incompressible Navier-Stokes (NS) equations. In primitive variables, they read as

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla^2 \mathbf{u} - \nabla p, \quad \nabla \cdot \mathbf{u} = 0, \quad (1)$$

where $\mathbf{u}$ denotes the velocity field, p represents the kinematic pressure, and ν is the kinematic viscosity. Direct simulations at high Reynolds numbers are not feasible because the convective term produces far too many scales of motion. Hence, in the foreseeable future, numerical simulations of turbulent flows will have to resort to models of the small scales. The most popular example thereof is the Large-Eddy Simulation (LES). Shortly, LES equations result from applying a spatial filter, with filter length Δ , to NS equations (1)

a) xavi@cttc.upc.edu

b) davidf@cttc.upc.edu

c) andrey@cttc.upc.edu

d) oliva@cttc.upc.edu

$$\partial_t \bar{\mathbf{u}} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = \nu \nabla^2 \bar{\mathbf{u}} - \nabla \bar{p} - \nabla \cdot \tau(\bar{\mathbf{u}}); \quad \nabla \cdot \bar{\mathbf{u}} = 0, \quad (2)$$

where $\bar{\mathbf{u}}$ is the filtered velocity and $\tau(\bar{\mathbf{u}})$ is the subgrid stress (SGS) tensor that approximates the effect of the under-resolved scales, i.e., $\tau(\bar{\mathbf{u}}) \approx \bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}$. It is assumed that the filter $\mathbf{u} \rightarrow \bar{\mathbf{u}}$ commutes with differentiation. Then, the closure problem consists of replacing (approximating) the tensor $\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}$ with a tensor depending only on $\bar{\mathbf{u}}$ (and not $\mathbf{u}$). Because of its inherent simplicity and robustness, the eddy-viscosity assumption is by far the most used closure model

$$\tau(\bar{\mathbf{u}}) \approx -2\nu_e \mathbf{S}(\bar{\mathbf{u}}), \quad (3)$$

where ν_e denotes the eddy-viscosity and $\mathbf{S}(\bar{\mathbf{u}}) = 1/2(\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T)$ is the rate-of-strain tensor. Notice that $\tau(\bar{\mathbf{u}})$ is considered traceless without the loss of generality, because the trace can be included as part of the filtered pressure, $\bar{p}$. Following the same notation as in Nicoud *et al.*,¹ the eddy-viscosity can be modeled in a natural way as follows:

$$\nu_e = (C_m \Delta)^2 D_m(\bar{\mathbf{u}}), \quad (4)$$

where C_m is the model constant, Δ is the subgrid characteristic length, and $D_m(\bar{\mathbf{u}})$ is the differential operator with units of frequency associated with the model. Most of the existing eddy-viscosity models can be represented by this formulation.¹ Hereafter, in this work, we consider that C_m in Eq. (4) is really a constant. Instead, one can also take $C_m = C_m(\bar{\mathbf{u}})$ following the dynamical procedure proposed by Germano *et al.*² where the coefficient C_m is computed with the help of the Jacobi identity (in least-square sense) as proposed by Lilly.³ However, it is well-known that this procedure leads to highly variable coefficient field with a significant fraction of negative values for ν_e . This can cause numerical instability in simulations. Thus, averaging with respect to homogeneous direction(s) and *ad hoc* clipping for ν_e are, in general, necessary. Therefore, the original dynamic procedure cannot be applied to geometrically complex flows without homogeneous directions. The dynamic localization model and the Lagrangian dynamic model, respectively, proposed by Ghosal *et al.*⁴ and Meneveau *et al.*⁵ were attempts to overcome these limitations. However, these two models require a significantly higher computational cost. More recently, Park *et al.*⁶ introduced two global dynamic approaches: a dynamic global model based on the Germano identity and a dynamic global model with two test filters based on the global equilibrium between the viscous dissipation and the SGS dissipation. Instead of using two test filters, You and Moin⁷ presented a dynamic global approach using only one test filter. However, Lee *et al.*⁸ showed that the assumption of the global equilibrium is not valid for freely decaying isotropic turbulence. Examples of very recent applications of these global dynamic approaches can be found in the literature.^{9,10} Since a global constant is found, global dynamic approaches need to rely on differential operators, $D_m(\bar{\mathbf{u}})$, that automatically vanish in near-wall regions. Hence, the models proposed in this paper are good potential candidates to be used within the framework of a global dynamic model. Although not considered here either, the proposed models could be also combined with the variational multi-scale methodology proposed by Hughes *et al.*¹¹ In this case, only the smallest resolved scales are directly affected by the SGS tensor. This approach also requires the construction of an explicit linear filter in order to separate the scales.

The rest of the paper is organized as follows. A framework where all the model differential operators, $D_m(\bar{\mathbf{u}})$, are represented as a combination of elements of a 5D phase space of invariants is proposed. The basic theory together with some useful relations between invariants is presented in Sec. II. Then, a list of well-known eddy-viscosity models for LES is represented within this framework in Sec. III. In this way, new models can be constructed by imposing appropriate restrictions in that space. This is addressed in Sec. IV with special emphasis to the near-wall behavior. The analysis leads to a family of eddy-viscosity models whose differential operators, $D_m(\bar{\mathbf{u}})$, have the proper cubic near-wall behavior, i.e., $\nu_e = O(y^3)$. However, the model constant, C_m , still needs to be determined somehow. This problem is addressed in Sec. V from both theoretical and numerical point-of-views. In Sec. VI, the performance of the proposed models is numerically evaluated for decaying isotropic turbulence and a turbulent channel flow. Finally, relevant results are summarized and conclusions are given.

II. THEORY

The essence of turbulence is the smallest scales of motion. They result from a subtle balance between convective transport and diffusive dissipation. Numerically, if the grid is not fine enough, this balance needs to be restored by a turbulence model. The success of a turbulence model depends on the ability to capture well this (im)balance. In this regard, many eddy-viscosity models for LES have been proposed in the last decades.^{12,13} In order to be frame invariant, most of them rely on differential operators that are based on the combination of invariants of a symmetric second-order tensor (with the proper scaling factors). To make them locally dependent, such tensors are derived from the gradient of the resolved velocity field, $\mathbf{G} \equiv \nabla \mathbf{u}$. This is a second-order traceless tensor, $\text{tr}(\mathbf{G}) = \nabla \cdot \mathbf{u} = 0$. Therefore, in 3D, this 3×3 tensor contains 8 independent elements and it can be characterized by 5 invariants (3 scalars are required to specify the orientation in 3D). Following the same criterion that in Refs. 14 and 15, this set of five invariants can be defined as follows:

$$\{Q_G, R_G, Q_S, R_S, V^2\}, \quad (5)$$

where $Q_A = 1/2\{\text{tr}^2(\mathbf{A}) - \text{tr}(\mathbf{A}^2)\}$ and $R_A = \det(\mathbf{A}) = 1/6\{\text{tr}^3(\mathbf{A}) - 3\text{tr}(\mathbf{A})\text{tr}(\mathbf{A}^2) + 2\text{tr}(\mathbf{A}^3)\}$ represent the second and third invariant of the second-order tensor $\mathbf{A}$, respectively. Moreover, the first invariant of $\mathbf{A}$ will be denoted as $P_A = \text{tr}(\mathbf{A})$. Notice that if $\mathbf{A}$ is traceless, $\text{tr}(\mathbf{A}) = 0$, these formulae reduce to $P_A = 0$, $Q_A = -1/2\text{tr}(\mathbf{A}^2)$, and $R_A = \det(\mathbf{A}) = 1/3\text{tr}(\mathbf{A}^3)$, respectively. Finally, $V^2 = 4(\text{tr}(\mathbf{S}^2\Omega^2) - 2Q_S Q_\Omega)$, where $\mathbf{S} = 1/2(\mathbf{G} + \mathbf{G}^T)$ and $\Omega = 1/2(\mathbf{G} - \mathbf{G}^T)$ are the symmetric and the skew-symmetric parts of the gradient tensor, $\mathbf{G}$, respectively. Notice that all these tensors are also traceless, $\text{tr}(\mathbf{S}) = \text{tr}(\Omega) = \text{tr}(\mathbf{G}) = 0$. The following relations between their principal invariants can be easily obtained:

$$P_G = P_S = P_\Omega = 0, \quad (6)$$

$$Q_G = Q_S + Q_\Omega, \quad (7)$$

$$R_G = R_S + \text{tr}(\Omega^2\mathbf{S}), \quad R_\Omega = 0. \quad (8)$$

Since the pioneering works in the early 1990s,^{14,16,17} these invariants have been studied from both theoretical and experimental/numerical point-of-views. For the so-called “restricted Euler equations” (where the pressure and viscous terms are neglected), exact transport equations for the invariants can be found.¹⁵ Namely,

$$\frac{dQ_G}{dt} = -3R_G; \quad \frac{dR_G}{dt} = \frac{2}{3}Q_G^2; \quad (9)$$

$$\frac{dQ_S}{dt} = -2R_S - R_G; \quad \frac{dR_S}{dt} = \frac{2}{3}Q_G Q_S + \frac{1}{4}V^2; \quad \frac{dV^2}{dt} = -\frac{16}{3}(R_S - R_G)Q_G, \quad (10)$$

where $d/dt = \partial/\partial t + (\mathbf{u} \cdot \nabla)$ is the Lagrangian derivative. This defines a complete dynamical system in the 5D phase space defined in (5). Despite the above-mentioned simplifications some important features observed in isotropic turbulence can be reproduced by this system. Namely, the preferential alignment of the vorticity vector, $\boldsymbol{\omega} = \nabla \times \mathbf{u}$, with the eigenvector corresponding to the intermediate eigenvalue of $\mathbf{S}$ and the tendency of this tensor to have one negative and two positive eigenvalues. On the other hand, numerical^{18,19} and experimental²⁰ studies for different configurations have revealed the “universal” teardrop shape of the joint probability density function of R_G and Q_G .

The identification of coherent structures is another example where the invariants play an important role.^{21–24} For instance, the invariant $Q_\Omega = 1/2(\Omega : \Omega) = 1/4|\boldsymbol{\omega}|^2$ is proportional to the enstrophy density; therefore, it identifies tube-like structures with high vorticity. The invariant $Q_S = -1/2(\mathbf{S} : \mathbf{S})$ is proportional to the local rate of viscous dissipation, $\varepsilon = 2\nu \mathbf{S} : \mathbf{S}$. Notice that $Q_\Omega \geq 0$ whereas $Q_S \leq 0$ and these two invariants are related to the invariant Q_G with identity (7); hence, positive values of the invariant $Q_G > 0$ are related to areas where enstrophy dominates whereas $Q_G < 0$ implies that the viscous dissipation dominates. The former correspond to vortex-like structures and justifies the widely adopted Q_G -criterion for flow visualization of turbulence. Finally, the invariant V^2 is equal to the L^2 -norm of the vortex-stretching vector, i.e., $V^2 = 4(\text{tr}(\mathbf{S}^2\Omega^2) - 2Q_S Q_\Omega) = 2((\mathbf{S} : \mathbf{S})(\Omega : \Omega) - 2\mathbf{S}\Omega : \mathbf{S}\Omega) = |\mathbf{S}\boldsymbol{\omega}|^2 \geq 0$. It is remarkable the role that these invariants play in other areas of research such as the visualization

of tensor fields,²⁵ in particular, in the analysis of diffusion tensor magnetic resonance images (see, for instance, Ennis and Kindlmann²⁶).

Starting from the classical Smagorinsky model,²⁷ most of the eddy-viscosity models for LES are based on invariants of second-order tensors that are derived from the gradient tensor, $\mathbf{G}$. Therefore, it seems natural to re-write them in terms of the 5D phase space defined in (5). This is addressed in Sec. III. However, for convenience, some other important invariants (or relations) in the context of eddy-viscosity models for LES are defined before. Namely,

$$\text{tr}(\mathbf{G}\mathbf{G}^T) = \text{tr}(\mathbf{S}^2) - \text{tr}(\mathbf{\Omega}^2) = 2(Q_\Omega - Q_S), \quad (11)$$

$$\text{tr}(\mathbf{S}^2\mathbf{\Omega}^2) = 1/8(\text{tr}(\mathbf{G}^4) - \text{tr}(\mathbf{G}\mathbf{G}^T\mathbf{G}\mathbf{G}^T)) = 1/8(2Q_G^2 - \text{tr}(\mathbf{G}\mathbf{G}^T\mathbf{G}\mathbf{G}^T)), \quad (12)$$

$$\text{tr}(\mathbf{S}^2\mathbf{\Omega}^2) = V^2/4 + 2Q_SQ_\Omega, \quad (13)$$

$$\text{tr}(\tilde{\mathbf{A}}^2) = \text{tr}(\mathbf{A}^2) - 1/3\text{tr}^2(\mathbf{A}), \quad (14)$$

where $\tilde{\mathbf{A}} = \mathbf{A} - 1/3\text{tr}(\mathbf{A})\mathbf{I}$ denotes the traceless part of tensor $\mathbf{A}$. In this context, it is also useful to define the three eigenvalues, $\lambda_1 \geq \lambda_2 \geq \lambda_3$ of $\mathbf{A}$. They are solutions of the characteristic equation

$$\det(\lambda\mathbf{I} - \mathbf{A}) = \lambda^3 - P_A\lambda^2 + Q_A\lambda - R_A = 0, \quad (15)$$

where

$$P_A = \lambda_1 + \lambda_2 + \lambda_3; \quad Q_A = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3; \quad R_A = \lambda_1\lambda_2\lambda_3, \quad (16)$$

whereas for traceless tensors, it simplifies to

$$P_{\tilde{\mathbf{A}}} = 0; \quad Q_{\tilde{\mathbf{A}}} = -1/2(\lambda_1\lambda_1 + \lambda_2\lambda_2 + \lambda_3\lambda_3); \quad R_{\tilde{\mathbf{A}}} = \lambda_1\lambda_2\lambda_3. \quad (17)$$

III. A UNIFIED FRAMEWORK FOR EDDY-VISCOSITY MODELS

In Subsections III A–III E, different eddy-viscosity models for LES are re-written in terms of the list of five invariants given in (5). For the sake of clarity, sometimes the invariant Q_Ω is also used. Notice that it can always be written in terms of Q_S , Q_G via identity (7). Starting from the classical Smagorinsky model, they are presented in chronological order.

A. Smagorinsky model

The Smagorinsky model²⁷ can be written in terms of the above-defined invariants as follows:

$$\nu_e^{Mag} = (C_S\Delta)^2|\mathbf{S}(\bar{\mathbf{u}})| = 2(C_S\Delta)^2(-Q_S)^{1/2}, \quad (18)$$

where C_S is the Smagorinsky constant, Δ is the filter length (related with the local grid size), and $|\mathbf{S}| = (2\mathbf{S} : \mathbf{S})^{1/2}$. Notice that the Frobenius norm of $\mathbf{S}$ is $\mathbf{S} : \mathbf{S} = \text{tr}(\mathbf{S}^2) = -2Q_S$.

B. WALE model

The wall-adapting local eddy (WALE) viscosity model was proposed by Nicoud and Ducros.²⁸ Following the same notation as in the original paper, it is based on the second invariant of the traceless part of the symmetric tensor $\mathbf{S}_d = 1/2(\mathbf{G}^2 + (\mathbf{G}^2)^T) = \mathbf{S}^2 + \mathbf{\Omega}^2$,

$$Q_{\tilde{\mathbf{S}}_d} = -1/2\text{tr}(\tilde{\mathbf{S}}_d^2). \quad (19)$$

Then, using identity (14), we can write $\text{tr}(\tilde{\mathbf{S}}_d^2)$ in terms of $\text{tr}(\mathbf{S}_d^2)$ and $\text{tr}(\mathbf{S}_d)$. Recalling that $\mathbf{S}_d = \mathbf{S}^2 + \mathbf{\Omega}^2$ and applying the Cayley-Hamilton theorem, we obtain

$$\text{tr}(\mathbf{S}_d) = \text{tr}(\mathbf{S}^2) + \text{tr}(\mathbf{\Omega}^2) = -2(Q_S + Q_\Omega) = -2Q_G, \quad (20)$$

$$\begin{aligned} \text{tr}(\mathbf{S}_d^2) &= \text{tr}(\mathbf{S}^4) + \text{tr}(\mathbf{\Omega}^4) + 2\text{tr}(\mathbf{S}^2\mathbf{\Omega}^2) \\ &= 2(Q_S^2 + Q_\Omega^2 + V^2/4 + 2Q_SQ_\Omega) = 2(Q_G^2 + V^2/4). \end{aligned} \quad (21)$$

Then, plugging Eqs. (20) and (21) into Eq. (19) leads to

$$Q_{\tilde{S}_d} = -1/2tr(\tilde{S}_d^2) = -1/2tr(S_d^2) + 1/6tr^2(S_d) = -(V^2/4 + Q_G^2/3). \quad (22)$$

Finally, in the WALE model proposed by Nicoud and Ducros,²⁸ the eddy-viscosity is given by

$$\nu_e^W = (C_W\Delta)^2 \frac{(-2Q_{\tilde{S}_d})^{3/2}}{(-2Q_S)^{5/2} + (-2Q_{\tilde{S}_d})^{5/4}}, \quad (23)$$

or, in terms of basic invariants,

$$\nu_e^W = (C_W\Delta)^2 \frac{(V^2/2 + 2Q_G^2/3)^{3/2}}{(-2Q_S)^{5/2} + (V^2/2 + 2Q_G^2/3)^{5/4}}. \quad (24)$$

C. Vreman's model

The Vreman's model²⁹ is based on the ratio between the second and the first invariant of the tensor $\mathbf{GG}^T$. With the help of identity (11), the latter can be written as follows:

$$P_{\mathbf{GG}^T} = tr(\mathbf{GG}^T) = 2(Q_\Omega - Q_S), \quad (25)$$

whereas the former is given by $Q_{\mathbf{GG}^T} = 1/2\{tr^2(\mathbf{GG}^T) - tr(\mathbf{GG}^T\mathbf{GG}^T)\}$. Then, with the help of identities (11) and (12), $Q_{\mathbf{GG}^T}$ can be expressed in terms of more basic invariants,

$$Q_{\mathbf{GG}^T} = 2(Q_\Omega - Q_S)^2 - Q_G^2 + 4tr(S^2\Omega^2), \quad (26)$$

and simplified further using (7) and (13),

$$Q_{\mathbf{GG}^T} = V^2 + Q_G^2. \quad (27)$$

In the Vreman's model, the eddy-viscosity is given by the following expression:

$$\nu_e^{Vr} = (C_{Vr}\Delta)^2 (Q_{\mathbf{GG}^T}/P_{\mathbf{GG}^T})^{1/2}. \quad (28)$$

Finally, plugging identities (25) and (27) leads to

$$\nu_e^{Vr} = (C_{Vr}\Delta)^2 \left(\frac{V^2 + Q_G^2}{2(Q_\Omega - Q_S)} \right)^{1/2}. \quad (29)$$

D. Verstappen's model

All the above-described models do not depend on the third invariants, R_S or R_G . Recently, Verstappen³⁰ proposed an eddy-viscosity model that is based on the third invariant of $\mathbf{S}$. It reads as

$$\nu_e^{Ve} = (C_{Ve}\Delta)^2 \frac{|R_S|}{-Q_S}; \quad (30)$$

therefore, it is already expressed in terms of invariants of $\mathbf{S}$.

E. σ -model

Even more recently, Nicoud *et al.*¹ proposed a new eddy-viscosity model. In this case, it is based on the singular values of the tensor $\mathbf{G}$. Namely,

$$\nu_e^\sigma = (C_\sigma\Delta)^2 \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2}, \quad (31)$$

where σ_i are the three singular eigenvalues of $\mathbf{G}$, i.e., $\sigma_i = \sqrt{\lambda_i}$, where λ_i is an eigenvalue of $\mathbf{GG}^T$, and $\sigma_1 \geq \sigma_2 \geq \sigma_3$. Hence, the eigenvalues of $\mathbf{GG}^T$ need to be determined. To do so, first, we need to compute the three invariants of $\mathbf{GG}^T$: the first two invariants, $P_{\mathbf{GG}^T}$ and $Q_{\mathbf{GG}^T}$, are, respectively, given by identities (25) and (27), whereas the third invariant of $\mathbf{GG}^T$ follows straightforwardly

$$R_{\mathbf{GG}^T} = \det(\mathbf{GG}^T) = \det(\mathbf{G})\det(\mathbf{G}^T) = R_G^2. \quad (32)$$

Finally, the eigenvalues of $\mathbf{GG}^T$ are obtained by solving its characteristic equation. Hence, the formula for the eddy-viscosity given in Eq. (31) can be computed in terms of the following four basic invariants: Q_G , Q_S , V^2 , and R_G . However, it requires the numerical solution of a cubic equation.

IV. NEAR-WALL BEHAVIOR AND OTHER FEATURES

The major drawback of the classical Smagorinsky model (see Eq. (18)) is that the differential operator it is based on does not vanish in near-wall regions (see Table I). First attempts to overcome this inherent problem of the Smagorinsky model made use of wall functions.^{31,32} However, the first outstanding improvement was the dynamic procedure proposed by Germano *et al.*² in the early 1990s. Alternatively, it is possible to build models based on invariants that do not have this limitation. Examples thereof are the WALE, the Vreman's, the Verstappen's, and the σ -model described in Sec. III. This list can be completed with a novel eddy-viscosity model recently proposed by Ryu and Iaccarino.³³ It is based on the volumetric strain-stretching tensor, which is constructed by the multiplication of diagonal components of the rate-of-strain tensor with its off-diagonal components and decays as $O(y^3)$ near solid walls.

At this point, it is interesting to observe that new models can be derived by imposing restrictions on the differential operators they are based on. For instance, let us consider models that are based on the invariants of the tensor $\mathbf{GG}^T$,

$$\nu_e = (C_{s3pqr}\Delta)^2 P_{\mathbf{GG}^T}^p Q_{\mathbf{GG}^T}^q R_{\mathbf{GG}^T}^r, \quad (33)$$

where $P_{\mathbf{GG}^T}$, $Q_{\mathbf{GG}^T}$, and $R_{\mathbf{GG}^T}$ are given by Eqs. (25), (27), and (32), respectively. This tensor is proportional to the gradient model³⁴ given by the leading term of the Taylor series expansion of the subgrid stress tensor $\tau(\bar{\mathbf{u}}) = (\Delta^2/12)\mathbf{GG}^T + O(\Delta^4)$. The local dissipation of gradient model is then proportional to $-\mathbf{GG}^T : \mathbf{S} = -tr(\mathbf{GG}^T \mathbf{S}) = 1/3(tr(\mathbf{G}^3) - 4tr(\mathbf{S}^3)) = R_G - 4R_S$. Hence, the local dissipation introduced by the model, i.e., $(\Delta^2/12)(R_G - 4R_S)$, can also take negative values; therefore, the gradient model cannot be used as a standalone LES model, since it produces a finite time blow-up of the kinetic energy.³⁵ From the asymptotic near-wall behavior of the basic invariants (see Table I), it is easy to deduce that $P_{\mathbf{GG}^T}$, $Q_{\mathbf{GG}^T}$, and $R_{\mathbf{GG}^T}$ scale $O(y^0)$, $O(y^2)$, and $O(y^6)$, and their units are $[T^{-2}]$, $[T^{-4}]$, and $[T^{-6}]$, respectively. Then, the exponents p , q , and r in Eq. (33), must satisfy the following equations:

$$-6r - 4q - 2p = -1; \quad 6r + 2q = s, \quad (34)$$

to guarantee that the differential operator has units of frequency, i.e., $[P_{\mathbf{GG}^T}^p Q_{\mathbf{GG}^T}^q R_{\mathbf{GG}^T}^r] = [T^{-1}]$ and a slope s for the asymptotic near-wall behavior, i.e., $O(y^s)$. Solutions for $q(p, s) = (1 - s)/2 - p$ and $r(p, s) = (2s - 1)/6 + p/3$ are displayed in Figure 1. The Vreman's model given in Eq. (28) corresponds to the solution with $s = 1$ (see Table I) and $r = 0$. However, it seems more appropriate

TABLE I. Top: near-wall behavior and units of the five basic invariants in the 5D phase space given in (5) together with the invariant Q_Ω defined in (7). Bottom: near-wall behavior of the Smagorinsky, the WALE, the Vreman's, the Verstappen's, and the σ -model.

	<i>Invariants</i>					
	Q_G	R_G	Q_S	R_S	V^2	Q_Ω
Wall-behavior	$O(y^2)$	$O(y^3)$	$O(y^0)$	$O(y^1)$	$O(y^2)$	$O(y^0)$
Units	$[T^{-2}]$	$[T^{-3}]$	$[T^{-2}]$	$[T^{-3}]$	$[T^{-4}]$	$[T^{-2}]$
	<i>Models</i>					
	Smagorinsky Eq. (18)	WALE Eq. (24)	Vreman's Eq. (29)	Verstappen's Eq. (30)	σ -model Eq. (31)	
Wall-behavior	$O(y^0)$	$O(y^3)$	$O(y^1)$	$O(y^1)$	$O(y^3)$

FIG. 1. Solutions for the linear system of Eq. (34) for $s=1$ (dashed line) and $s=3$ (solid line). Each (r, q, p) solution represents an eddy-viscosity model of the form given in Eq. (33).

to look for solutions with the proper cubic near-wall behavior,³⁶ i.e., $s=3$ (solid lines in Figure 1). This leads to a family of p -dependent eddy-viscosity models,

$$\nu_e^{S3PQR} = (C_{s3pq}\Delta)^2 P_{GGT}^p Q_{GGT}^{-(p+1)} R_{GGT}^{(p+5/2)/3}. \quad (35)$$

Hereafter, this family of models will be referred as S3PQR-model. Restricting ourselves to solutions involving only two invariants of $\mathbf{GG}^T$, three models are found. Namely,

$$\nu_e^{S3PQ} = (C_{s3pq}\Delta)^2 P_{GGT}^{-5/2} Q_{GGT}^{3/2}, \quad (36)$$

$$\nu_e^{S3PR} = (C_{s3pr}\Delta)^2 P_{GGT}^{-1} R_{GGT}^{1/2}, \quad (37)$$

$$\nu_e^{S3QR} = (C_{s3qr}\Delta)^2 Q_{GGT}^{-1} R_{GGT}^{5/6}, \quad (38)$$

for $p = -5/2$, $p = -1$, and $p = 0$, respectively. These three solutions are also represented in Figure 1. Notice that with this notation the Vreman's model would be named S1PQ-model. Vreman also introduced a family of models equivalent to S_sPQ which includes the S3PQ-model (take $q = 3/2$ in Eq. (31) in Ref. 29). However, only the S1PQ-model was tested.

Apart from the proper near-wall behavior, the list of desirable properties that an eddy-viscosity model should meet is usually completed based on physical, numerical, and practical arguments. Nicoud *et al.*¹ summarized most of these properties and derived the σ -model given in Eq. (31) that meets all of them. Table II shows the properties of all the models described in Sec. III together with the p -dependent model proposed in Eq. (35). The first property, following the same notation as Nicoud *et al.*¹ is denoted as **Property P0**, includes both positiveness and locality. Although from a physical point-of-view, negative values of ν_e can be justified with the backscatter phenomenon, from a numerical point-of-view, the condition $\nu_e \geq 0$ is, in general, considered appropriate because it guarantees stability. On the other hand, LES equations should be Galilean invariant. In order to preserve this physical principle, eddy-viscosity models are usually based on the combination of invariants of a symmetric second-order tensor that depends on the gradient of the resolved velocity field, $\mathbf{G}$. Doing so, the condition of locality is also achieved; from a practical point-of-view, this is a desirable feature especially if the model aims to be applied in complex flows. This property is achieved by all the models displayed in Table II. The second property [**Property P1**] is the above-mentioned cubic near-wall behavior, i.e., $\nu_e = O(y^3)$. It can be shown that due to the no-slip condition and the incompressibility constraint, the production of turbulent kinetic energy follows a cubic behavior near the wall,³⁶ i.e., $y^+ \lesssim 5$. Hence, similar to the WALE and the σ -model, it seems

TABLE II. Properties of the Smagorinsky, the WALE, the Vreman's, the Verstappen's, the σ -model, and the S3PQR models. Namely, **P0**: $\nu_e \geq 0$, locality and frame invariant; **P1**: near-wall behavior; **P2**: $\nu_e = 0$ for 2D flows; **P3**: ν_e for the canonical axisymmetric flow $\mathbf{G} = \text{diag}(2\Delta, -\Delta, -\Delta)$; **P4**: well-conditioned and low computational cost.

Model	Smagorinsky	WALE	Vreman's	Verstappen's	σ -model	S3PQR-model
Formula	Equation (18)	Equation (24)	Equation (29)	Equation (30)	Equation (31)	Equation (35)
Constant	$C_S = 0.165$	$C_W = \sqrt{0.5}$	$C_{Vr} = \sqrt{0.07}$	$C_{Ve} = 1/\pi\sqrt{3/2}$	$C_\sigma = 1.35$	$C_{s3pqr} = \sqrt{3}C_{Vr}$
P0	Yes	Yes	Yes	Yes	Yes	Yes
P1	$O(y^0)$	$O(y^3)$	$O(y^1)$	$O(y^1)$	$O(y^3)$	$O(y^3)$
P2	No	No	No	Yes	Yes	Yes (if $p > -5/2$)
P3	≈ 0.094	≈ 0.075	≈ 0.086	≈ 0.101	0	$0.07(2^{5/3}/3)p^{+1}$
P4	++++	++	+++	+++	+	+++

appropriate that the eddy-viscosity mimics this behavior. As mentioned above, the proposed model also meets this property.

The last two properties proposed by Nicoud *et al.*¹ correspond to physical situations where no subgrid activity is expected. Namely, the eddy-viscosity should be exactly zero for 2D flows [**Property P2**] and for pure axisymmetric or isotropic expansion (or contraction) [**Property P3**]. Property **P2** can be justified from the absence of vortex-stretching for 2D flows whereas property **P3** corresponds to canonical laminar flow configurations. Moreover, 2D resolved scales are not compatible with a 3D subgrid scale activity in the long run because the subgrid scales interact with the smallest resolved scales. This is an additional argument to justify property **P2**. In this case, only the Verstappen's model and the σ -model meet with property **P2**. A simple analysis shows that only the third invariant of $\mathbf{GG}^T$, i.e., $R_{\mathbf{GG}^T}$, vanishes for 2D flows. Therefore, the S3PQR model proposed in Eq. (35) also meets **P2** with the condition that $p > -5/2$. Regarding the property **P3**, Table II displays the value of ν_e for the canonical axisymmetric flow $\mathbf{G} = \text{diag}(2\Delta, -\Delta, -\Delta)$. Doing so, the results do not depend on the subgrid characteristic length, Δ . In this case, only the σ -model vanishes whereas the rest of models have similar values. In our case, the result (weakly) depends on p giving values between ≈ 0.064 ($p = -5/2$) and ≈ 0.076 ($p = 1/2$), slightly lower than the rest of models. Isotropic expansions (or contractions) are not considered because they are not compatible with the divergence-free condition, $\nabla \cdot \bar{\mathbf{u}} = 0$. To complete the list of properties proposed by Nicoud *et al.*,¹ it is also desirable that models are always well-conditioned and have a low (or moderate) computational cost [**Property P4**]. In this regard, most of them rely on the computation of the invariants of a second-order tensor that depends on the gradient of the resolved velocity field. The computational cost of this type of operations is rather small and only special attention is required for indeterminate forms of type 0/0. Except for the Smagorinsky model, this is the case of all the models shown in Table II. More cumbersome is the computation of the σ -model: it also requires the solution of a cubic equation (see Sec. III E, for details). Apart from being computationally more expensive, solving a cubic equation, it may be a numerically ill-conditioned problem.

V. FINDING PROPER BOUNDS FOR THE MODEL CONSTANT

The model constant for an eddy-viscosity model needs to be determined in some way. In the case of the Smagorinsky model, it is possible to obtain a value of C_S by assuming that the cut-off wave number $k_c = \pi/\Delta$ lies within the inertial range for a classical Kolmogorov energy spectrum $E(k) = C_K \varepsilon^{2/3} k^{-5/3}$. Following Lilly's approach,³⁷ $C_S = (2/3C_K)^{3/4}/\pi$ is found by assuming that the model dissipation is equal to the turbulent kinetic energy dissipation, ε . Then, taking a value of $C_K \approx 1.58$ for the Kolmogorov constant³⁸ leads to $C_S \approx 0.17$. Unfortunately, in general, this theoretical analysis cannot be extended for other SGS models. Instead, the model constant can be numerically evaluated by assuming that the new model gives the same average dissipation that the Smagorinsky model. This has been done either using fields of homogeneous isotropic turbulence²⁸

or using a large sample of random velocity gradient tensor.¹ In both cases, simulations of a freely decaying isotropic turbulence were carried out to find more accurate estimations of the model constant. Alternatively, a theoretical analysis using the inequalities between the invariants may allow to find upper bounds for the model constant. This was the approach followed by Vreman²⁹ to bound his model constant in terms of the Smagorinsky constant. A similar approach was followed by Verstappen;³⁰ in this case, he found an upper bound using the Poincaré's inequality. Moreover, using the inequalities between the invariants Q_S and R_S , he could also show that his model dissipation is upper bounded by the Smagorinsky model. Both types of analysis (theoretical and numerical) are considered in the next paragraphs.

Let us consider a symmetric second-order tensor, $\mathbf{A} = \mathbf{A}^T$. In this case, all the eigenvalues are real-valued, i.e., $\lambda_i \in \mathbb{R}$, $i = 1, 2, 3$. Since the eigenvalues of $\mathbf{A}$ are solutions of its characteristic equation (see Eq. (15)), the discriminant of the cubic equation

$$D \equiv 18PQR - 4P^3R + P^2Q^2 - 4Q^3 - 27R^2 \quad (39)$$

must be non-negative, $D \geq 0$. In this case, the sub-indices of the invariants have been dropped for simplicity. The following quadratic equation for R is obtained by imposing that $D = 0$:

$$27R^2 + (4P^3 - 18PQ)R + (4Q^3 + P^2Q^2) = 0. \quad (40)$$

Since $d^2D/dR^2 = -54 < 0$, the third invariant R is bounded by the two solutions of Eq. (40). Namely,

$$R_a \leq R \leq R_b, \quad (41)$$

where $R_a = 1/3P(Q - 2/9P^2) - 2/27(P^2 - 3Q)^{3/2}$ and $R_b = 1/3P(Q - 2/9P^2) + 2/27(P^2 - 3Q)^{3/2}$. Moreover, R_a and R_b must be real-valued; therefore, $P^2 - 3Q \geq 0$. This leads to the following inequality between the first and the second invariant:

$$3Q \leq P^2. \quad (42)$$

Inequalities (41) and (42) are valid for any symmetric second-order tensor. Hereafter, we restrict our analysis to symmetric tensors with non-negative invariants, i.e., $P, Q, R \geq 0$. In this case, it can be shown that given a P (or a Q), the maximum value for R_b is always given by $P^2 = 3Q$. Plugging this into inequality (41) leads to

$$0 \leq R \leq P^3/27 \quad \text{and} \quad 0 \leq R \leq (Q/3)^{3/2}. \quad (43)$$

For convenience, we can also consider the product between the first and the third invariant,

$$0 \leq RP \leq R_bP \leq Q^3/3. \quad (44)$$

At this point, we are ready to analyze the following dimensionless invariant,

$$A^{S3PQR} \equiv P_{\text{GG}^T}^{p+1/2} Q_{\text{GG}^T}^{-(p+3/2)} R_{\text{GG}^T}^{(p+5/2)/3} \quad (45)$$

that represents the quotient between the invariant $P_{\text{GG}^T}^p Q_{\text{GG}^T}^{-(p+1)} R_{\text{GG}^T}^{(p+5/2)/3}$ of the $S3PQR$ -models given in Eq. (35) and the invariant $P_{\text{GG}^T}^{-1/2} Q_{\text{GG}^T}^{1/2}$ of the Vreman's model given in Eq. (28). The tensor GG^T is symmetric and its invariants are all non-negative (see Eqs. (25), (27), and (32)); therefore, inequalities (42)–(44) hold for P_{GG^T} , Q_{GG^T} , and R_{GG^T} . Assuming that $p \geq -5/2$, we can use inequality (43) to find an upper bound for A^{S3PQR} ,

$$0 \leq A^{S3PQR} \leq (1/3)^{(p+5/2)/2} P_{\text{GG}^T}^{p+1/2} Q_{\text{GG}^T}^{-(p+1/2)/2} \quad \text{if } -5/2 \leq p. \quad (46)$$

Then, using inequality (42) and assuming that $p \leq -1/2$ lead to

$$0 \leq A^{S3PQR} \leq 1/3 \quad \text{if } -5/2 \leq p \leq -1/2. \quad (47)$$

On the other hand, we can use inequality (44) to find a upper bound for $p \geq -1/2$,

$$0 \leq A^{S3PQR} \leq (1/3)^{(p+1/2)} Q_{\text{GG}^T}^{(p-1/2)} R_{\text{GG}^T}^{-2(p-1/2)/3} \quad \text{if } -1/2 \leq p. \quad (48)$$

FIG. 2. Values for the model constant, C_{s3pqr} , defined in Eq. (35) as a function of the exponent p . Solid line corresponds to those values that lead to the same averaged dissipation as for the Smagorinsky model given in Eq. (18) with $C_S = 0.165$. Horizontal dashed line corresponds to the upper limit found in inequality (50) with $C_{Vr} = \sqrt{0.07}$.

Then, using inequality (43) and assuming that $p \leq 1/2$ lead to $0 \leq A^{S3PQR} \leq 1/3$ if $-1/2 \leq p \leq 1/2$. Hence, combined with previous inequality (47) leads to

$$0 \leq A^{S3PQR} \leq 1/3 \quad \text{if } -5/2 \leq p \leq 1/2. \quad (49)$$

Therefore, the model constant C_{s3pqr} can be related to the Vreman's constant, C_{Vr} , with the following inequality:

$$0 \leq \frac{(C_{Vr})^2}{(C_{s3pqr})^2} \frac{\nu_e^{S3PQR}}{\nu_e^{Vr}} \leq \frac{1}{3} \quad \text{if } -5/2 \leq p \leq 1/2. \quad (50)$$

Hence, imposing $C_{s3pqr} = \sqrt{3}C_{Vr}$ guarantees both numerical stability and that the models have less or equal dissipation than Vreman's model, i.e.,

$$0 \leq \nu_e^{S3PQR} \leq \nu_e^{Vr} \quad \text{if } -5/2 \leq p \leq 1/2. \quad (51)$$

Figure 2 displays the values for the model constant, C_{s3pqr} , as a function of the exponent p . The values reported has been obtained by equating the averaged dissipation of the Smagorinsky model, i.e., $\langle 2\nu_e^{S3PQR} \mathbf{S} : \mathbf{S} \rangle = \langle 2\nu_e^{Smag} \mathbf{S} : \mathbf{S} \rangle$, for a large enough sample of random traceless velocity gradient tensors. This simple random procedure is able to produce fairly good predictions for other models: namely, for a Smagorinsky constant of $C_S = 0.165$, it leads to $C_{Vr} \approx 0.266$, $C_W \approx 0.569$, and $C_\sigma \approx 1.378$, for the Vreman's, the WALE, and the Sigma models, respectively. These values are in very good agreement with the values obtained by Nicoud *et al.*¹ using the same procedure and very close to the values proposed in the original papers.^{1,28,29} Applying the same procedure for the Verstappen's model³⁰ leads to $C_{Ve} \approx 0.527$, significantly above the value proposed in the original paper, i.e., $C_{Ve} = 1/\pi\sqrt{3/2} \approx 0.345$. Moreover, the upper limit given in inequality (50) with $C_{Vr} = \sqrt{0.07}$ is also shown in Figure 2. As expected for the whole range of $-5/2 \leq p \leq 1/2$, this value is smaller than the value obtained by equating the averaged dissipation of the Smagorinsky model. Simulations of decaying isotropic turbulence confirm these values in Sec. VI.

VI. NUMERICAL EXPERIMENTS

A family of p -dependent eddy-viscosity models has been proposed in Sec. IV. In short, the eddy-viscosity, ν_e^{S3PQR} , is given by Eq. (35) where P_{GG^T} , Q_{GG^T} , and R_{GG^T} are, respectively, the first, second, and third invariants of the second-order tensor $\mathbf{GG}^T$, and $\mathbf{G} \equiv \nabla \mathbf{u}$ is the gradient

of the resolved velocity field. In terms of the 5D phase space defined in (5), these three invariants are given by Eqs. (25), (27), and (32), respectively. Regarding the value of the model constant, C_{s3pqr} , two criteria have been analyzed in Sec. V; namely, the upper bound given by inequality (50), i.e., $C_{s3pqr} = \sqrt{3}C_{Vr}$ with $C_{Vr} = \sqrt{0.07}$, guarantees that the models have less or equal dissipation than Vreman's model. On the other hand, values obtained by equating the averaged dissipation with the Smagorinsky model are displayed in Figure 2. In this case, the value of C_{s3pqr} depends on the exponent p . In this section, several numerical experiments are carried out to assess the performance of the proposed method and to check the adequacy of these bounds.

A. Decaying isotropic turbulence

The numerical simulation of decaying isotropic turbulence has been chosen as a first test-case. The configuration corresponds to the classical experimental results obtained by Comte-Bellot and Corrsin³⁹ (hereafter denoted as CBC) using the grid turbulence with a mesh size $M = 5.08$ cm and a free-stream velocity $U_0 = 10$ m/s. The Taylor micro-scale Reynolds number at $tU_0/M = 42$ (initial state) is $Re_\lambda = u_{rms}\lambda/\nu = 71.6$ with $u_{rms} = 22.2$ cm/s and decreases to 60.6 at $tU_0/M = 171$. The results are non-dimensionalized with the following reference length and velocity: $L_{ref} = 11M/(2\pi)$ and $u_{ref} = \sqrt{3/2}u_{rms}|_{tU_0/M=42}$. The LES equations are solved with a pseudo-spectral code using the 3/2 dealiasing rule. An explicit second-order Adams-Bashforth scheme is used for time-integration. The simulations are carried out in a computational cube of $(11M)^3$, and the energy spectra of the divergence-free initial field at $tU_0/M = 42$ correspond with the experimental data of CBC.

Time-evolution of the resolved kinetic energy and the three-dimensional energy spectra at $tU_0/M = 42, 98$, and 171 are, respectively, shown in Figures 3 and 4. LES results have been obtained with a 32^3 mesh and with two sets of model constants. Results without model are not shown because the simulation is unstable. First, the upper bound given by inequality (50) leads to $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3}C_{Vr} \approx 0.458$ with $C_{Vr} = \sqrt{0.07}$. This guarantees that the proposed models have less or equal dissipation as the Vreman's model (also shown for comparison). Figures 3 (top) and 4 (top) clearly show that the S3PQR models do not introduce enough dissipation. A second approach has also been studied in Sec. V: in this case, the model constants are obtained by equating the averaged dissipation with the dissipation of the Smagorinsky model. This leads to the p -dependent results displayed in Figure 2, in particular to $C_{s3pq} = 0.572$ ($p = -5/2$), $C_{s3pr} = 0.709$ ($p = -1$), and $C_{s3qr} = 0.762$ ($p = 0$), respectively. Results displayed in Figures 3 (bottom) and 4 (bottom) show a good agreement with the experimental data of CBC indicating that this second set of constants introduce the right amount of SGS dissipation. Note that the results for the three models proposed here (S3PQ, S3PR, and S3QR) are virtually the same, showing that the performance for this test-case is sensitive to the model constant but not to the model itself. Hereafter, all the numerical simulations are carried out with this set of constants, i.e., $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, and $C_{s3qr} = 0.762$, respectively.

B. Turbulent channel flow

To test the performance of the proposed model with the presence of walls, a turbulent channel flow has been considered. In this case, the code is based on a fourth-order symmetry-preserving finite volume discretization⁴⁰ of the incompressible Navier-Stokes equations on structured staggered grids. A second-order self-adapting explicit scheme⁴¹ is used for the time integration and the pressure-velocity coupling is solved by means of a classical fractional step projection method. For details about the numerical algorithms and the verification of this code, the reader is referred to Gorobets *et al.*⁴² Regarding the spatial discretization of the eddy-viscosity models, the novel approach proposed by Trias *et al.*⁴³ has been used. A standard approach would consist on discretizing the term $\nabla \cdot (\nu_e(\nabla \mathbf{u})^T)$ directly. However, this implies many *ad hoc* interpolations, especially on staggered grids, that tend to smear the eddy-viscosity, ν_e . This may (negatively?) influence the performance of eddy-viscosity especially near the walls. Instead, an alternative form was proposed in our previous work.⁴³ Shortly, with the help of vector calculus it can be shown that

FIG. 3. Time evolution of the resolved kinetic energy for the decaying isotropic turbulence corresponding to the Comte-Bellot and Corrsin³⁹ experiment. LES results have been obtained with a 32^3 mesh. Symbols are the experimental measurements at $tU_0/M = 42, 98$, and 171 . Top: model constants are $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3}C_{Vr} \approx 0.458$ and $C_{Vr} = \sqrt{0.07}$. Bottom: model constants are $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, and $C_{s3qr} = 0.762$, respectively.

$$\nabla \cdot (v_e(\nabla \mathbf{u})^T) = \nabla(\nabla \cdot (v_e \mathbf{u})) - \nabla \cdot (\mathbf{u} \otimes \nabla v_e). \quad (52)$$

Then, recalling that the flow is incompressible, the second term in the right-hand-side can be written as $\nabla \cdot (\mathbf{u} \otimes \nabla v_e) = (\mathbf{u} \cdot \nabla) \nabla v_e$, i.e.,

$$\nabla \cdot (v_e(\nabla \mathbf{u})^T) = \nabla(\nabla \cdot (v_e \mathbf{u})) - (\mathbf{u} \cdot \nabla) \nabla v_e. \quad (53)$$

This provides an alternative form to construct consistent approximations of Eqs. (2) and (3) without introducing new interpolation operators. From a numerical point-of-view, the most remarkable property of this form is that it can be straightforwardly implemented by simply re-using operators that are already available in any code. Moreover, for constant viscosity, formulations constructed via Eq. (53) become identical to the original formulation because both terms exactly vanish. Numerical tests⁴³ showed the capability of the method to compute fourth-order accurate approximations on staggered Cartesian grids and second-order accurate approximations on collocated unstructured grids. Moreover, the computational costs of evaluating Eq. (53) can be significantly reduced by simply ignoring the first-term in the right-hand-side, $\nabla(\nabla \cdot (v_e \mathbf{u}))$. Since it is a gradient of a scalar field, this term can be absorbed into the pressure, $\pi = p - \nabla \cdot (v_e \mathbf{u})$.

FIG. 4. Three-dimensional energy spectra for the decaying isotropic turbulence corresponding to the Comte-Bellot and Corrsin³⁹ experiment. LES results have been obtained with a 32^3 mesh. Symbols are the experimental measurements at $tU_0/M = 42, 98$, and 171 . Top: model constants are $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3}C_{Vr} \approx 0.458$ and $C_{Vr} = \sqrt{0.07}$. Bottom: model constants are $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, and $C_{s3qr} = 0.762$, respectively.

Figure 5 shows the performance of the proposed models for a turbulent channel flow at $Re_\tau = 395$ in conjunction with the discretization methods for eddy-viscosity models proposed by Trias *et al.*⁴³ The results are compared with the direct numerical simulation (DNS) data of Moser *et al.*⁴⁴ The dimensions of the channel are taken equal to those of the DNS, i.e., $2\pi \times 2 \times \pi$. The computational grid is reduced in a significant manner; namely, the DNS was performed on a $256 \times 193 \times 192$ grid whereas the LES results have been obtained with a 32^3 mesh, i.e., the DNS uses about 290 times more grid points than the present LES. They are uniformly distributed in the stream-wise and the span-wise directions whereas the wall-normal points are distributed using a piece-wise hyperbolic sine functions. For lower-half of the channel, the distribution of points is given by

$$y_j = \sinh(\gamma j/N_y) / \sinh(\gamma/2) \quad j = 0, 1, \dots, N_y/2, \quad (54)$$

where N_y denotes the number of grid points in the wall-normal direction. The stretching parameter, γ , is taken equal to 7. Then, the grid points in the upper-half are computed by means of symmetry. With this distribution and $N_y = 32$, the first off-wall grid point is located at $y^+ \approx 2.6$, i.e., inside

FIG. 5. Results for a turbulent channel flow at $Re_\tau = 395$ obtained with a 32^3 mesh for LES and a 96^3 mesh without model, i.e., $\nu_e = 0$. Solid line corresponds to the DNS by Moser *et al.*⁴⁴ Top: average stream-wise velocity, $\langle u \rangle$. Bottom: root-mean-square of the fluctuating velocity components (from top to bottom, u_{rms} , w_{rms} and v_{rms} , respectively.).

the viscous sublayer ($y^+ < 5$). In this case, the subgrid characteristic length is computed as the cube root of the cell volume, i.e., $\Delta \equiv (\Delta x \Delta y \Delta z)^{1/3}$. Averages over the four statistically invariant transformations (time, stream-wise and span-wise directions, and central plane symmetry) are carried out for all the fields. The standard notation $\langle \cdot \rangle$ is used to denote this averaging procedure. The averaging over time starts after a start-up period. This period as well as the time-span over which the results are averaged, 60 time-units (based on the skin friction velocity, u_τ , and the channel width), is identical for all the simulations presented here.

The results displayed in Figure 5 are in good agreement with the DNS data. To illustrate the contribution of the eddy-viscosity models to improve the quality of the solution, the results obtained with a 96^3 mesh without model, i.e., $\nu_e = 0$, are also shown. The performance of the three models proposed here (S3PQ, S3PR, and S3QR) is essentially the same and no significant differences are observed between them. Compared with the Vreman's model, they tend to improve the results for the mean velocity in the buffer layer region ($5 < y^+ < 30$) whereas the quality of the solutions in the outer layer ($y^+ > 50$) is very similar. Although some discrepancies are observed, the root-mean-square of the fluctuating velocity components (see Figure 5, bottom) is also in rather good agreement with the DNS results. In this case, the proposed models outperform the solution obtained with the Vreman's model for all the regions. The latter do not predict accurately the

FIG. 6. Averaged eddy-viscosity, $\langle \nu_e \rangle$, divided by the kinematic viscosity, ν . Results for a turbulent channel flow at $Re_\tau = 395$ obtained with a 32×32 (top) and a $32 \times 96 \times 32$ mesh (bottom) for different LES models.

position of the peak for u_{rms} , and clearly under-predict the solution for both v_{rms} and w_{rms} . In this case, the solution obtained without model seems accurate; however, the clearly over-predicted friction velocity (if results were normalized by the mean stream-wise velocity) compensates an over-prediction of the velocity fluctuations. These results support the idea that the Vreman's model tends to over-dissipate especially in the near-wall region where the eddy-viscosity, ν_e , does not follow the proper cubic behavior (see Table II). To illustrate this, the average eddy-viscosity, $\langle \nu_e \rangle$, divided by the kinematic viscosity, ν , is displayed in Figure 6. In this case, results using the classical Smagorinsky model are also shown for comparison. As expected, the proposed models follow a cubic near-wall behavior whereas the Vreman's model predict much higher values in the buffer layer region ($5 < y^+ < 30$). The same qualitative behavior is observed for both the 32^3 mesh and a mesh with 3 times more grid points in the wall normal directions, i.e., $32 \times 96 \times 32$. As expected, a finer grid always leads to smaller values of ν_e ; however, it decreases faster for the proposed models.

VII. CONCLUDING REMARKS AND FUTURE RESEARCH

In the present work, a general framework for eddy-viscosity models for LES has been presented. It is based on the 5D phase space of invariants given in (5). In this way, new models

can be constructed by imposing appropriate restrictions in this space. Examples thereof are the three new eddy-viscosity models proposed in Eqs. (36)–(38). Likewise the Vreman's model given in Eq. (28), they are also based on the invariants of the second-order tensor $\mathbf{GG}^T$. However, they have the proper cubic near-wall behavior. Moreover, it has been analytically shown that relating the models constants to the Vreman's model constant via $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3}C_{Vr} \approx 0.458$ guarantees both numerical stability and that the models have less or equal dissipation than Vreman's model, i.e., $0 \leq \nu_e \leq \nu_e^{Vr}$. On the other hand, higher constant values have been obtained by equating the averaged dissipation of the models with the dissipation of the Smagorinsky model for a large sample of random velocity gradient tensors, $\mathbf{G}$. This approach leads to $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, and $C_{s3qr} = 0.762$. Simulations of decaying isotropic turbulence have shown that the latter set of values provides the right amount of SGS dissipation. The performance of the proposed models has also been successfully tested for a turbulent channel flow. Although no significant differences have been observed between them, recalling that only R_{GG^T} -dependent models switch off for 2D flows, S3PR and S3QR models are preferable in this regard. Furthermore, apart from fulfilling a set of desirable properties (positiveness, locality, Galilean invariance, proper near-wall behavior, and automatically switch-off for laminar, 2D, and axisymmetric flows), the proposed models are well-conditioned, and have a low computational cost and no intrinsic limitations for statistically inhomogeneous flows. Therefore, the proposed models seem to be well suited for engineering applications. In this regard, several issues may significantly affect their performance. The proper calculation of the subgrid characteristic length on unstructured grids or the (global dynamic?) determination of model constant is examples thereof. Moreover, it should be noted that although the theory developed is probably well justified for compressible flows in the low subsonic regime, it is strictly valid only for incompressible flows. All these issues are part of our future research plans to test these models for complex flows.

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- ¹ F. Nicoud, H. B. Toda, O. Cabrit, S. Bose, and J. Lee, "Using singular values to build a subgrid-scale model for large eddy simulations," *Phys. Fluids* **23**(8), 085106 (2011).
- ² M. Germano, U. Piomelli, P. Moin, and W. H. Cabot, "A dynamic subgrid-scale eddy viscosity model," *Phys. Fluids* **3**, 1760–1765 (1991).
- ³ D. K. Lilly, "A proposed modification of the Germano subgrid-scale closure method," *Phys. Fluids A* **4**, 633–635 (1992).
- ⁴ S. Ghosal, T. S. Lund, P. Moin, and K. Akselvoll, "A dynamic localization model for large-eddy simulation of turbulent flows," *J. Fluid Mech.* **286**, 229–255 (1995).
- ⁵ C. Meneveau, T. S. Lund, and W. H. Cabot, "A Lagrangian dynamic subgrid-scale model of turbulence," *J. Fluid Mech.* **319**, 353–385 (1996).
- ⁶ N. Park, S. Lee, J. Lee, and H. Choi, "A dynamic subgrid-scale eddy viscosity model with a global model coefficient," *Phys. Fluids* **18**(12), 125109 (2006).
- ⁷ D. You and P. Moin, "A dynamic global-coefficient subgrid-scale eddy-viscosity model for large-eddy simulation in complex geometries," *Phys. Fluids* **19**(6), 065110 (2007).
- ⁸ J. Lee, H. Choi, and N. Park, "Dynamic global model for large eddy simulation of transient flow," *Phys. Fluids* **22**(7), 075106 (2010).
- ⁹ R. W. C. P. Verstappen, S. T. Bose, J. Lee, H. Choi, and P. Moin, "A dynamic eddy-viscosity model based on the invariants of the rate-of-strain," in *Proceedings of Summer Program 2010* (Center for Turbulence Research, Stanford University, 2011), pp. 183–192.
- ¹⁰ N. S. Ghaisas, D. A. Shetty, and S. H. Frankel, "Large eddy simulation of thermal driven cavity: Evaluation of sub-grid scale models and flow physics," *Int. J. Heat Mass Transfer* **56**(1-2), 606–624 (2013).
- ¹¹ T. J. R. Hughes, L. Mazzei, A. A. Oberai, and A. A. Wray, "The multiscale formulation of large eddy simulation: Decay of homogeneous isotropic turbulence," *Phys. Fluids* **13**(2), 505–512 (2001).
- ¹² L. C. Berselli, T. Ilescu, and W. Layton, *Mathematics of Large Eddy Simulation of Turbulent Flows*, 1st ed. (Springer, 2006).
- ¹³ P. Sagaut, *Large Eddy Simulation for Incompressible Flows: An Introduction*, 3rd ed. (Springer, 2005).
- ¹⁴ B. J. Cantwell, "Exact solution of a restricted Euler equation for the velocity gradient tensor," *Phys. Fluids A* **4**, 782–793 (1992).

- ¹⁵ J. Martin, A. Ooi, M. S. Chong, and J. Soria, "Dynamics of the velocity gradient tensor invariants in isotropic turbulence," *Phys. Fluids* **10**, 2336–2346 (1998).
- ¹⁶ M. Chong, E. Perry, and B. Cantwell, "A general classification of three-dimensional flow fields," *Phys. Fluids A* **2**, 765–777 (1990).
- ¹⁷ B. J. Cantwell, "On the behavior of velocity gradient tensor invariants in direct numerical simulations of turbulence," *Phys. Fluids A* **5**, 2008–2013 (1993).
- ¹⁸ J. Soria, R. Sondergaard, B. J. Cantwell, M. S. Chong, and A. E. Perry, "A study of the fine-scale motions of incompressible time-developing mixing layers," *Phys. Fluids* **6**(2), 871–884 (1994).
- ¹⁹ G. E. Elsinga and I. Marusic, "Evolution and lifetimes of flow topology in a turbulent boundary layer," *Phys. Fluids* **22**(1), 015102 (2010).
- ²⁰ A. Tsinober, L. Shtilman, and H. Vaisburd, "A study of properties of vortex stretching and enstrophy generation in numerical and laboratory turbulence," *Fluid Dyn. Res.* **21**(6), 477–494 (1997).
- ²¹ J. Jeong and F. Hussain, "On the identification of a vortex," *J. Fluid Mech.* **285**, 69–94 (1995).
- ²² P. Chakraborty, S. Balachandar, and R. J. Adrian, "On the relationships between local vortex identification schemes," *J. Fluid Mech.* **535**, 189–214 (2005).
- ²³ C. B. da Silva and J. C. F. Pereira, "Invariants of the velocity-gradient, rate-of-strain, and rate-of-rotation tensors across the turbulent/nonturbulent interface in jets," *Phys. Fluids* **20**(5), 055101 (2008).
- ²⁴ B. Pierce, P. Moin, and T. Sayadi, "Application of vortex identification schemes to direct numerical simulation data of a transitional boundary layer," *Phys. Fluids* **25**(1), 015102 (2013).
- ²⁵ J. Weickert and H. Hagen, *Visualization and Processing of Tensor Fields* (Springer, 2006).
- ²⁶ D. B. Ennis and G. Kindlmann, "Orthogonal tensor invariants and the analysis of diffusion tensor magnetic resonance images," *Magn. Reson. Med.* **55**, 136–146 (2006).
- ²⁷ J. Smagorinsky, "General circulation experiments with the primitive equations," *Mon. Weather Rev.* **91**, 99–164 (1963).
- ²⁸ F. Nicoud and F. Ducros, "Subgrid-scale stress modelling based on the square of the velocity gradient tensor," *Flow, Turbul. Combust.* **62**(3), 183–200 (1999).
- ²⁹ A. W. Vreman, "An eddy-viscosity subgrid-scale model for turbulent shear flow: Algebraic theory and applications," *Phys. Fluids* **16**(10), 3670–3681 (2004).
- ³⁰ R. Verstappen, "When does eddy viscosity damp subfilter scales sufficiently?," *J. Sci. Comput.* **49**(1), 94–110 (2011).
- ³¹ P. Moin and J. Kim, "Numerical investigations of turbulent channel flow," *J. Fluid Mech.* **118**, 341–377 (1982).
- ³² U. Piomelli, J. Ferziger, P. Moin, and J. Kim, "New approximate boundary conditions for large eddy simulations of wall-bounded flows," *Phys. Fluids A* **1**, 1061–1068 (1989).
- ³³ S. Ryu and G. Iaccarino, "A subgrid-scale eddy-viscosity model based on the volumetric strain-stretching," *Phys. Fluids* **26**(6), 065107 (2014).
- ³⁴ R. A. Clark, J. H. Ferziger, and W. C. Reynolds, "Evaluation of subgrid-scale models using an accurately simulated turbulent flow," *J. Fluid Mech.* **91**, 1–16 (1979).
- ³⁵ B. Vreman, B. Geurts, and H. Kuerten, "Large-eddy simulation of the temporal mixing layer using the Clark model," *Theor. Comput. Fluid Dyn.* **8**, 309–324 (1996).
- ³⁶ D. R. Chapman and G. D. Kuhn, "The limiting behaviour of turbulence near a wall," *J. Fluid Mech.* **170**, 265–292 (1986).
- ³⁷ D. K. Lilly, "The representation of small scale turbulence in numerical simulation experiments," in *IBM Scientific Computing Symposium on Environmental Sciences*, edited by H. H. Goldstine (IBM, Yorktown Heights, NY, 1967), pp. 195–210.
- ³⁸ D. A. Donzis and K. R. Sreenivasan, "The bottleneck effect and the Kolmogorov constant in isotropic turbulence," *J. Fluid Mech.* **657**, 171–188 (2010).
- ³⁹ G. Comte-Bellot and S. Corrsin, "Simple Eulerian time correlation of full- and narrow-band velocity signals in grid-generated, 'isotropic' turbulence," *J. Fluid Mech.* **48**, 273–337 (1971).
- ⁴⁰ R. W. C. P. Verstappen and A. E. P. Veldman, "Symmetry-preserving discretization of turbulent flow," *J. Comput. Phys.* **187**, 343–368 (2003).
- ⁴¹ F. X. Trias and O. Lehmkuhl, "A self-adaptive strategy for the time-integration of Navier-Stokes equations," *Numer. Heat Transfer, Part B* **60**(2), 116–134 (2011).
- ⁴² A. Gorobets, F. X. Trias, M. Soria, and A. Oliva, "A scalable parallel Poisson solver for three-dimensional problems with one periodic direction," *Comput. Fluids* **39**, 525–538 (2010).
- ⁴³ F. X. Trias, A. Gorobets, and A. Oliva, "A simple approach to discretize the viscous term with spatially varying (eddy-) viscosity," *J. Comput. Phys.* **253**, 405–417 (2013).
- ⁴⁴ R. D. Moser, J. Kim, and N. N. Mansour, "Direct numerical simulation of turbulent channel flow up to $Re_\tau = 590$," *Phys. Fluids* **11**, 943–945 (1999).