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New differential operators and discretization methods for eddy-viscosity models for LES

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Abstract

The incompressible Navier-Stokes equations constitute an excellent mathematical modelization of turbulence. Unfortunately, attempts at performing direct numerical simulations (DNS) are limited to relatively low-Reynolds numbers. Therefore, dynamically less complex mathematical formulations are necessary for coarse-grain simulations. Eddy-viscosity models for Large-Eddy Simulation (LES) is an example 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...). In the present work, several differential operators are derived from the criterion that vortex-stretching mechanism must stop at the smallest grid scale. 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 models will be assessed by means of direct comparison to DNS reference results.

Keywords: LES, eddy-viscosity, DNS, Symmetry-preserving, MPI+OpenMP

Nomenclature

$\textbf{C}(\mathbf{u}_s)$ discrete convective operator
$\textbf{D}$ discrete diffusive operator
$\mathbf{u}$ velocity field
$D_m$ differential operator associated with the model
$M$ discrete divergence operator
$p$ pressure
$Q$ invariant of $S$, $-1/2\text{tr}(S^2)$
$R$ invariant of $S$, $-1/3\text{tr}(S^3) = -\text{det}(S)$
$S$ rate-of-strain tensor, $S = 1/2(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$
$\epsilon$ filter length
$\nu$ kinematic viscosity
$\nu_e$ eddy-viscosity
$\tau(\mathbf{u})$ subgrid stress tensor
$\omega$ vorticity, $\nabla \times \mathbf{u}$
$\Omega$ diagonal matrix with sizes of control volumes

Greek symbols

$\delta$ subgrid characteristic length

Subscripts and superscripts

\textsuperscript{c} cell-centered discrete field
\textsuperscript{s} staggered discrete field
\textsuperscript{(-)} spatial linear filter

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1. Introduction

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

\[
\partial_t u + C(u, u) = Du - \nabla p, \quad \nabla \cdot u = 0,
\]

where \( u \) denotes the velocity field, \( p \) represents the pressure, the non-linear convective term is given by \( C(u, v) = (u \cdot \nabla)v \), and the diffusive term reads \( Du = \nu \Delta u \), where \( \nu \) 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 equations in space

\[
\partial_t \overline{u} + C(\overline{u}, \overline{u}) = D\overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) ; \quad \nabla \cdot \overline{u} = 0,
\]

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

\[
\tau(\overline{u}) \approx -2\nu_e S(\overline{u}),
\]

where \( \nu_e \) denotes the eddy-viscosity. Notice that \( \tau(\overline{u}) \) 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

\[
\nu_e = (C_m \delta)^2 D_m(\overline{u}),
\]

where \( C_m \) is the model constant, \( \delta \) 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 equations, \( C \), is replaced by a smoother approximation, \( \tilde{C} \),

\[
\partial_t u_e + \tilde{C}(u_e, u_e) = Du_e - \nabla p_e, \quad \nabla \cdot u_e = 0.
\]

The first outstanding approach in this direction goes back to Leray [2]. The Navier-Stokes-\( \alpha \) 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].

2. Restraining the production of small scales

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. Both regularization modeling and LES aim to do that by decreasing the non-linear transport and increasing the dissipation, respectively. Hence, in our opinion, the success of any turbulence model strongly depends on the ability to capture well this (im)balance.

Let us consider an arbitrary part of the domain flow, \( \Omega \), with periodic boundary conditions. The inner product is defined in the usual way: \( (a, b) = \int_{\Omega} a \cdot bd\Omega \). Then, taking the \( L^2 \) inner product of (1) with \( -\Delta u \) leads to the enstrophy equation

\[
\frac{1}{2} \frac{d}{dt} \| \omega \|^2 = (\omega, C(\omega, u)) - \nu(\nabla \omega, \nabla \omega),
\]

where \( \omega = \nabla \times u \).
where \(||\omega||^2 = (\omega, \omega)\) and the convective term contribution \((C(u, \omega), \omega) = 0\) vanishes because of the skew-symmetry of the convective operator. Following the same arguments than in [6], the vortex-stretching term can be expressed in terms of the invariant \(R = -1/3tr(S^3) = -det(S)\)

\[
(\omega, C(\omega, u)) = -\frac{4}{3} \int_{\Omega} tr(S^3) d\Omega = 4 \int_{\Omega} Rd\Omega = 4\tilde{R}, \tag{7}
\]

whereas the diffusive terms may be bounded in terms of the invariant \(Q = -1/2tr(S^2)\)

\[
(\nabla\omega, \nabla\omega) = -Q(\omega, \omega) = -\lambda_{\Delta}(\omega, \omega) = 4\lambda_{\Delta} \int_{\Omega} Q d\Omega = 4\lambda_{\Delta}\tilde{Q}, \tag{8}
\]

where \(\lambda_{\Delta} < 0\) is the largest (smallest in absolute value) non-zero eigenvalue of the Laplacian operator \(\Delta\) on \(\Omega\) and \(\tilde{\cdot}\) denotes the integral over \(\Omega\). However, it relies on the accurate estimation of \(\lambda_{\Delta}\) on \(\Omega\). The latter may be cumbersome, especially on unstructured grids. Alternatively, it may be (numerically) computed directly from \((\nabla\omega, \nabla\omega)\) or, even easier, by simply noticing that \((\nabla\omega, \nabla\omega) = 4 \int_{\Omega} Q(\omega) d\Omega = 4\tilde{Q}(\omega)\). However, from a numerical point-of-view, this type of integrations are not straightforward. Instead, recalling that \(\nabla \times \nabla \times u = \nabla (\nabla \cdot u) - \Delta u\) and \(\nabla \cdot u = 0\), a more appropriate expression can be obtained as follows

\[
(\nabla\omega, \nabla\omega) = -(\omega, \Delta \omega) = (\omega, \nabla \times \nabla \times \omega) = (\nabla \times \omega, \nabla \times \omega) = (\Delta u, \Delta u) = ||\Delta u||^2. \tag{9}
\]

Then, to prevent a local intensification of vorticity, i.e. \(||\omega||_t \leq 0\), the inequality \(H_{\Omega} \leq v(\Delta u, \Delta u)/(\omega, S\omega)\) must be satisfied, where \(H_{\Omega}\) denotes the overall damping introduced by the model in the (small) part of the domain \(\Omega\). Additionally, the dynamics of the large scales should not be significantly affected by the (small) scales contained within the domain \(\Omega\), i.e. \((\omega, S\omega) < 0\). Hence, to confine the dynamics of the small scales suffices to modify the previous inequality by simply taking the absolute value of its right-hand-side. Then, from Eq.(7) and noticing that

\[
\lambda_{\Delta} \leq t \Omega = \max \left\{ v ||\Delta u||^2/||\tilde{R}||, 1 \right\}. \tag{10}
\]

This differential operator satisfies a list of desirable properties. Namely, it automatically switches off \((R \to 0)\) for laminar flows (no vortex-stretching), 2D flows \((\lambda_{\Delta} = 0 \to R = 0)\) and in the wall (the near-wall behavior of the invariants is \(R \propto y^4\) and \(Q \propto y^0\), where \(y\) is the distance to the wall). Notice that these features would be automatically inherit by any type of model based on this differential operator.

2.1. Regularization modeling

Following the same notation than in [4], the action of a regularization model within the (small) part of the domain \(\Omega\) (see above) can be approximated as follows

\[
(\omega, C(\omega, u)) \approx f_{\Omega}(\omega, C(\omega, u)), \tag{11}
\]

where the damping factor, \(f_{\Omega}\), depends on the specific regularization method and the kernel of the filter (see [4, 5], for details). Hence, the criterion proposed in Eq.(10) can be applied for regularization modeling equating \(f_{\Omega}\) and \(H_{\Omega}\), i.e.

\[
f_{\Omega} = H_{\Omega} = \min \left\{ v ||\Delta u||^2/||\tilde{R}||, 1 \right\}. \tag{12}
\]

For implementation details the reader is referred to [5].

2.2. Towards a simple LES

An eddy-viscosity model, \(\tau(\overline{u}) = -2\nu S(\overline{u})\), adds the dissipation term \((\nabla\omega, \nu_{\varepsilon} \nabla\omega)\) to the enstrophy equation. Then, the eddy-viscosity, \(\nu_{\varepsilon}\), would result from a simple balance in order to prevent the local intensification of vorticity, \(||\omega||^2 \leq 0\),

\[
\nu_{\varepsilon} = \max \left\{ \frac{4||\tilde{R}|| - v ||\Delta \overline{u}||^2}{||\Delta \overline{u}||^2}, 0 \right\}. \tag{13}
\]
This analysis can be extended further for other differential operators. For instance, \( \tau'(\overline{u}) = 2\nu' S(\Delta \overline{u}) \) and \( \tau''(\overline{u}) = -2\nu'' S(\Delta \overline{u}) \), where \( \Delta^2 \equiv \Delta \Delta \) is the bi-Laplacian, lead to the following hyperviscosity terms in the enstrophy equation

\[
-(\nabla \omega, \nu' \nabla \Delta \overline{\omega}) \quad \text{and} \quad (\nabla \omega, \nu'' \nabla \Delta^2 \overline{\omega}),
\]

(14)

Then, following similar reasonings, \( \nu' \) and \( \nu'' \) follow

\[
\nu' = \max \left\{ \frac{4|\Delta| - \nu\|\Delta \omega\|^2}{-(\Delta \overline{\omega}, \Delta^2 \overline{\omega})}, 0 \right\} \quad \text{and} \quad \nu'' = \max \left\{ \frac{4|\Delta| - \nu\|\Delta \omega\|^2}{\|\Delta^2 \overline{\omega}\|^2}, 0 \right\}.
\]

(15)

It is noticeable that, apart from the computation of \( R \), all these models can be straightforwardly implemented by simply re-using the discrete diffusive operator.

### 3. Numerical methods for eddy-viscosity models for LES

The incompressible NS equations (1) with constant physical properties are discretized on a staggered grid using a fourth-order symmetry-preserving discretization [7]. Doing so, the symmetry properties of the underlying differential operators are preserved: the convective operator, \( C(u_s) \), 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, \( u_s \in \mathbb{R}^m \), is governed by the following operator-based finite-volume discretization of Eqs.(1)

\[
\Omega_s \frac{d u_s}{dt} + C(u_s) u_s + D u_s - M^T p_s = 0_s, \quad M u_s = 0_c,
\]

(16)

where \( p_s \in \mathbb{R}^n \) 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 [7]. The resulting convective matrix, \( C(u_s) \in \mathbb{R}^{m \times m} \), is skew-symmetric, \( i.e. C(u_s) + C^T(u_s) = 0 \). The skew-symmetry of \( C(u_s) \) implies that

\[
C(u_s) v_s \cdot w_s = v_s \cdot C^T(u_s) w_s = -v_s \cdot C(u_s) w_s,
\]

(17)

for any discrete velocity vectors \( u_s \) (if \( Mu_s = 0_c \), \( v_s \), and \( w_s \)). Then, the evolution of the discrete energy, \( \|u_s\|^2 = u_s \cdot \Omega_s u_s \), is governed by

\[
\frac{d}{dt} \|u_s\|^2 = -u_s \cdot (D + D^T) u_s < 0,
\]

(18)

where the convective and the pressure gradient contributions cancel because of Eq.(17) and the incompressibility constraint, \( Mu_s = 0_c \), 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.

#### 3.1. 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, \( \nu_e \), is not constant neither on space and time. To obtain the Eq.(1) (with \( \nu \) replaced by \( \nu + \nu_e \)) from Eqs.(2)-(3) with constant \( \nu_e \), notice that \( 2\nabla \cdot S(u) = \nabla \cdot \nabla u + \nabla \cdot (\nabla u)^T \) and recall the vector calculus identity \( \nabla \cdot (\nabla u)^T = \nabla (\nabla \cdot u) \) to cancel out the second term. However, for non-constant \( \nu_e \), the discretization of \( \nabla \cdot (\nu_e (\nabla u)^T) \) needs to be addressed. This can be quite cumbersome especially for staggered formulations.

The standard approach consists on discretizing the term \( \nabla \cdot (\nu_e (\nabla u)^T) \) directly. However, this implies many *ad hoc* interpolations that tends to smear the eddy-viscosity, \( \nu_e \). This may (negatively?) influence the performance of
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.(20) can be discretized as follows
\[
-M^T \Omega_c^{-1} \tilde{M}_s, \quad \text{where} \quad \tilde{[u]}_f = [v_s]_f, \quad (21)
\]
where \( \Omega_c \in \mathbb{R}^{n \times n} \) is a diagonal matrix containing the sizes of the cell-centered control volumes and \([v_s]_f \) is the value of \( v_s(x,t) \) evaluated at the face \( f \). This term, like the continuous counterpart, (i) vanishes for constant \( v_s \) (\( \tilde{M}_s = v_s \tilde{M}_s = \tilde{0}_s \)) and (ii) its contribution to the total kinetic energy is also null (\( u_s^T M^T \Omega_c^{-1} \tilde{M}_s = (\tilde{M}_s)^T \Omega_c^{-1} \tilde{M}_s = 0 \)). Regarding the second term, \( C(\tilde{u}, \nabla v_c) \), it can be discretized as follows
\[
C(\tilde{u}, (-\Omega_c^{-1} M^T v_c)), \quad (22)
\]
where \( v_c \in \mathbb{R}^n \) is a cell-centered vector containing the values of \( v_c(x,t) \). In this case, it also vanishes for constant \( v_c \) (\( M^T v_c = v_c M^T I_s = \tilde{0}_s \)). We can conclude that the alternative form given in Eq.(20) discretized by the expressions given in (21) and (22) is a consistent discretization of the term \( \nabla \cdot (v_c (\nabla u)^T) \) without introducing new discrete operators. Moreover, in the case with constant \( v_c \) these two terms vanish. In summary, combining Eqs.(21) and (22), the term \( \nabla \cdot (v_c (\nabla u)^T) \) can be discretized as follows
\[
\frac{-M^T \Omega_c^{-1} \tilde{M}_s - C(\tilde{u}, (-\Omega_c^{-1} M^T v_c))}{\approx \nabla \cdot \nabla (v_c)} \approx C(\tilde{u}, \nabla v_c) \quad (23)
\]
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.(23) 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 have already been presented in [8] (see also Figure 1, left). Moreover, the computational costs of evaluating Eq.(20) can be significantly reduced by simply ignoring the first-term in the right-hand-side, \( \nabla (\nabla \cdot (v_c u)) \).

Since it is a gradient of a scalar field, this term can be absorbed into the pressure, \( \pi = p - \nabla \cdot (v_c u) \).

4. Concluding remarks and future research

A family of new differential operators for turbulence modeling has been derived by considering the balance between the vortex-stretching contribution and the dissipation in the enstrophy equation. They are suitable to be used for both regularization and LES modeling. In the context of LES, three eddy-viscosity-type models have been obtained. Namely, (i) \( \tau(\tilde{u}) = -2v_s \tilde{S}(\tilde{u}) \), (ii) \( \tau'(\tilde{u}) = 2v'_s \tilde{S}(\Delta \tilde{u}) \) and (iii) \( \tau''(\tilde{u}) = -2v''_s \tilde{S}(\Delta^2 \tilde{u}) \), where \( v_s, v'_s \) and \( v''_s \) are given by Eqs.(13) and (15), respectively. They can be related with already existing approaches. Firstly, the model (i) is almost the same than the recently proposed \( QR \)-model [6]. Essentially, they only differ on the calculation of the diffusive contribution to the enstrophy equation: instead of making use of the equality (9) it is bounded by means of the inequality (8), therefore, the eddy-viscosity is given by \( v_s \propto \lambda_4^\Delta |\tilde{R}|/Q \) instead of Eq.(13). Regarding the models (ii) and (iii) they can be respectively related to the well-known small-large and small-small variational multiscale methods [10] by noticing that \( u'' = -e^2/24 \Delta u + O(e^4) \). All these models switch off (\( R \to 0 \)) for laminar (no vortex-stretching), 2D flows (\( \lambda_3 = 0 \to R = 0 \)) and near the wall (\( R \propto y^3 \)). To test the performance of these new turbulence models is part of our research plans. In particular, we plan to test them for a turbulent flow through a square duct at \( Re = 1200 \) (see Figure 1, right) by means of direct comparison with the DNS results presented in a companion paper [9]. Shortly, the dimensions of the computational domain are \( 2\pi \times 1 \times 1 \) in the stream-wise and wall-normal
directions, respectively. With regard to the numerical methods, the incompressible NS equations have been discretized by a fourth-order symmetry preserving discretization [7], whereas the time-integration method is a second-order fully-explicit one-leg scheme [11]. We have used a $640 \times 518 \times 518$ staggered grid to cover the computational domain and it has been carried out using 392 CPUs on the MareNostrum supercomputer. The code makes use of a two-level hybrid MPI+OpenMP parallelization strategy with an OpenCL-based extension for its use on GPGPU architectures. Parallelization issues and implementation details are presented and discussed in the companion paper [12].

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