NEW DIFFERENTIAL OPERATORS AND DISCRETIZATION METHODS FOR LARGE-EDDY SIMULATION AND REGULARIZATION MODELING

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Abstract. Direct numerical simulations (DNS) of the incompressible Navier-Stokes equations are limited to relatively low-Reynolds numbers. Therefore, dynamically less complex mathematical formulations are necessary for coarse-grain simulations. Regularization and eddy-viscosity models for Large-Eddy Simulation are examples thereof. They rely on differential operators that should be able to capture well different flow configurations (laminar and 2D flows, near-wall behavior, transitional regime...). Most of them are based on the combination of invariants of a symmetric second-order tensor that is derived from the gradient of the resolved velocity field. In the present work, they are presented in a framework where all the models are represented as a combination of elements of a 5D phase space of invariants. In this way, new models can be constructed by imposing appropriate restrictions in this space. Moreover, since the discretization errors may play an important role, a novel approach to discretize the viscous term with spatially varying eddy-viscosity is used. It is based on basic operators; therefore, the implementation is straightforward even for staggered formulations. The performance of the proposed methods will be assessed by means of direct comparison to DNS reference results.

1 INTRODUCTION

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

$$\partial_t \boldsymbol{u} + \mathcal{C}(\boldsymbol{u}, \boldsymbol{u}) = \mathcal{D}\boldsymbol{u} - \nabla p, \qquad \nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

where $\boldsymbol{u}$ denotes the velocity field, p represents the kinematic pressure, the non-linear convective term is given by $\mathcal{C}(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u} \cdot \nabla) \boldsymbol{v}$, and the diffusive term reads $\mathcal{D}\boldsymbol{u} = \nu \Delta \boldsymbol{u}$, where 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 filtering the NS Eqs.(1) in space

$$\partial_t \overline{\boldsymbol{u}} + \mathcal{C}(\overline{\boldsymbol{u}}, \overline{\boldsymbol{u}}) = \mathcal{D}\overline{\boldsymbol{u}} - \nabla \overline{p} - \nabla \cdot \tau(\overline{\boldsymbol{u}}) \; ; \quad \nabla \cdot \overline{\boldsymbol{u}} = 0, \tag{2}$$

where $\overline{\boldsymbol{u}}$ is the filtered velocity and $\tau(\overline{\boldsymbol{u}})$ is the subgrid stress tensor and aims to approximate the effect of the under-resolved scales, *i.e.* $\tau(\overline{\boldsymbol{u}}) \approx \overline{\boldsymbol{u} \otimes \boldsymbol{u}} - \overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}$. Then, the closure problem consists on replacing (approximating) the tensor $\overline{\boldsymbol{u} \otimes \boldsymbol{u}}$ with a tensor depending only on $\overline{\boldsymbol{u}}$ (and not $\boldsymbol{u}$). Because of its inherent simplicity and robustness, the eddy-viscosity assumption is by far the most used closure model

$$\tau(\overline{\boldsymbol{u}}) \approx -2\nu_e S(\overline{\boldsymbol{u}}), \tag{3}$$

where ν_e denotes the eddy-viscosity. Notice that $\tau(\overline{\boldsymbol{u}})$ is considered traceless without the loss of generality, because the trace can be included as part of the pressure, $\overline{p}$. Following the same notation than in [1], the eddy-viscosity can be modeled in a natural way as follows

$$\nu_e = (C_m \delta)^2 D_m(\overline{\boldsymbol{u}}), \tag{4}$$

where C_m is the model constant, δ is the subgrid characteristic length and D_m is a differential operator associated with the model. This provides a framework where most of the existing eddy-viscosity models can be represented [1].

Alternatively, regularizations of the non-linear convective term basically reduce the transport towards the small scales: the convective term in the NS Eqs.(1), $\mathcal{C}$, is replaced by a smoother approximation, $\tilde{\mathcal{C}}$,

$$\partial_t \boldsymbol{u}_\epsilon + \tilde{\mathcal{C}}(\boldsymbol{u}_\epsilon, \boldsymbol{u}_\epsilon) = \mathcal{D}\boldsymbol{u}_\epsilon - \nabla p_\epsilon, \qquad \nabla \cdot \boldsymbol{u}_\epsilon = 0. \tag{5}$$

The first outstanding approach in this direction goes back to Leray [2]. The Navier-Stokes-α model also forms an example thereof [3]. More recently, a family of regularization methods that exactly preserve the symmetry and conservation properties of the convective term was proposed in [4]. In this way, the production of smaller and smaller scales of motion is restrained in an unconditionally stable manner. A very recent application of this regularization approach can be found in [5]. The criterion the determine the local filter length, ϵ, is also based on a differential operator. Like most of the eddy-viscosity models for LES, they are based on the combination of invariants of a symmetric second-order tensor that is derived from the gradient of the resolved velocity field.

In this context, a framework where all the models are represented as a combination of elements of a 5D phase space of invariants is presented. The basic theory together with some useful relations between invariants is presented in the next section. Then, a list of

eddy-viscosity models for LES is represented within this framework in Section 3. In this way, new models can be constructed by imposing appropriate restrictions in this space. This is addressed in Section 4 with special emphasis to the near-wall behavior. Moreover, since the discretization errors may play an important role a novel approach to discretize the viscous term with spatially varying eddy-viscosity is presented in Section 5. It is based on basic operators; therefore, the implementation is straightforward even for staggered formulations. Finally, relevant results are summarized and conclusions are given.

2 THEORY

The essence of turbulence are 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 turbulence eddy-viscosity models for LES have been proposed in the last decades (see [6], for a review). 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, $\mathsf{G} \equiv \nabla \overline{\boldsymbol{u}}$. This is a second-order traceless tensor, $tr(\mathsf{G}) = \nabla \cdot \overline{\boldsymbol{u}} = 0$. Therefore, it 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 [7, 8], this set of five invariants can be defined as follows

$$\{Q_\mathsf{G}, R_\mathsf{G}, Q_\mathsf{S}, R_\mathsf{S}, V^2\}, \tag{6}$$

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

$$P_\mathsf{G} = P_\mathsf{S} = P_\Omega = 0, \tag{7}$$

$$Q_\mathsf{G} = Q_\mathsf{S} + Q_\Omega, \tag{8}$$

$$R_\mathsf{G} = R_\mathsf{S} + tr(\Omega^2\mathsf{S}), \quad R_\Omega = 0. \tag{9}$$

Since the pioneering works in the early 90s [7, 9, 10] 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 (see [8], for instance). Namely,

$$\frac{dQ_{\mathsf{G}}}{dt} = -3R_{\mathsf{G}}; \qquad \frac{dR_{\mathsf{G}}}{dt} = \frac{2}{3}Q_{\mathsf{G}}^2, \tag{10}$$

$$\frac{dQ_{\mathsf{S}}}{dt} = -2R_{\mathsf{S}} - R_{\mathsf{G}}; \quad \frac{dR_{\mathsf{S}}}{dt} = \frac{2}{3}Q_{\mathsf{G}}Q_{\mathsf{S}} + \frac{1}{4}V^2; \quad \frac{dV^2}{dt} = -\frac{16}{3}(R_{\mathsf{S}} - R_{\mathsf{G}})Q_{\mathsf{G}}. \tag{11}$$

This defines a complete dynamical system in the 5D phase space defined in (6). 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, $\boldsymbol{\omega} = \nabla \times \boldsymbol{u}$, with the eigenvector corresponding to the intermediate eigenvalue of S and the tendency of this tensor to have one negative and two positive eigenvalues. On the other hand, numerical and experimental 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. For instance, the invariant $Q_{\Omega} = 1/4|\boldsymbol{\omega}|^2$ is proportional to the enstrophy density; therefore, it identifies tube-like structures with high vorticity. The invariant $Q_{\mathsf{S}} = -1/2(\mathsf{S} : \mathsf{S})$ is proportional to the local rate of viscous dissipation, $\varepsilon = 2\nu\mathsf{S} : \mathsf{S}$. Notice that $Q_{\Omega} \geq 0$ whereas $Q_{\mathsf{S}} \leq 0$ and these two invariants are related with the invariant Q_{G} with the identity (8); hence, positive values of the invariant $Q_{\mathsf{G}} > 0$ are related with areas where enstrophy dominates whereas $Q_{\mathsf{G}} < 0$ 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. It is remarkable the role that these invariants play in other areas of research such as the visualization of tensor fields [11], in particular in the analysis of diffusion tensor magnetic resonance images (see [12], for instance).

Starting from the classical Smagorinsky model [13], most of the eddy-viscosity models for LES are based on invariants of second-order tensors that are derived from the gradient tensor, G. Therefore, it seems natural to re-write them in terms of the 5D phase space defined in (6). This is addressed in the next section. However, for convenience some other important invariants (or relations) in the context of eddy-viscosity models for LES are defined before. Namely,

$$tr(\mathsf{G}\mathsf{G}^T) = tr(\mathsf{S}^2) - tr(\Omega^2) = 2(Q_{\Omega} - Q_{\mathsf{S}}), \tag{12}$$

$$tr(\mathsf{S}^2\Omega^2) = 1/8(tr(\mathsf{G}^4) - tr(\mathsf{G}\mathsf{G}^T\mathsf{G}\mathsf{G}^T)) = 1/8(2Q_{\mathsf{G}}^2 - tr(\mathsf{G}\mathsf{G}^T\mathsf{G}\mathsf{G}^T)), \tag{13}$$

$$Z^2 = V^2 - 2Q_{\mathsf{S}}Q_{\Omega}, \tag{14}$$

$$tr(\tilde{\mathsf{A}}^2) = tr(\mathsf{A}^2) - 1/3tr^2(\mathsf{A}), \tag{15}$$

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

characteristic equation

$$det(\lambda I - A) = \lambda^3 - P_A\lambda^2 + Q_A\lambda - R_A = 0, \tag{16}$$

where

$$P_A = \lambda_1 + \lambda_2 + \lambda_3; \quad Q_A = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3; \quad R_A = \lambda_1\lambda_2\lambda_3, \tag{17}$$

whereas for traceless tensors it simplifies to

$$P_{\tilde{A}} = 0; \quad Q_{\tilde{A}} = -1/2\left(\lambda_1\lambda_1 + \lambda_2\lambda_2 + \lambda_3\lambda_3\right); \quad R_{\tilde{A}} = \lambda_1\lambda_2\lambda_3. \tag{18}$$

3 A UNIFIED FRAMEWORK FOR EDDY-VISCOSITY MODELS

In the next subsections, different eddy-viscosity models for LES are re-written in terms of the list of five invariants given in (6). For the sake of clarity, sometimes the invariants Q_Ω and Z^2 are also used. Notice that they can always be written in terms of Q_S, Q_G and V^2 via the identities (8) and (14), respectively. Starting from the classical Smagorinsky model, they are presented in chronological order.

3.1 Smagorinsky model

The Smagorinsky model [13] can be written in terms of the above-defined invariants as follows

$$\nu_e^{Smag} = (C_S\delta)^2|S(\overline{u})| = 2(C_S\delta)^2(-Q_S)^{1/2}, \tag{19}$$

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

3.2 WALE model

The wall-adapting local eddy viscosity (WALE) model was originally proposed in [14]. Following the same notation than the original paper, it is based on the second invariant of the traceless part of the symmetric tensor $S_d = 1/2(G^2 + (G^2)^T) = S^2 + \Omega^2$,

$$Q_{\tilde{S}_d} = -1/2tr(\tilde{S}_d^2). \tag{20}$$

Then, using the identity (15) we can write the $tr(\tilde{S}_d^2)$ in terms of $tr(S_d^2)$ and $tr(S_d)$. Recalling that $S_d = S^2 + \Omega^2$, and applying the Caley-Hamilton theorem we obtain

$$tr(S_d) = tr(S^2) + tr(\Omega^2) = -2(Q_S + Q_\Omega) = -2Q_G, \tag{21}$$

$$tr(S_d^2) = tr(S^4) + tr(\Omega^4) + 2tr(S^2\Omega^2) = 2(Q_S^2 + Q_\Omega^2 + V^2). \tag{22}$$

Then, plugging Eqs.(21) and (22) into Eq.(20) leads to

$$Q_{\tilde{S}_d} = -1/2tr(\tilde{S}_d^2) = -1/2tr(S_d^2) + 1/6tr^2(S_d) \tag{23}$$

$$= -(Q_S^2 + Q_\Omega^2 + V^2) + 2/3Q_G^2. \tag{24}$$

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However, at this point it is more appropriate to write it in terms of the invariant Z^2 defined in Eq.(14), *i.e.*

$$Q_{\tilde{\mathsf{S}}_d} = -1/3Q_{\mathsf{G}}^2 - Z^2. \tag{25}$$

Finally, in the WALE model the eddy-viscosity is given by

$$\nu_e^W = (C_W\delta)^2 \frac{(-2Q_{\tilde{\mathsf{S}}_d})^{3/2}}{(-2Q_{\mathsf{S}})^{5/2} + (-2Q_{\tilde{\mathsf{S}}_d})^{5/4}}, \tag{26}$$

or, in terms of basic invariants,

$$\nu_e^W = (C_W\delta)^2 \frac{(2/3Q_{\mathsf{G}}^2 + Z^2)^{3/2}}{(-2Q_{\mathsf{S}})^{5/2} + (2/3Q_{\mathsf{G}}^2 + Z^2)^{5/4}}. \tag{27}$$

3.3 Vreman's model

The Vreman's model [15] is based on the ratio between the second and the first invariants of the tensor $\mathsf{G}\mathsf{G}^T$. With the help of the identity (12), the latter can be written as follows

$$P_{\mathsf{G}\mathsf{G}^T} = tr(\mathsf{G}\mathsf{G}^T) = 2(Q_\Omega - Q_{\mathsf{S}}), \tag{28}$$

whereas the former is given by $Q_{\mathsf{G}\mathsf{G}^T} = 1/2\{tr^2(\mathsf{G}\mathsf{G}^T) - tr(\mathsf{G}\mathsf{G}^T\mathsf{G}\mathsf{G}^T)\}$. Then, with the help of the identities (12) and (13), $Q_{\mathsf{G}\mathsf{G}^T}$ can be expressed in terms of more basic invariants

$$Q_{\mathsf{G}\mathsf{G}^T} = 2(Q_\Omega - Q_{\mathsf{S}})^2 - Q_{\mathsf{G}}^2 + 4V^2, \tag{29}$$

and simplified further using (8) and (14)

$$Q_{\mathsf{G}\mathsf{G}^T} = Q_{\mathsf{G}}^2 + 4Z^2. \tag{30}$$

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

$$\nu_e^{Vr} = (C_{Vr}\delta)^2 \left(Q_{\mathsf{G}\mathsf{G}^T}/P_{\mathsf{G}\mathsf{G}^T} \right)^{1/2}. \tag{31}$$

Finally, plugging identities (28) and (30) leads to

$$\nu_e^{Vr} = (C_{Vr}\delta)^2 \left(\frac{Q_{\mathsf{G}}^2 + 4Z^2}{2(Q_\Omega - Q_{\mathsf{S}})} \right)^{1/2}. \tag{32}$$

3.4 R_{S}-based model

All the above-described models do not depend on the third invariants, R_{S} or R_{G}. Recently, Verstappen [16] proposed an eddy viscosity model that is based on the third invariant of S. It reads,

$$\nu_e^R = (C_R\delta)^2 \frac{|R_{\mathsf{S}}|}{-Q_{\mathsf{S}}}, \tag{33}$$

therefore, it is already expressed in terms of basic invariants of S.

	Invariants						
	Q_{G}	R_{G}	Q_{S}	R_{S}	V^2	Q_Ω	Z^2
Wall-behavior	$\mathcal{O}(y^2)$	$\mathcal{O}(y^3)$	$\mathcal{O}(y^0)$	$\mathcal{O}(y^1)$	$\mathcal{O}(y^0)$	$\mathcal{O}(y^0)$	$\mathcal{O}(y^2)$
Units	$[T^{-2}]$	$[T^{-3}]$	$[T^{-2}]$	$[T^{-3}]$	$[T^{-4}]$	$[T^{-2}]$	$[T^{-4}]$
	Models						
	Smagorinsky		WALE	Vreman's	R_{S}-based	σ-model	
	Eq.(19)		Eq.(27)	Eq.(32)	Eq.(33)	Eq.(34)	
Wall-behavior	$\mathcal{O}(y^0)$		$\mathcal{O}(y^3)$	$\mathcal{O}(y^1)$	$\mathcal{O}(y^1)$	$\mathcal{O}(y^3)$	

Table 1: Top: near-wall behavior and units of the five basic invariants in the 5D phase space given in (6) together with the invariants Q_Ω and Z^2 defined in (8) and (14), respectively. Bottom: near-wall behavior of the Smagorinsky, the WALE, the Vreman's, the R_{S}-based and the σ-models.

3.5 σ-model

Even more recently, in [1] a new eddy-viscosity model was proposed. In this case, it is based on the singular values of the tensor G. Namely,

$$\nu_e^\sigma = (C_\sigma \delta)^2 \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2}, \tag{34}$$

where σ_i are the three singular eigenvalues of G, *i.e.* $\sigma_i = \sqrt{\lambda_i}$ where λ_i is an eigenvalue of $\mathsf{G}\mathsf{G}^T$, and $\sigma_1 \geq \sigma_2 \geq \sigma_3$. The eigenvalues of $\mathsf{G}\mathsf{G}^T$ can be easily related with its invariants using Eqs.(17). The first two invariants, $P_{\mathsf{G}\mathsf{G}^T}$ and $Q_{\mathsf{G}\mathsf{G}^T}$ are given by the identities (28) and (30), respectively. Finally, the third invariant of $\mathsf{G}\mathsf{G}^T$ follows straightforwardly

$$R_{\mathsf{G}\mathsf{G}^T} = det(\mathsf{G}\mathsf{G}^T) = det(\mathsf{G})det(\mathsf{G}^T) = R_{\mathsf{G}}^2. \tag{35}$$

Hence, the formula for the eddy-viscosity given in Eq.(34) can be written in terms of the following four basic invariants: Q_{G}, Q_{S}, V^2 and R_{G}.

4 NEAR-WALL BEHAVIOR AND OTHER FEATURES

The major drawback of the classical Smagorinsky model (see Eq. 19) is that the differential operator it is based on does not vanish in near-wall regions (see Table 1). First attempts to overcome this inherent problem of the Smagorinsky model made use of wall functions. However, the first outstanding improvement was the dynamic procedure proposed by Germano *et al.* [17] in the early 90s. 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 R_{S}-based and the σ-model described in the previous section.

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 $\mathsf{G}\mathsf{G}^T$

$$\nu_e = (C_M \delta)^2 P_{\mathsf{G}\mathsf{G}^T}^p Q_{\mathsf{G}\mathsf{G}^T}^q R_{\mathsf{G}\mathsf{G}^T}^r, \tag{36}$$
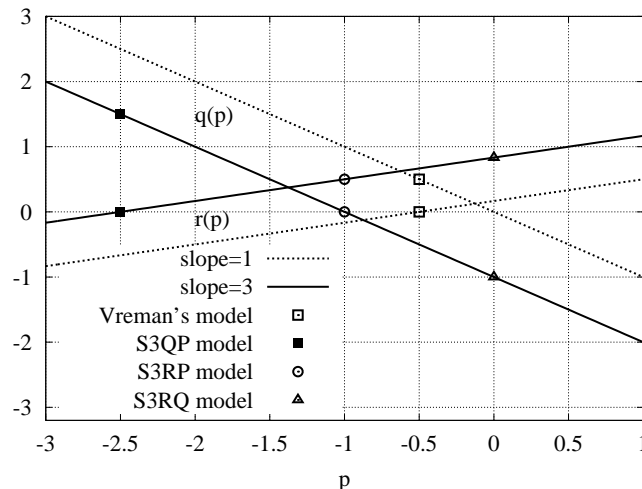
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Figure 1: Solutions for the linear system of Eqs.(37) for $s = 1$ (dashed line) and $s = 3$ (solid line). Each (r, q, p) solution represents an eddy-viscosity model of the form given in Eq.(36).

where P_{GG^T}, Q_{GG^T} and R_{GG^T} are given by Eqs.(28), (30) and (35), respectively. Then, from the asymptotic near-wall behavior of the basic invariants (see Table 1) it is easy to deduce that they scale $\mathcal{O}(y^0)$, $\mathcal{O}(y^2)$ and $\mathcal{O}(y^6)$, and their units are $[T^{-2}]$, $[T^{-4}]$ and $[T^{-6}]$, respectively. Since the differential operator, $[D_m(\overline{\boldsymbol{u}})] = [T^{-1}]$ the exponents have the following restrictions

$$-6r - 4q - 2p = -1; \qquad 6r + 2q = s, \tag{37}$$

where s is the slope for the asymptotic near-wall behavior, *i.e.* $\mathcal{O}(y^s)$. 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.(31) corresponds to the solution with $s = 1$ (see Table 1) and $r = 0$. However, it seems more appropriate to look for solutions with the proper near-wall behavior, *i.e.* $s = 3$ (solid lines in Figure 1). Restricting ourselves to solutions involving only two invariants of GG^T we find three new models,

$$\nu_e^{S3QP} = (C_{s3qp}\delta)^2 P_{\mathsf{GG}^T}^{-5/2} Q_{\mathsf{GG}^T}^{3/2}, \tag{38}$$

$$\nu_e^{S3RP} = (C_{s3rp}\delta)^2 P_{\mathsf{GG}^T}^{-1} R_{\mathsf{GG}^T}^{1/2}, \tag{39}$$

$$\nu_e^{S3RQ} = (C_{s3rq}\delta)^2 Q_{\mathsf{GG}^T}^{-1} R_{\mathsf{GG}^T}^{5/6}. \tag{40}$$

These three solutions are also represented in Figure 1. Notice that with this notation the Vreman's would be named S1QP model.

5   NUMERICAL METHODS FOR EDDY-VISCOSITY MODELS FOR LES

The incompressible NS Eqs.(1) with constant physical properties are discretized on a staggered grid using a fourth-order symmetry-preserving discretization [18]. Doing so, the

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symmetry properties of the underlying differential operators are preserved: the convective operator, $\mathsf{C}\left(\boldsymbol{u}_s\right)$, is represented by a skew-symmetric matrix and the diffusive operator, D, by a symmetric positive-definite matrix. In short, the temporal evolution of the spatially discrete staggered velocity vector, $\boldsymbol{u}_s \in \mathbb{R}^m$, is governed by the following operator-based finite-volume discretization of Eqs.(1)

$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_s + \mathsf{D}\boldsymbol{u}_s - \mathsf{M}^T\boldsymbol{p}_c = \mathbf{0}_s, \qquad \mathsf{M}\boldsymbol{u}_s = \mathbf{0}_c, \qquad (41)$$

where $\boldsymbol{p}_c \in \mathbb{R}^n$ is the cell-centered pressure scalar field. The dimension of these vectors, n and m, are the number of control volumes and faces on the computational domain, respectively. The sub-indices c and s refer to whether the variables are cell-centered or staggered at the faces. The diagonal matrix, $\Omega_s \in \mathbb{R}^{m \times m}$, describes the sizes of the staggered control volumes and the convective flux is discretized as in [18]. The resulting convective matrix, $\mathsf{C}\left(\boldsymbol{u}_s\right) \in \mathbb{R}^{m \times m}$, is skew-symmetric, *i.e.* $\mathsf{C}\left(\boldsymbol{u}_s\right) + \mathsf{C}^T\left(\boldsymbol{u}_s\right) = \mathsf{0}$. The skew-symmetry of $\mathsf{C}\left(\boldsymbol{u}_s\right)$ implies that

$$\mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{v}_s \cdot \boldsymbol{w}_s = \boldsymbol{v}_s \cdot \mathsf{C}^T\left(\boldsymbol{u}_s\right)\boldsymbol{w}_s = -\boldsymbol{v}_s \cdot \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{w}_s, \qquad (42)$$

for any discrete velocity vectors $\boldsymbol{u}_s$ (if $\mathsf{M}\boldsymbol{u}_s = \mathbf{0}_c$), $\boldsymbol{v}_s$ and $\boldsymbol{w}_s$. Then, the evolution of the discrete energy, $\|\boldsymbol{u}_s\|^2 = \boldsymbol{u}_s \cdot \Omega_s \boldsymbol{u}_s$, is governed by

$$\frac{d}{dt}\|\boldsymbol{u}_s\|^2 = -\boldsymbol{u}_s \cdot \left(\mathsf{D} + \mathsf{D}^T\right)\boldsymbol{u}_s < 0, \qquad (43)$$

where the convective and the pressure gradient contributions cancel because of Eq.(42) and the incompressibility constraint, $\mathsf{M}\boldsymbol{u}_s = \mathbf{0}_c$, respectively. Therefore, even for coarse grids, the energy of the resolved scales of motion is convected in a stable manner, *i.e.* the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should be from a physical point-of-view. This discretization has already been successfully tested for many direct numerical simulations (DNS). The most recent example thereof can be found in [5] where a DNS of turbulent flow in air-filled differentially heated cavity was carried out.

5.1 Discretization of the viscous term with spatially varying eddy-viscosity

In this work we propose to apply the same ideas to discretize the eddy-viscosity model (3) for LES (2). In this case, in general the (eddy-)viscosity, ν_e, is not constant neither on space and time. To obtain the Eq.(1) (with ν replaced by $\nu + \nu_e$) from Eqs.(2)-(3) with constant ν_e notice that $2\nabla \cdot S(\boldsymbol{u}) = \nabla \cdot \nabla \boldsymbol{u} + \nabla \cdot (\nabla \boldsymbol{u})^T$ and recall the vector calculus identity $\nabla \cdot (\nabla \boldsymbol{u})^T = \nabla(\nabla \cdot \boldsymbol{u})$ to cancel out the second term. However, for non-constant ν_e, the discretization of $\nabla \cdot (\nu_e(\nabla \boldsymbol{u})^T)$ needs to be addressed. This can be quite cumbersome especially for staggered formulations.

The standard approach consists on discretizing the term $\nabla \cdot (\nu_e(\nabla \boldsymbol{u})^T)$ directly. However, this implies many *ad hoc* interpolations that tends 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 [19]. Shortly, with the help of vector calculus it can be shown that

$$\nabla \cdot (\nu_e (\nabla \boldsymbol{u})^T) = \nabla(\nabla \cdot (\nu_e \boldsymbol{u})) - \nabla \cdot (\boldsymbol{u} \otimes \nabla \nu_e). \tag{44}$$

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

$$\nabla \cdot (\nu_e (\nabla \boldsymbol{u})^T) = \nabla(\nabla \cdot (\nu_e \boldsymbol{u})) - \mathcal{C}(\boldsymbol{u}, \nabla \nu_e). \tag{45}$$

This provides an alternative form to construct consistent approximations of Eqs.(2)-(3) without introducing new interpolation operators. Namely, the first term in the right-hand-side of Eq.(45) can be discretized as follows

$$-\mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{\boldsymbol{u}}_s \qquad \text{where} \quad [\tilde{\boldsymbol{u}}_s]_f = [\boldsymbol{\nu}_s]_f [\boldsymbol{u}_s]_f, \tag{46}$$

where $\Omega_c \in \mathbb{R}^{n \times n}$ is a diagonal matrix containing the sizes of the cell-centered control volumes and $[\boldsymbol{\nu}_s]_f$ is the value of $\nu_e(\boldsymbol{x}, t)$ evaluated at the face f. This term, like the continuous counterpart, (i) vanishes for constant ν_e ($\mathsf{M}\tilde{\boldsymbol{u}}_s = \nu_e \mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c$) and (ii) its contribution to the total kinetic energy is also null ($\boldsymbol{u}_s^T \mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{\boldsymbol{u}}_s = (\mathsf{M}\boldsymbol{u}_s)^T \Omega_c^{-1} \mathsf{M} \tilde{\boldsymbol{u}}_s = 0$). Regarding the second term, $\mathcal{C}(\boldsymbol{u}, \nabla \nu_e)$, it can be discretized as follows

$$\mathsf{C}(\boldsymbol{u}_s)(-\Omega_s^{-1} \mathsf{M}^T \boldsymbol{\nu}_c), \tag{47}$$

where $\boldsymbol{\nu}_c \in \mathbb{R}^n$ is a cell-centered vector containing the values of $\nu_e(\boldsymbol{x}, t)$. In this case, it also vanishes for constant ν_e ($\mathsf{M}^T \boldsymbol{\nu}_c = \nu_e \mathsf{M}^T \mathbf{1}_c = \boldsymbol{0}_s$). We can conclude that the alternative form given in Eq.(45) discretized by the expressions given in (46) and (47) is a consistent discretization of the term $\nabla \cdot (\nu_e (\nabla \boldsymbol{u})^T)$ without introducing new discrete operators. Moreover, in the case with constant ν_e these two terms vanish. In summary, combining Eqs.(46) and (47), the term $\nabla \cdot (\nu_e (\nabla \boldsymbol{u})^T)$ can be discretized as follows

$$\underbrace{-\mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{\boldsymbol{u}}_s}_{\approx \nabla(\nabla \cdot (\nu_e \boldsymbol{u}))} - \underbrace{\mathsf{C}(\boldsymbol{u}_s)(-\Omega_s^{-1} \mathsf{M}^T \boldsymbol{\nu}_c)}_{\approx \mathcal{C}(\boldsymbol{u}, \nabla \nu_e)}. \tag{48}$$

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.(48) become identical to the original formulation because both terms exactly vanish. Numerical results showing the capability of the method to compute fourth-order accurate approximations on staggered Cartesian grids were presented in [19] (see also Figure 2). Moreover, the computational costs of evaluating Eq.(45) can be significantly reduced by simply ignoring the first-term in the right-hand-side, $\nabla(\nabla \cdot (\nu_e \boldsymbol{u}))$. Since it is a gradient of a scalar field, this term can be absorbed into the pressure, $\pi = p - \nabla \cdot (\nu_e \boldsymbol{u})$.
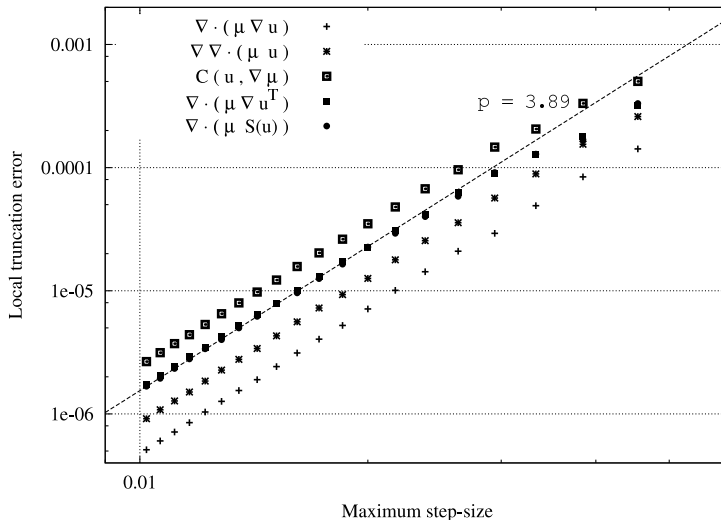
Figure 2: Norm of the local truncation error versus the maximum step-size. Results correspond to the 4th-order staggered discretization on structured Cartesian grids. Details can be found in [19].

6   CONCLUDING REMARKS AND FUTURE RESEARCH

In the present work, a general framework for eddy-viscosity (also regularization) models for LES has been presented. It is based on the 5D phase space of invariants given in (6). In this way, new models can be constructed by imposing appropriate restrictions in this space. Example thereof are the three new eddy-viscosity models proposed in Eqs. (38), (39) and (40). Like the Vreman's model given in Eq.(31), they are also based on the invariants of the tensor $\mathsf{G}\mathsf{G}^T$. However, the have the proper cubic near-wall behavior. Moreover, since the discretization errors may play an important role, a novel approach to discretize the viscous term with spatially varying eddy-viscosity has also been presented. It is based on basic operators; therefore, the implementation is straightforward even for staggered formulations. The performance of the proposed methods will be assessed by means of direct comparison to DNS results.

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