



Statistical behavior of the orthogonal subgrid scale stabilization terms in the finite element large eddy simulation of turbulent flows



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ABSTRACT

Numerical simulations have proved that Variational Multiscale Methods (VMM) perform well as pure numerical large eddy simulation (LES) models. In this paper we focus on the orthogonal subgrid scale (OSS) finite element method and make an analysis of the statistical behavior of its stabilization terms in the quasi static approximation. This is done by resorting to results from classical statistical fluid mechanics concerning two point velocity, pressure and combined correlation functions of various orders. Given a fine enough mesh with characteristic element size h in the inertial subrange of a turbulent flow, it is shown that the rate of transfer of subgrid kinetic energy provided by the OSS stabilization terms does not depend on h and that it equals the molecular physical dissipation rate (up to a dimensionless constant that only depends on the finite element shapes) for a proper redesign of the standard parameters of the formulation. This is a noteworthy fact taking into account that the subgrid stabilization terms do not arise from physical considerations, but from the mathematical necessity to allow equal interpolation for the pressure and velocity fields, as well as to control convection. Therefore, the obtained results contribute somehow to the line of reasoning supporting that pure numerical approaches (i.e., without introducing additional physical models) could probably suffice in the LES simulation of turbulent flows.

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1. Introduction

Two parallel lines have been followed in the past years to simulate incompressible turbulent flows that can be of engineering interest. On the one side, the drawbacks of RANS (Reynolds Averaged Navier–Stokes) models combined with the impossibility to perform DNS (Direct Numerical Simulation) computations for large Reynolds number problems led to the development of LES (large eddy simulation) strategies (see e.g., [1]). On the other side, the numerical problems that arise when trying to solve the discrete differential or weak versions of CDR (Convection–Diffusion–Reaction) equations have motivated the development of several stabilization strategies to mitigate them. A landmark in the development of these stabilization methods was the appearance of the *subgrid scale* stabilization approach or, as originally termed, the *variational multiscale* method (VMM), in the framework of finite element methods [2,3]. Both approaches, LES and VMM applied to fluid dynamics, share some features like being based on a scale decomposition of the continuous velocity and pressure fields of the Navier–Stokes equations. However, in the former case this scale

separation is performed at the continuous level, whilst in the latter case it is inherently carried out in the discretization process. The relation between both methods is not fully understood at present and it is not clear whether they should be used together or independently in the simulation of turbulent flows. As it will be detailed below, in this paper we aim at gaining some further insight on this connection through the analysis of the statistical behavior of the VMM stabilization terms. In particular, the subgrid scale terms of the quasi-static approximation in the Orthogonal Subgrid Scale (OSS) finite element method will be considered [4].

In conventional LES the scale decomposition between large and small flow scales has been traditionally performed by means of a filtering process (see e.g., [5–7]) defined through a convolution operation. The filter is applied to the Navier–Stokes equations usually assuming that it commutes with the differential operators and a new equation for the filtered velocity and pressure fields is derived. However, this equation contains the divergence of the so-called *residual stress* tensor that depends on the exact velocity field. This term has to be modeled somehow to obtain a closed system of equations only depending on filtered quantities. Once a physical LES model is chosen, the resulting filtered equation is finally discretized and solved.

This standard LES approach suffers from several mathematical difficulties such as knowing the error introduced when the filtering and differentiation operators are assumed to commute

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[8], knowing which should be the appropriate choice for the LES boundary conditions and, what is probably more important, knowing which is the relation between the errors introduced by the physical LES model and by the discretization procedure. Some of these subjects have received recent attention both from analytical (see e.g., [9,10]) and numerical points of view (see e.g., [11–15]). In [16] a review of several LES models was performed and some interesting conclusions were drawn out, such as the fact that filtering is not indispensable to achieve LES models, that aiming at an exact closure for the residual stress tensor is a paradoxical program and that some LES models have the remarkable propriety of being more regular than the original Navier–Stokes equations, leading to problems for which uniqueness of solutions can be proved. In this sense, it was concluded that a LES model should fulfill with two main requisites, namely, it should regularize the Navier–Stokes equations yielding to well-posed problems and it should lead to *suitable* weak solutions (i.e., physically acceptable solutions). In an attempt to provide a first step towards a mathematical definition of LES, the notion of *suitable approximations* to the Navier–Stokes equations was then introduced in [17]. In this context, it is worthwhile mentioning that a DNS using the Galerkin method with low order finite elements constitutes a suitable approximation to the Navier–Stokes equations, which may justify the fact that sometimes better results are achieved for low-order methods when no LES model is employed [18].

In the VMM or subgrid scale approach to solve turbulent flows, the scale separation is carried out by means of a projection onto the finite element space. Two equations are then obtained respectively governing the dynamics of the large and small scales. Large scales are those that can be captured by the computational mesh, while small or subgrid scales are those not captured by the mesh. Modeling takes place when giving an approximated solution for the subgrid scales equation, which is to be inserted in the large scale equation to account for its effects. One could then view the VMM method as an alternative approach to simulate large eddies in turbulent flows, giving place to pure *numerical* LES in contrast to traditional or *physical* LES. However, in what concerns terminology and unless otherwise specified, throughout this work we will generally use the plain acronym LES to refer to conventional or physical LES, which involves filtering and finding a closure for the residual stress tensor. As far as the authors know, the possibility of using a VMM model as a numerical LES approach was originally proposed in [4] and applied successfully for the first time in [19].

It should be noted that the initial motivation of the VMM method was to solve some of the numerical problems associated with the simulation of the discrete Navier–Stokes equations, such as the necessity to satisfy the *inf-sup* condition (which implies the use of different interpolation spaces for the velocity and pressure fields) or the numerical instabilities appearing for convective dominated flows. Consequently, when the VMM was first applied to the simulation of turbulent flows a physical LES model (Smagorinsky’s model) was still included, although solely acting on the subgrid scale equation [20–22]. As mentioned above, the idea that the stabilization terms in the VMM approach could be sufficient to simulate turbulent flows was already pointed out in the framework of orthogonal subgrid scale (OSS) stabilization methods [4] (see also [23]) as a natural extension to that work. Later it was re-introduced in [24,25] and further elaborated in [26]. A quite definite step supporting the approach has been the very good results obtained in the simulation of various turbulence benchmark problems such as isotropic turbulence, turbulent channel flows or surface mounted objects, with the sole use of numerical stabilization (see [19] and also [27–30]). Actually, to the best of our knowledge, this “numerical” line of thinking initiated with the MILES (Monotone Integrated LES) approach [31] c.f. [15] (see also [1

and references therein). We shall come back to this point in Section 5.

In this paper we aim at analyzing the relation between pure *numerical* LES based on the VMM formulation and *physical* LES from a different perspective. We would like to make use of *existing* statistics [32] for isotropic turbulence and check how the stabilization terms of the quasi-static OSS method [33,34,4] behave according to them. For a fine enough computational mesh so that its characteristic element size h lies in the inertial subrange of a turbulent flow, we make use of the two point correlation functions of various orders for the pressure and velocity fields, as well as for their combination. To do so we assume that the finite element OSS solution is close at the nodes to the interpolant, which is reasonable, so that the statistics for the exact velocity and pressure fields also apply to the OSS solution. The analysis will reveal that the contribution to the energy balance equation from the OSS stabilization terms are proportional to the physical dissipation rate and independent of h to dominant order, for an appropriate redesign of the formulation parameters. Therefore, the OSS method satisfies an important point a closure LES model requires, namely that the rate of kinetic energy transferred from the filtered large scales to the small ones is proportional to the physical dissipation rate at the Kolmogorov length scale (see e.g., [35,36]). The property described is a noteworthy fact given that the stabilization terms arise in the discrete weak Navier–Stokes equations from purely numerical considerations regarding stability issues, so there is no a priori need for them to behave in the appropriate physical way. Besides, we would like to remark that the forthcoming results are not to be confused with a mere scaling analysis. Many numerical strategies include stabilization terms, which are obviously dimensionally correct, but this does not imply that they can be related to existing turbulence statistics that support their behavior in the inertial subrange.

The paper is organized as follows. In Section 2 the energy balance equations for the continuous Navier–Stokes and LES problems are presented together with their discrete counterparts using the Galerkin and OSS finite element methods. The problem we would like to address is established and the OSS terms accounting for the transfer of kinetic energy to subscales that should be proportional to the physical dissipation rate are identified. In Section 3 we proceed to the explicit discretization of these terms, showing that their ensemble average can be written as products of geometrical factors multiplying two point second and fourth-order nodal velocity correlations, second order pressure correlations and triple-order velocity–pressure correlations. In Section 4, results from statistical fluid mechanics are used to relate these correlations to the physical dissipation rate, which is the main goal of the paper. Some general comments and remarks, together with references to numerical experiments supporting the pure numerical approach to solve turbulent flows are given in Section 5. Conclusions are finally drawn in Section 6.

2. Energy balance equations

2.1. Energy balance equation for the Navier–Stokes problem

The strong formulation of the Navier–Stokes equations problem consists in solving their differential version in a given domain $\Omega \subset \mathbb{R}^d$ (where $d = 2, 3$ is the number of space dimensions) with boundary $\partial\Omega$ and prescribed initial and boundary conditions. We will only consider homogeneous Dirichlet conditions on the boundary ($\partial\Omega \equiv \Gamma_D$) for simplicity and use the conservative form of the equations. Throughout the work we will concentrate on the three dimensional case ($d = 3$). The problem to be solved then reads

$$\partial_t \mathbf{u} - 2\nabla \cdot [\nu \mathbf{S}(\mathbf{u})] + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + \nabla p = \mathbf{f} \quad \text{in } \Omega \times (0, T), \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \times (0, T), \quad (2)$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad \text{in } \Omega, t = 0, \quad (3)$$

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{0} \quad \text{on } \Gamma_D \times (0, T), \quad (4)$$

where \mathbf{u} stands for the flow velocity, p for the pressure, ν represents the kinematic fluid viscosity (taken constant hereafter), $\mathbf{S}(\mathbf{u}) := \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ the rate of strain tensor, \mathbf{f} the external force and $(0, T)$ is the time interval of analysis.

Use is made of the following notation to introduce the weak form associated to problem (1)–(4). $L^p(\Omega)$ designates the spaces of functions whose p power ($1 \leq p < \infty$) is integrable in Ω , with $p = \infty$ corresponding to the space of bounded functions in Ω . For $p = 2$ we have a Hilbert space with scalar product

$$(\mathbf{u}, \mathbf{v}) := \int_{\Omega} \mathbf{u}(\mathbf{x}) \mathbf{v}(\mathbf{x}) d\Omega \quad (5)$$

and induced norm $\|\mathbf{u}\|_{L^2(\Omega)} \equiv \|\mathbf{u}\| = (\mathbf{u}, \mathbf{u})^{1/2}$. From a physical point of view, $L^2(\Omega)$ can be identified with the space of velocity fields with bounded kinetic energy, given that $\|\mathbf{u}\|^2 = 2E(\mathbf{u})$, with $E(\mathbf{u})$ standing for the kinetic energy per unit mass.

$H^m(\Omega)$ denotes the space of functions whose distributional derivatives up to order m lay in $L^2(\Omega)$. The case $m = 1$ is of special interest as it is also a Hilbert space and can be physically identified with the space of velocity and vorticity fields having bounded energy and enstrophy [37]. On the other hand, $H_0^1(\Omega)$ stands for the functions in $H^1(\Omega)$ vanishing on Γ_D . $H^{-1}(\Omega)$ denotes the topological dual of $H_0^1(\Omega)$ and the brackets, $\langle \cdot, \cdot \rangle$, will be used for the duality pairing between these spaces or, more generally, for the integral of the product of two functions in Ω . A subscript ω will be used if this integral is performed in a subdomain $\omega \subset \Omega$. $\|\cdot\|_X$ designates the norm in a Banach space, X , and $L^p(0, T; X)$ is the space of time dependent functions such that their X -norm is $L^p(0, T)$. A bold character is used for the vector counterpart of all these spaces.

The weak form of problem (1)–(4) can be formulated as: find $[\mathbf{u}, p] \in \mathbf{L}^2(0, T; \mathbf{H}_0^1(\Omega)) \times \mathcal{D}'(0, T; L^2(\Omega)/\mathbb{R})$ (\mathcal{D}' being the space of distributions) such that

$$(\partial_t \mathbf{u}, \mathbf{v}) + 2\nu(\mathbf{S}(\mathbf{u}), \mathbf{S}(\mathbf{v})) + \langle \nabla \cdot (\mathbf{u} \otimes \mathbf{u}), \mathbf{v} \rangle - (p, \nabla \cdot \mathbf{v}) = (\mathbf{f}, \mathbf{v}), \quad (6)$$

$$(q, \nabla \cdot \mathbf{u}) = 0 \quad (7)$$

for all $[\mathbf{v}, q] \in \mathbf{H}_0^1(\Omega) \times L^2(\Omega)/\mathbb{R}$, and satisfying the initial condition in a weak sense.

For each $t \in (0, T)$, setting $\mathbf{v} = \mathbf{u}$, $q = p$ in (6), (7) and taking into account that we have limited the analysis to homogeneous Dirichlet boundary conditions, we obtain the energy balance equation

$$\frac{d}{dt} \left(\frac{1}{2} \|\mathbf{u}\|^2 \right) = -2\nu \|\mathbf{S}(\mathbf{u})\|^2 + (\mathbf{f}, \mathbf{u}). \quad (8)$$

Eq. (8) states that the time variation of the flow kinetic energy depends on two factors, namely, the molecular dissipation due to viscosity (which is clearly negative) and the power exerted by the external force that can be either positive or negative. Identifying the pointwise kinetic energy as $k := \mathbf{u} \cdot \mathbf{u}/2$, the pointwise molecular dissipation as $\varepsilon_{\text{mol}} := 2\nu[\mathbf{S}(\mathbf{u}) : \mathbf{S}(\mathbf{u})]$ and the pointwise power of the external force as $P_f := \mathbf{f} \cdot \mathbf{u}$, we can rewrite (8) as

$$\int_{\Omega} \frac{dk}{dt} d\Omega = - \int_{\Omega} \varepsilon_{\text{mol}} d\Omega + \int_{\Omega} P_f d\Omega. \quad (9)$$

According to the Kolmogorov description of the energy cascade in turbulent flows [38] cf. [36], the flow can be viewed as driven by the external forces acting at the large scales (low wave numbers) and generating kinetic energy, which is transferred to the low scales (high wave numbers) by non-linear processes. When the

Kolmogorov length is reached, the viscous dissipation, ε_{mol} , in the r.h.s of (9) takes part transforming the flow kinetic energy into internal energy (heat is released).

2.2. Energy balance equation for a large eddy simulation model

In the standard large eddy simulation (LES) of turbulent flows, a scale separation between large and small scales for the velocity and pressure fields in the Navier–Stokes equations is carried out. As commented in the Introduction, this has been done traditionally by means of a convolution of the latter fields with a low pass filter operator, $(\bar{\cdot}) : v \mapsto \bar{v}$, so that the decomposition $[\mathbf{u}, p] = [\bar{\mathbf{u}}, \bar{p}] + [\mathbf{u}', p']$ is obtained (see e.g., [5] cf. [36,1]). $[\bar{\mathbf{u}}, \bar{p}]$ stands for the large, filtered, scales while $[\mathbf{u}', p']$ represent the small, residual, scales.

Without getting into details on the type of filter used for the scale separation and assuming that the filtering operator commutes with differentiation (although this will be certainly a source of errors [39,40,8]), the following differential problem is obtained for the filtered velocity and pressure fields $[\bar{\mathbf{u}}, \bar{p}]$:

$$\partial_t \bar{\mathbf{u}} - 2\nabla \cdot [\nu \mathbf{S}(\bar{\mathbf{u}})] + \nabla \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) + \nabla \bar{p} = \mathbf{f} - \nabla \cdot \mathcal{R} \quad \text{in } \Omega \times (0, T), \quad (10)$$

$$\nabla \cdot \bar{\mathbf{u}} = 0 \quad \text{in } \Omega \times (0, T), \quad (11)$$

$$\bar{\mathbf{u}}(\mathbf{x}, 0) = \bar{\mathbf{u}}_0(\mathbf{x}) \quad \text{in } \Omega, t = 0, \quad (12)$$

$$\bar{\mathbf{u}}(\mathbf{x}, t) = \mathbf{0} \quad \text{on } \Gamma_D \times (0, T), \quad (13)$$

which is analogous to (1)–(4) except for the divergence of the tensor \mathcal{R} appearing in the r.h.s of (10). The tensor $\mathcal{R} := \bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}$ is usually named the *residual stress tensor* or the *subgrid scale tensor* and an expression for it in terms of $\bar{\mathbf{u}}$ is needed to close the system of Eqs. (10)–(13). The different options for \mathcal{R} give place to different LES models.

The weak formulation of problem (10)–(13) can be stated as: find $[\bar{\mathbf{u}}, \bar{p}] \in \mathbf{L}^2(0, T; \mathbf{H}_0^1(\Omega)) \times \mathcal{D}'(0, T; L^2(\Omega)/\mathbb{R})$ such that

$$(\partial_t \bar{\mathbf{u}}, \mathbf{v}) + 2\nu(\mathbf{S}(\bar{\mathbf{u}}), \mathbf{S}(\mathbf{v})) + \langle \nabla \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}), \mathbf{v} \rangle - (\bar{p}, \nabla \cdot \mathbf{v}) = (\bar{\mathbf{f}}, \mathbf{v}) + \langle \mathcal{R}, \nabla \mathbf{v} \rangle, \quad (14)$$

$$(q, \nabla \cdot \bar{\mathbf{u}}) = 0 \quad (15)$$

for all $[\mathbf{v}, q] \in \mathbf{H}_0^1(\Omega) \times L^2(\Omega)/\mathbb{R}$, and satisfying the initial condition in a weak sense. Taking into account that \mathcal{R} is symmetric, we can rewrite the second term in the r.h.s of (14) as $\langle \mathcal{R}, \nabla \mathbf{v} \rangle = \langle \mathcal{R}, \mathbf{S}(\mathbf{v}) \rangle$. In addition, and without loss of generality, we will consider \mathcal{R} deviatoric, its volumetric part being absorbed in the pressure term.

Assuming again continuity in time, if we next set $\mathbf{v} = \bar{\mathbf{u}}$, $q = \bar{p}$, for each $t \in (0, T)$ in 14,15 we can obtain an energy balance for the filtered Navier–Stokes equations:

$$\frac{d}{dt} \left(\frac{1}{2} \|\bar{\mathbf{u}}\|^2 \right) = -2\nu \|\mathbf{S}(\bar{\mathbf{u}})\|^2 + \langle \mathcal{R}, \mathbf{S}(\bar{\mathbf{u}}) \rangle + (\bar{\mathbf{f}}, \bar{\mathbf{u}}). \quad (16)$$

We can now define the filtered pointwise kinetic energy $\bar{k} := \bar{\mathbf{u}} \cdot \bar{\mathbf{u}}/2$, the pointwise filtered molecular dissipation $\bar{\varepsilon}_{\text{mol}} := 2\nu[\mathbf{S}(\bar{\mathbf{u}}) : \mathbf{S}(\bar{\mathbf{u}})]$, the rate of production of residual kinetic energy $\bar{\mathcal{P}}_r := -\mathcal{R} : \mathbf{S}(\bar{\mathbf{u}})$ and the pointwise power of the external filtered force $\bar{P}_f := \bar{\mathbf{f}} \cdot \bar{\mathbf{u}}$, so that we can rewrite (16) as

$$\frac{d}{dt} \int_{\Omega} \bar{k} d\Omega = - \int_{\Omega} \bar{\varepsilon}_{\text{mol}} d\Omega - \int_{\Omega} \bar{\mathcal{P}}_r d\Omega + \int_{\Omega} \bar{P}_f d\Omega. \quad (17)$$

For a fully developed turbulent flow with the filter width in the inertial subrange, the filtered field accounts for almost all the kinetic energy of the flow. Thus, $\int_{\Omega} \bar{k} d\Omega \approx \int_{\Omega} k d\Omega$ and the first terms in (9) and (17) become nearly equal. If the external force mainly acts on the large scales of the flow, it will also happen that $\int_{\Omega} \bar{P}_f d\Omega \approx \int_{\Omega} P_f d\Omega$. On the other hand, the energy dissipated by the filtered field, $\bar{\varepsilon}_{\text{mol}}$ is relatively small and can be neglected [36]. Consequently, comparing Eq. (17) with Eq. (9), we observe

that in order for the LES model to behave correctly it should happen that $\int_{\Omega} \bar{\mathcal{P}}_r d\Omega \approx \int_{\Omega} \varepsilon_{\text{mol}} d\Omega$. That is, the rate of production of residual kinetic energy should equal, in the mean, the energy dissipated by viscous processes at the very small scales (Kolmogorov length), which is the point of view expressed by Lilly [35].

In the case of some celebrated LES models, such as the Smagorinsky model [41], $\bar{\mathcal{P}}_r$ is always positive and there is no backscatter, i.e., the energy is always transferred from the filtered scales to the residual ones, but not vice versa. It is quite customary then to term $\bar{\mathcal{P}}_r$ as *subgrid or residual dissipation* and to denote it by ε_{SGS} , see e.g., [15]. However, this may lead to confusion, especially when introducing the discrete stabilized numerical version of the original and filtered Navier–Stokes equations, so we will keep the notation $\bar{\mathcal{P}}_r$ in this work.

2.3. Energy balance equations in discrete problems: stabilized numerical approach of the original and filtered Navier–Stokes equations

2.3.1. Galerkin finite element approach

Consider a partition $\{\Omega_e\}$ of the computational domain, with e ranging from 1 to the number of elements n_e . Let $\mathcal{V}_{0,h} \subset H_0^1(\Omega)$, and $\mathcal{V}_{0,h}^d$ the vector counterpart. The Galerkin finite element approximation to problem (6) and (7) can be stated as: given the finite dimensional spaces $\mathcal{V}_{0,h}^d \subset \mathbf{H}_0^1(\Omega)$ and $\mathcal{Q}_{0,h} \subset L^2(\Omega)/\mathbb{R}$, find $[\mathbf{u}_h(t), p_h(t)] \in \mathbf{L}^2(0, T; \mathcal{V}_{0,h}^d) \times \mathcal{D}(0, T; \mathcal{Q}_{0,h})$ such that

$$\begin{aligned} (\partial_t \mathbf{u}_h, \mathbf{v}_h) + 2\nu(\mathcal{S}(\mathbf{u}_h), \mathcal{S}(\mathbf{v}_h)) + \langle \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h), \mathbf{v}_h \rangle \\ - (p_h, \nabla \cdot \text{bf } \mathbf{v}_h) = (\mathbf{f}, \mathbf{v}_h), \end{aligned} \quad (18)$$

$$(q_h, \nabla \cdot \mathbf{u}_h) = 0 \quad (19)$$

for all $[\mathbf{v}_h, q_h] \in \mathcal{V}_{0,h}^d \times \mathcal{Q}_{0,h}$.

Note that Eqs. (18) and (19) are still continuous in time. However, for the developments to be presented hereafter time discretization will be not required, so no explicit expression for it will be given. Anyway, and whichever time discrete scheme is used, it is well known that the Galerkin finite element approach (18) and (19) presents several difficulties. On the one hand, numerical instabilities are encountered when the non-linear convective term in the equation dominates the viscous one at high Reynolds number problems. On the other hand, a compatibility condition (*inf-sup* or *LBB* condition) is required to control the pressure term. This condition does not allow to use equal order interpolations to approximate the velocity and pressure fields.

Several stabilization strategies have been developed to circumvent the above numerical instabilities of the Galerkin finite element solution to the Navier–Stokes equations. As mentioned in the introduction, we will concentrate here on the *subgrid scale* approach (also termed *variational multiscale method* or *residual-based stabilization*) originally developed by Hughes [2,3] for the scalar convection–diffusion–reaction equation, and latter extended to other equations by many authors. In particular we will focus on the orthogonal subgrid scale (OSS) approach developed in [33,34,4,23], with quasi-static subscales.

2.3.2. Orthogonal subgrid scale stabilization

The subgrid scale finite element stabilization method applied to the present problem consists in first splitting the continuous spatial spaces where the solution is found as $\mathbf{H}_0^1(\Omega) = \mathcal{V}_{0,h}^d \oplus \tilde{\mathcal{V}}_0^d$ and $L^2(\Omega)/\mathbb{R} = \mathcal{Q}_{h,0} \oplus \tilde{\mathcal{Q}}_0$, with $\tilde{\mathcal{V}}_0^d$ and $\tilde{\mathcal{Q}}_0$ being any infinite dimensional spaces that respectively complete the finite element spaces $\mathcal{V}_{0,h}^d$ and $\mathcal{Q}_{h,0}$ in $\mathbf{H}_0^1(\Omega)$ and $L^2(\Omega)/\mathbb{R}$. The velocity and pressure fields can then be decomposed as $\mathbf{u} = \mathbf{u}_h + \tilde{\mathbf{u}}$ and $p = p_h + \tilde{p}$ (the same holds for the test functions $\mathbf{v} = \mathbf{v}_h + \tilde{\mathbf{v}}, q = q_h + \tilde{q}$).

The weak form of the Navier–Stokes equations can now be split into two systems of equations. This is done by first substituting $\mathbf{u} = \mathbf{u}_h + \tilde{\mathbf{u}}$ and $p = p_h + \tilde{p}$ in (6) and (7) and taking $[\mathbf{v}, q] = [\mathbf{v}_h, q_h]$, which corresponds to projecting (6) and (7) onto

the finite element spaces. Then, a second equation is obtained by projecting (6) and (7) onto the finite element complementary spaces by setting $[\mathbf{v}, q] = [\tilde{\mathbf{v}}, \tilde{q}]$.

After integrating some terms by parts and neglecting terms involving integrals over interelement boundaries, the equation corresponding to the large scales (projection onto the finite element spaces) becomes [4,23],

$$\begin{aligned} (\partial_t \mathbf{u}_h, \mathbf{v}_h) + 2\nu(\mathcal{S}(\mathbf{u}_h), \mathcal{S}(\mathbf{v}_h)) + \langle \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h), \mathbf{v}_h \rangle \\ - (p_h, \nabla \cdot \mathbf{v}_h) + (q_h, \nabla \cdot \mathbf{u}_h) \\ - \sum_e (\tilde{\mathbf{u}}, 2\nu \nabla \cdot \mathcal{S}(\mathbf{v}_h) + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{v}_h) + \nabla q_h)_{\Omega_e} \\ + (\partial_t \tilde{\mathbf{u}}, \mathbf{v}_h) + \langle \nabla \cdot (\tilde{\mathbf{u}} \otimes \mathbf{u}_h), \mathbf{v}_h \rangle \\ + (\tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}}, \mathbf{v}_h) \\ - (\tilde{p}, \nabla \cdot \mathbf{v}_h) = (\mathbf{f}, \mathbf{v}_h), \end{aligned} \quad (20)$$

where \sum_e stands for the sum for all elements. The first two lines of (20) contain the Galerkin terms previously found in (18) and (19). The third line includes terms that are already obtained in the stabilization of the linearized and stationary version of the Navier–Stokes equations [33,34] (Oseen problem). These terms avoid the convection instabilities of the Galerkin formulation and also allow to use equal interpolations for the velocity and the pressure. The first term in the fourth line accounts for the time derivative of the subscales, while the second term provides global momentum conservation [23]. The term in the fifth line has a quadratic dependence on the velocity subscales. Although it can play a role in the simulation of turbulence [23] it will be neglected in this work. This is so for two reasons. The first one is practical given that the term yields expressions for which no statistical results are known. The second is that it is argued in [24] that this term has very little influence on the results. Neglecting the fifth line in (20) constitutes one of the simplifying hypotheses of our work. Finally, the term in the sixth line accounts for the effects of the pressure subscales.

To solve (20) we need some expressions for the velocity and pressure subscales $[\tilde{\mathbf{u}}, \tilde{p}]$. These expressions can be found from the solution of the small subgrid scales equation (projection onto the finite element complementary spaces). Given that the latter equation cannot be solved exactly, an approximation for its solution is required. The different ways in how this approximated solution is obtained give place to different subgrid scale stabilization models. We will use here the orthogonal subgrid scale (OSS) approach, which is based on choosing the spaces orthogonal to the finite element ones as the complimentary spaces in the above formulation. Moreover *quasi-static* subscales will be considered, leading to the approximation [33,34]:

$$\tilde{\mathbf{u}} \approx \tau_1 \mathbf{r}_{u,h}, \quad (21)$$

$$\tilde{p} \approx \tau_2 r_{p,h}, \quad (22)$$

where $\mathbf{r}_{u,h}$ and $r_{p,h}$ represent the orthogonal projection of the residuals of the finite element components \mathbf{u}_h and p_h

$$\begin{aligned} \mathbf{r}_{u,h} &= -\Pi_h^\perp [\partial_t \mathbf{u}_h - 2\nu \nabla \cdot \mathcal{S}(\mathbf{u}_h) + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h - \mathbf{f}] \\ &= -\Pi_h^\perp [-2\nu \nabla \cdot \mathcal{S}(\mathbf{u}_h) + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h], \end{aligned} \quad (23)$$

$$r_{p,h} = -\Pi_h^\perp [\nabla \cdot \mathbf{u}_h]. \quad (24)$$

Π_h^\perp in the above equations stands for the orthogonal projection, $\Pi_h^\perp := I - \Pi_h$, with I being the identity and Π_h the L^2 projection onto the appropriate finite element space. In fact, the numerical analysis of the stationary and linearized problem is greatly simplified if this projection is weighted elementwise by the stabilization parameters, as shown in [42]. However, this is not essential for the following developments.

In the second line of (23) we have used precisely the fact that, once discretized, $\partial_t \mathbf{u}_h \subset \mathcal{V}_{0,h}^d$. We have also considered that the external force belongs to $\mathcal{V}_{0,h}^d$ i.e., it only acts at the large scales

of the flow in accordance with the simplified vision of the energy cascade presented at the end of Section 2.1. We have also introduced another simplification in the expressions for the velocity residual as only the finite element component has been considered in the advective velocity term. Note, in addition, that no implicit time dependence of the subscales has been considered (*quasi-static* approach). On the other hand, the viscous term in the above equations has to be evaluated elementwise.

Even though we will restrict ourselves to quasi-static subscales because our focus is the dissipation they introduce, let us mention that the *dynamic* approach has interesting properties. From the theoretical point of view, it is shown in [43] that the resulting approximation has the desired long-term behavior for the finite element solution plus additional control on the subscales. In particular, it can be shown that the finite element component belongs to an absorbing set and so does the subscale. For the former, the absorbing case can be shown to be a global attractor in the two-dimensional case. From the physical point of view, dynamic subscales allow one to model backscatter, as shown in [44].

The stabilization parameters appearing in (21) and (22) can be obtained from arguments based on a Fourier analysis for the subscales [4] that yield,

$$\tau_1 = \left[\left(c_1 \frac{v}{h^2} \right)^2 + \left(c_2 \frac{U_{1e}}{h} \right)^2 \right]^{-1/2}, \quad (25)$$

$$\tau_2 = \frac{h^2}{c_1} \left[\left(c_1 \frac{v}{h^2} \right)^2 + \left(c_2 \frac{U_{2e}}{h} \right)^2 \right]^{1/2}, \quad (26)$$

c_1 and c_2 in (25) and (26) are algorithmic parameters with recommended values of $c_1 = 4$ and $c_2 = 2$ for linear elements [45], while h stands for a characteristic mesh element size. U_{1e} and U_{2e} in (25) and (26) stand for some characteristic scalar element velocities, so that τ_1 and τ_2 can be considered constant within each element. U_{1e} and U_{2e} are often given the same value, for instance the mean of the velocity moduli at each element node, though this does not need to be necessarily the case. As it will be shown at the end of Section 4, the choice of U_{1e} and U_{2e} turns to be crucial to achieve the expected behavior of the OSS formulation in the inertial subrange. Besides, note that we have neglected the subscale contribution in the advective velocity of τ_1 . The choice (25) and (26) for the stabilization parameters guarantees that the kinetic energy of the modeled subscales approximates the kinetic energy of the exact subscales [4].

Eq. (20) together with the approximation (21) and (22) for the subscales constitute the proposed numerical approach to solve the incompressible Navier–Stokes equations.

2.3.3. Energy balance for the orthogonal subgrid scale finite element approach to the Navier–Stokes problem

In order to find an energy balance equation for the OSS numerical approach to the Navier–Stokes equations we can now set $\mathbf{v}_h = \mathbf{u}_h$ and $q_h = p_h$ in (20). This yields (no approximation for the subscales is considered for the moment)

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{u}_h\|^2 &= -2\nu \|\mathbf{S}(\mathbf{u}_h)\|^2 - \sum_e \langle \tilde{\mathbf{u}}, 2\nu \mathbf{S}(\mathbf{u}_h) + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) \\ &\quad + \nabla p_h \rangle_{\Omega_e} + \sum_e \langle \tilde{p}, \nabla \cdot \mathbf{u}_h \rangle_{\Omega_e} + \langle \mathbf{f}, \mathbf{u}_h \rangle. \end{aligned} \quad (27)$$

If we now consider the subscales approximation (21)–(24) in (27) we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{u}_h\|^2 &= -2\nu \|\mathbf{S}(\mathbf{u}_h)\|^2 + \langle \mathbf{f}_h, \mathbf{u}_h \rangle - \sum_e \tau_1 (\Pi_h^\perp [-2\nu \nabla \cdot \mathbf{S}(\mathbf{u}_h) \\ &\quad + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h], 2\nu \nabla \cdot \mathbf{S}(\mathbf{u}_h) + \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h)_{\Omega_e} \\ &\quad - \sum_e \tau_2 (\Pi_h^\perp (\nabla \cdot \mathbf{u}_h), \nabla \cdot \mathbf{u}_h)_{\Omega_e}. \end{aligned} \quad (28)$$

Since we are interested in high Reynolds numbers, all the stabilization terms multiplied by the viscosity will be neglected, from where we obtain the following energy balance equation for the OSS stabilized finite element approach to the Navier–Stokes equations:

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{u}_h\|^2 &= -2\nu \|\mathbf{S}(\mathbf{u}_h)\|^2 + \langle \mathbf{f}_h, \mathbf{u}_h \rangle - \sum_e \tau_1 (\Pi_h^\perp [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) \\ &\quad + \nabla p_h], \nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h)_{\Omega_e} \\ &\quad - \sum_e \tau_2 (\Pi_h^\perp (\nabla \cdot \mathbf{u}_h), \nabla \cdot \mathbf{u}_h)_{\Omega_e}. \end{aligned} \quad (29)$$

Let us define the pointwise numerical kinetic energy of the flow as $k^h := \frac{1}{2} \|\mathbf{u}_h\|^2$, the pointwise molecular numerical dissipation for the large scales as $\varepsilon_{\text{mol}}^h := 2\nu \mathbf{S}(\mathbf{u}_h) : \mathbf{S}(\mathbf{u}_h)$ and the pointwise numerical power for the external force as $P_f^h := \mathbf{f}_h \cdot \mathbf{u}_h$. We will also identify $\mathcal{P}_r^{h\tau}$ within each element with

$$\mathcal{P}_r^{h\tau} := \tau_1 \mathcal{P}_r^{h\tau_1} + \tau_2 \mathcal{P}_r^{h\tau_2} \quad (30)$$

where

$$\mathcal{P}_r^{h\tau_1} := \Pi_h^\perp [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h] \cdot [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h], \quad (31)$$

$$\mathcal{P}_r^{h\tau_2} := \Pi_h^\perp (\nabla \cdot \mathbf{u}_h) (\nabla \cdot \mathbf{u}_h). \quad (32)$$

Equipped with these definitions, Eq. (29) can be rewritten as

$$\frac{d}{dt} \int_\Omega k^h d\Omega = - \int_\Omega \varepsilon_{\text{mol}}^h d\Omega - \sum_e \int_{\Omega_e} \mathcal{P}_r^{h\tau} d\Omega_e + \int_\Omega P_f^h d\Omega, \quad (33)$$

which can be compared with the energy balance equation of the continuous problem (9), using similar arguments to those in Section 2.2.

It is clear that k^h will account for nearly the whole pointwise kinetic energy of the flow so that $\int_\Omega k^h d\Omega \approx \int_\Omega k d\Omega$. On the other hand, it will also occur that $\int_\Omega P_f^h d\Omega \approx \int_\Omega P_f d\Omega$, given that the force only acts at the large scales. In addition the numerical molecular dissipation of the large scales will be negligible, so that $\int_\Omega \varepsilon_{\text{mol}}^h d\Omega \approx 0$.

The next, crucial, question is if it should happen that $\sum_e \int_{\Omega_e} \mathcal{P}_r^{h\tau} d\Omega \approx \int_\Omega \varepsilon_{\text{mol}} d\Omega$ for the OSS formulation to be a good numerical approach for the Navier–Stokes equations, in the case of fully developed turbulence. Actually, this should not be necessarily the case for all the terms in $\mathcal{P}_r^{h\tau}$, given that they have arisen in the equation motivated by pure numerical stabilization necessities. However, it would be desirable that at least some of these terms should account for the appropriate physical behavior and that their domain integration should approximate the mean molecular dissipation in (9). It will be the main result of this work to show, by means of heuristic reasoning, that actually the whole $\mathcal{P}_r^{h\tau}$ satisfies this assumption. It should be also noted that in the definition of $\mathcal{P}_r^{h\tau}$, the approximation for high Reynolds number flows was already performed (stabilization terms multiplied by the viscosity have been neglected).

2.3.4. Energy balance for the orthogonal subgrid scale finite element approach to a LES model

We could now proceed to discretize the LES Eqs. (14) and (15) using the OSS approach. The usual way to do so is by simply adding the Navier–Stokes stabilization terms to the Galerkin discretization of the LES equations, i.e., terms containing the residual stress tensor, \mathcal{R} , are not included in the stabilization terms (see e.g., [15]). This approach is in fact non consistent unless linear elements are used. However, in the OSS method this approach still makes sense given that the consistency error becomes optimal (see [42]).

The following discrete energy balance equation for the LES model analogous to (33) is obtained

$$\int_\Omega \frac{d\bar{k}^h}{dt} d\Omega = - \int_\Omega \bar{\varepsilon}_{\text{mol}}^h d\Omega - \sum_e \int_{\Omega_e} \bar{\mathcal{P}}_r^{h\tau} d\Omega_e - \int_\Omega \bar{\mathcal{P}}_r^h d\Omega + \int_\Omega \bar{P}_f^h d\Omega, \quad (34)$$

with $k^h := \frac{1}{2} |\bar{\mathbf{u}}_h|^2$, $\bar{e}_{\text{mol}}^h := 2\nu \mathbf{S}(\bar{\mathbf{u}}_h) : \mathbf{S}(\bar{\mathbf{u}}_h)$, $\bar{P}_r^h := \bar{\mathbf{f}}_h \cdot \bar{\mathbf{u}}_h$, $\bar{P}_r^h := -\mathcal{R} : \mathcal{S}(\bar{\mathbf{u}}_h)$ and the term $\bar{P}_r^{h\tau} := -\sum_e \tau_1 (\Pi_h^{\perp} [\nabla \cdot (\bar{\mathbf{u}}_h \otimes \bar{\mathbf{u}}_h) + \nabla \bar{p}_h] : \nabla \cdot (\bar{\mathbf{u}}_h \otimes \bar{\mathbf{u}}_h) + \nabla \bar{p}_h)_{\Omega_e} - \sum_e \tau_2 (\Pi_h^{\perp} (\nabla \cdot \bar{\mathbf{u}}_h), \nabla \cdot \bar{\mathbf{u}}_h)_{\Omega_e}$. Following the argumentation lines in the above sections it is clear that the kinetic energy term will approximate the one in the exact energy balance Eq. (9). The same will prove true for the external force power and, again, \bar{e}_{mol}^h will be negligible. However, we are now left with the curious fact that the two terms involving $\bar{P}_r^{h\tau}$ and \bar{P}_r^h should equal, in the mean, the molecular physical dissipation. This seems at least redundant if the term containing $\bar{P}_r^{h\tau}$ that arises from the discretization of the original Navier–Stokes equation already presents this behavior. In other words, the process of first filtering at the continuum level, modeling, and then proceeding to discretization (LES method) may look unnecessary if an appropriate numerical discretization scheme is used. Obviously, for an inaccurate discretization scheme the addition of extra dissipation as that provided by LES could be useful, but this should not be the case. In the following sections we aim at giving support to this idea.

3. Numerical subgrid kinetic energy transfer for high Reynolds numbers using the OSS stabilized FEM

3.1. Elemental ensemble average of $\mathcal{P}_r^{h\tau}$ for high Reynolds numbers

3.1.1. Elemental ensemble average of $\mathcal{P}_r^{h\tau_1}$

Let us designate by $\Pi_i^h [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h]$ the i th component of the projector in the definition of the numerical subgrid kinetic energy transfer term $\mathcal{P}_r^{h\tau_1}$ in (31) and denote the i th velocity component by u_{hi} .

We consider a finite element partition of the domain Ω having n_p pressure nodes, n_u velocity nodes and n_e elements. Following similar lines of what is done in [46] (although with a very different objective) we define the average value in a mesh element Ω_e of $\mathcal{P}_r^{h\tau_1}$ in (31) as

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle &= \frac{1}{V_e} \int_{\Omega_e} (\mathcal{P}_r^{h\tau_1}) d\Omega_e \\ &= \frac{1}{V_e} \int_{\Omega_e} \Pi^{h,\perp} [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h] \cdot [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h] d\Omega_e. \end{aligned} \quad (35)$$

An ensemble average (or time average under the ergodic assumption) of this quantity can be performed to obtain

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle = \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h] \cdot [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h) + \nabla p_h] d\Omega_e \right\rangle. \quad (36)$$

(Brackets $\langle \cdot \rangle$ are used in this section to denote ensemble average instead of duality pairing). We next identify the terms $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$, $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$, $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP}$ and $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP}$ in (36) that will be treated independently in the analysis. We have

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU} &:= \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] \cdot [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \partial_i (u_{hi} u_{hj}) \partial_k (u_{hk} u_{hj}) d\Omega_e \right\rangle \\ &\quad - \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi_j^h [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] \partial_k (u_{hk} u_{hj}) d\Omega_e \right\rangle, \end{aligned} \quad (37)$$

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU} &:= \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} (\nabla p_h) \cdot [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \partial_i p_h \partial_j (u_{hj} u_{hi}) d\Omega_e \right\rangle \\ &\quad - \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi_i^h (\nabla p_h) \partial_j (u_{hj} u_{hi}) d\Omega_e \right\rangle, \end{aligned} \quad (38)$$

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP} &:= \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] \cdot \nabla p_h d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \partial_i (u_{hi} u_{hj}) \partial_j p_h d\Omega_e \right\rangle \\ &\quad - \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi_j^h [\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)] \partial_j p_h d\Omega_e \right\rangle \end{aligned} \quad (39)$$

and

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP} &:= \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} (\nabla p_h) \cdot \nabla p_h d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \partial_i p_h \partial_i p_h d\Omega_e \right\rangle \\ &\quad - \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi_i^h (\nabla p_h) \partial_i p_h d\Omega_e \right\rangle. \end{aligned} \quad (40)$$

Above and in the following, summation is understood over spatial repeated indexes.

Obviously, we have

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle = \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP}. \quad (41)$$

3.1.2. Elemental ensemble average of $\mathcal{P}_r^{h\tau_2}$

Proceeding analogously to what has been done in the previous section but for the $\mathcal{P}_r^{h\tau_2}$ term defined in (32), it can readily be checked that the elemental ensemble average of $\mathcal{P}_r^{h\tau_2}$ becomes

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_2} \rangle &:= \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^{h,\perp} (\nabla \cdot \mathbf{u}_h) (\nabla \cdot \mathbf{u}_h) d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left\langle \int_{\Omega_e} (\partial_i u_{hi})^2 d\Omega_e \right\rangle - \frac{1}{V_e} \left\langle \int_{\Omega_e} \Pi^h (\nabla \cdot \mathbf{u}_h) (\partial_i u_{hi}) d\Omega_e \right\rangle. \end{aligned} \quad (42)$$

3.1.3. Elemental ensemble average of $\mathcal{P}_r^{h\tau}$

From (30), (36) and (42), we can define the ensemble average of the rate of production of kinetic energy $\mathcal{P}_r^{h\tau}$ for high Reynolds numbers as

$$\langle \mathcal{P}_{r,e}^{h\tau} \rangle := \tau_1 \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle + \tau_2 \langle \mathcal{P}_{r,e}^{h\tau_2} \rangle. \quad (43)$$

3.2. FEM solution and treatment of the L^2 projection in $\langle \mathcal{P}_{r,e}^{h\tau} \rangle$

3.2.1. FEM solution for the velocity and pressure fields and L^2 projection

The components of the discrete velocity field \mathbf{u}_h can be expanded as usual for a mesh having n_u nodes as

$$u_{hi}(\mathbf{x}) = \sum_{a=1}^{n_u} N_u^a(\mathbf{x}) U_i^a, \quad (44)$$

where the velocity shape functions $\{N_u^a(\mathbf{x}), a = 1, \dots, n_u\}$ are a basis of $\mathcal{V}_{0,h}$ and U_i^a are the velocity nodal values, i.e., at the nodal points, $\mathbf{x}^b, b = 1, \dots, n_u$, it holds that

$$u_{hi}(\mathbf{x}^b) = U_i^b. \quad (45)$$

In case of \mathbf{u}_h being the finite element interpolant, the nodal values are exact and

$$u_{hi}(\mathbf{x}^b) = U_i^b = u_i(\mathbf{x}^b) \equiv u_i^b. \quad (46)$$

Let us also assume the following interpolation for the Reynolds stresses (see e.g., [47])

$$u_{hi} u_{hj}(\mathbf{x}) = \sum_{b=1}^{n_u} N_u^b(\mathbf{x}) U_i^b U_j^b \quad (47)$$

in order to have simpler expressions and to make some of the forthcoming results useful from a computational point of view.

Concerning the discrete pressure field, p_h , it will be expanded as

$$p_h(\mathbf{x}) = \sum_{a=1}^{n_p} N_p^a(\mathbf{x}) P^a, \quad (48)$$

where the pressure shape functions $\{N_p^a(\mathbf{x}), a = 1, \dots, n_p\}$ are a basis of $\mathcal{Q}_{h,0}$ and P^a denotes the pressure nodal value at node \mathbf{x}^a . We note that one of the advantages of using a stabilized finite element method such as the OSS in Section 2.3.2 is that one can choose $N_u^a = N_p^a \equiv N^a$, hence circumventing the necessity of using different interpolations for the velocity and pressure fields as demanded by the *inf-sup* condition (see e.g. [2,3,33,34,4]).

On the other hand, it will be necessary to give explicit expressions for the projected terms $\Pi_i^h[\nabla \cdot (\mathbf{u}_h \otimes \mathbf{u}_h)]$ and $\Pi_i^h(\nabla p_h)$ appearing in (37)–(40). This can be done as follows. Consider a function ψ_h computed from the finite element interpolation, not necessarily continuous. Its $L^2(\Omega)$ projection onto $\mathcal{V}_{0,h}$ can be written as

$$\Pi(\psi_h) = \sum_{a=1}^{n_u} N^a(\mathbf{x}) \Pi^a, \quad (49)$$

with the coefficients Π^a being given by the solution of the linear system

$$\sum_{a=1}^{n_u} M^{ba} \Pi^a = \int_{\Omega} N^b \psi_h d\Omega, \quad b = 1, \dots, n_u \quad (50)$$

$$M^{ba} := \int_{\Omega} N^b N^a d\Omega. \quad (51)$$

To simplify the notation, suppose that the mass matrix \mathbf{M} in (51) can be approximated by means of a diagonal matrix $\text{diag}(\mathcal{M}_{11}, \dots, \mathcal{M}_{n_u n_u})$ using a nodal quadrature rule. In this case

$$\Pi^b = \mathcal{M}_{bb}^{-1} \int_{\Omega} N^b \psi_h d\Omega, \quad (52)$$

so (49) becomes

$$\Pi(\psi_h) = \sum_{a=1}^{n_u} \mathcal{M}_{aa}^{-1} N^a \int_{\Omega} N^a \psi_h d\Omega. \quad (53)$$

3.2.2. $\langle \mathcal{P}_{r,e}^{h\tau} \rangle$ in terms of the finite element velocity and pressure fields

We next have to substitute the above expansions for the discrete velocity and pressure fields in the expressions for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$, $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$, $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP}$, $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP}$ and $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$, respectively given by Eqs. (37)–(40).

Convective term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$ corresponding to the velocity subscales (37). We will first address the term in the second line of (37), which will be denoted by $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,1}$. Substituting (47) in this term yields

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,1} &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \left[\sum_a \partial_i N^a U_i^a U_j^a \sum_b \partial_k N^b U_k^b U_j^b \right] d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left[\sum_{a,b} \langle U_i^a U_j^a U_k^b U_j^b \rangle \int_{\Omega_e} \partial_i N^a \partial_k N^b d\Omega_e \right]. \end{aligned} \quad (54)$$

The term in the third line of (37) will be denoted by $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,2}$. After substituting (47) and (53) in it, we get

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,2} &= -\frac{1}{V_e} \left\langle \int_{\Omega_e} \left[\sum_{a,c} \mathcal{M}_{cc}^{-1} N^c \int_{\Omega} N^c \partial_i N^a U_i^a U_j^a d\Omega \sum_b \partial_k N^b U_k^b U_j^b \right] d\Omega_e \right\rangle \\ &= -\frac{1}{V_e} \left\{ \sum_{a,b} \langle U_i^a U_j^a U_k^b U_j^b \rangle \int_{\Omega_e} \left[\partial_k N^b \sum_c \mathcal{M}_{cc}^{-1} N^c \int_{\Omega} N^c \partial_i N^a d\Omega \right] d\Omega_e \right\}. \end{aligned} \quad (55)$$

To facilitate the notation in expressions (54) and (55) we define the geometric factors

$$I_{ij}^{ab} := \int_{\Omega_e} \partial_j N^b \partial_i N^a d\Omega_e \quad (56)$$

and

$$G_{ij}^{ab} := \int_{\Omega_e} \left[\partial_j N^b \sum_c \mathcal{M}_{cc}^{-1} N^c \int_{\Omega} N^c \partial_i N^a d\Omega \right] d\Omega_e. \quad (57)$$

Both factors depend on the element Ω_e . However, while I_{ij}^{ab} has a *local* character in the sense that it only depends on the shape functions and the type of element being used, G_{ij}^{ab} has a *global* character because it involves an integration over the whole computational domain Ω . This global character is due to the fact that a projection is involved in $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,2}$.

We will also denote the velocity correlation function as

$$B_{ij}^{ab} = \langle U_i^a U_j^b \rangle \quad (58)$$

and the two point fourth moment of the velocity field by

$$B_{ij,kl}^{ab} = \langle U_i^a U_j^b U_k^c U_l^d \rangle. \quad (59)$$

Using the notation (56)–(59) in Eqs. (54) and (55), we obtain the following expansion for the convective term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$:

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU} = \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,1} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU,2} = \frac{1}{V_e} \sum_{a,b} B_{ij,kj}^{ab} (I_{ik}^{ab} - G_{ik}^{ab}), \quad (60)$$

where summation on the spatial dimension indexes i, j, k is assumed whereas summation on nodes will be explicitly indicated throughout the text for the sake of clarity.

Pressure–velocity terms $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$ and $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP}$ corresponding to the velocity subscales (38), (39). It will be next found an expression similar to (60) starting with the pressure term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$. Making use of (47) and (48) in (38), we get for the term in the second line of (38), which we denote $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU,1}$,

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU,1} &= \frac{1}{V_e} \left\langle \int_{\Omega_e} \left[\sum_a \partial_i N^a P^a \sum_b \partial_j N^b U_j^b U_i^b \right] d\Omega_e \right\rangle \\ &= \frac{1}{V_e} \left[\sum_{a,b} \langle P^a U_j^b U_i^b \rangle \int_{\Omega_e} \partial_i N^a \partial_j N^b d\Omega_e \right]. \end{aligned} \quad (61)$$

Using now (47), (48) and (53) in the third line of (38), we obtain

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU,2} &= -\frac{1}{V_e} \left\langle \int_{\Omega_e} \left[\sum_{a,c} \mathcal{M}_{cc}^{-1} N^c \int_{\Omega} N^c \partial_i N^a P^a d\Omega \sum_b \partial_j N^b U_j^b U_i^b \right] d\Omega_e \right\rangle \\ &= -\frac{1}{V_e} \left\{ \sum_{a,b} \langle P^a U_j^b U_i^b \rangle \int_{\Omega_e} \left[\partial_j N^b \sum_c \mathcal{M}_{cc}^{-1} N^c \int_{\Omega} N^c \partial_i N^a d\Omega \right] d\Omega_e \right\}. \end{aligned} \quad (62)$$

Given the geometric factors (56) and (57) and defining the two point triple velocity–pressure correlation as

$$B_{p,ij}^{ab} = \langle P^a U_i^b U_j^b \rangle, \quad (63)$$

we can rewrite $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$ as

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU} = \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU,1} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU,2} = \frac{1}{V_e} \sum_{a,b} B_{p,ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}), \quad (64)$$

with summation implied on indexes i, j .

In what concerns the term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP}$, we can proceed analogously to what has been done for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$. Taking into account that for homogeneous isotropic turbulence $B_{p,ij}^{ab} = B_{p,ij}^{ba}$ (see e.g., Eq.

(106) below) it follows that $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP} = \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$. Consequently

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU} + \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UP} = \frac{2}{V_e} \sum_{a,b} B_{p,ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}), \quad (65)$$

Pressure term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP}$ corresponding to the velocity subscales (40). Inserting (48) in (40) and taking into account the factors (56) and (57) we get

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP} = \frac{1}{V_e} \sum_{a,b} B_{pp}^{ab} (I_{ii}^{ab} - G_{ii}^{ab}), \quad (66)$$

with

$$B_{pp}^{ab} = \langle P^a P^b \rangle, \quad (67)$$

standing for the two-point second-order pressure correlation.

Divergence term $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$ corresponding to the pressure subscales (42). It can be readily checked that the expression analogous to (60) and (64) for the term $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$ in (42) is given by

$$\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle = \frac{1}{V_e} \sum_{a,b} B_{ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}), \quad (68)$$

with B_{ij}^{ab} being the second-order velocity correlations (58).

Finite element expression for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle$. Using the developments (60), (65), (66) and (68) in Eqs. (41) and (43) we obtain the finite element expression for the ensemble average of the rate of production of subgrid kinetic energy

$$\begin{aligned} \langle \mathcal{P}_{r,e}^{h\tau} \rangle &= \tau_1 \langle \mathcal{P}_{r,e}^{h\tau_1} \rangle + \tau_2 \langle \mathcal{P}_{r,e}^{h\tau_2} \rangle \\ &= \frac{1}{V_e} \sum_{a,b} [\tau_1 (B_{ij,kj}^{ab} + 2B_{p,ik}^{ab} + B_{pp}^{ab} \delta_{ik}) + \tau_2 B_{ik}^{ab}] (I_{ik}^{ab} - G_{ik}^{ab}) \end{aligned} \quad (69)$$

4. Relation between the numerical subgrid kinetic energy transfer and the molecular physical dissipation in the inertial subrange

4.1. Two point fourth-order velocity correlations for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$

Given that I_{ij}^{ab} and G_{ij}^{ab} in (56), (57) are pure geometric factors, in order to relate expression (69) for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle$ with the molecular physical dissipation, ε_{mol} , we will have to relate the second-order and fourth-order velocity correlations $B_{ij}^{ab}, B_{ij,kl}^{ab}$, the two point triple velocity–pressure correlation $B_{p,ij}^{ab}$ and the two point second-order pressure correlation B_{pp}^{ab} to it.

To do so, use will be made in what follows of some results of statistical fluid mechanics and in particular of statistics concerning homogeneous isotropic turbulence. Although the various correlations $B_{ij}^{ab}, B_{ij,kl}^{ab}, B_{p,ij}^{ab}$ and B_{pp}^{ab} do not involve the whole velocity and pressure fields at the nodes, but their OSS finite element approximation, we will consider that the results from statistical fluid mechanics can be still applied to them, similarly to what is assumed for the filtered velocity in a LES model. Note that in the case of $[\mathbf{u}_h, p_h]$ being the interpolant, see (46), no approximation would be needed. We then guess that the velocity and pressure from the OSS finite element solution will not differ substantially from the interpolant, at least in what concerns their statistical behavior. This is also implicitly assumed in practical implementations of the results in [46].

Let us start with the two point fourth moment velocity correlation $B_{ij,kl}^{ab}$, which by virtue of its definition (59) fulfills

$$B_{ij,kl}^{ab} = B_{ji,kl}^{ab} = B_{ji,lk}^{ab} = B_{ij,lk}^{ab}. \quad (70)$$

Use can be made of the quasi-normal approximation (Millionshchikov zero-fourth-cumulant hypothesis, see e.g., [32]) in order to relate the fourth-order velocity correlations with second-order velocity correlations. For the particular case of velocities being considered at just two points, the quasi-normal approximation for the exact velocity field establishes

$$\langle u_i^a u_j^a u_k^b u_l^b \rangle = \langle u_i^a u_j^a \rangle \langle u_k^b u_l^b \rangle + \langle u_i^a u_k^b \rangle \langle u_j^a u_l^b \rangle + \langle u_i^a u_l^b \rangle \langle u_j^a u_k^b \rangle. \quad (71)$$

Assuming that this relation holds true for the finite element velocity field, we can rewrite it using the notation (58) and (59) to obtain

$$B_{ij,kl}^{ab} = B_{ij}^{aa} B_{kl}^{bb} + B_{ik}^{ab} B_{jl}^{ab} + B_{il}^{ab} B_{jk}^{ab}. \quad (72)$$

In our case, the two-point fourth-order velocity correlation in (60) and (69) is contracted on the second and fourth indexes so that

$$B_{ij,kj}^{ab} = B_{ij}^{aa} B_{kj}^{bb} + B_{ik}^{ab} B_{jj}^{ab} + B_{ij}^{ab} B_{jk}^{ab}. \quad (73)$$

The second-order velocity correlations can be related to the second-order velocity structure function D_{ij}^{ab} defined by (see e.g., [32,36])

$$D_{ij}^{ab} = \langle (U_i^b - U_i^a)(U_j^b - U_j^a) \rangle. \quad (74)$$

Developing (74) and under the assumption of homogeneous isotropic turbulence (which implies that $B_{ij}^{ab} = B_{ij}^{ba}, B_{ij}^{aa} = B_{ij}^{bb}$, see for example [32]) it is straightforward to see that

$$B_{ij}^{ab} = B_{ij}^{aa} - \frac{1}{2} D_{ij}^{ab} = \frac{1}{3} u'^2 \delta_{ij} - \frac{1}{2} D_{ij}^{ab}, \quad (75)$$

with u' representing the flow r.m.s (root mean square) velocity (see e.g., [36]).

Substituting (75) into (73) yields

$$B_{ij,kj}^{ab} = \frac{5}{9} u'^4 \delta_{ik} - \frac{5}{6} u'^2 D_{ik}^{ab} - \frac{1}{6} u'^2 \delta_{ik} D_{jj}^{ab} + \frac{1}{4} (D_{jj}^{ab} D_{ik}^{ab} + D_{ij}^{ab} D_{jk}^{ab}). \quad (76)$$

The first term in (76) can be neglected in what follows given that it will vanish when finally inserted in (60). This is so because it can be factorized out of the summation on nodes in this expression. The summation can be carried inside the integrals in (56) and (57), which will then contain terms of the type $\partial_i (\sum_a N^a)$. Given that the shape functions form a partition of unity, $\sum_a N^a = 1$ and the derivative of this term is obviously zero (velocity boundary conditions need not to be considered at this point).

As previously mentioned, a computational mesh with its characteristic length h lying in the inertial subrange $[l_{D1}, l_{E1}]$ is considered in this paper. Combining the Kolmogorov first and second similarity hypothesis, an expression for the second order structure function D_{ij}^{ab} can be found solely in terms of ε_{mol} and the distance between nodes \mathbf{x}^a and $\mathbf{x}^b, r^{ab} = \|\mathbf{x}^a - \mathbf{x}^b\|$, for $r^{ab} \in [l_{D1}, l_{E1}]$. The expression is given by (see e.g., [32,36])

$$D_{ij}^{ab} = 2C(\varepsilon_{\text{mol}} r^{ab})^{2/3} \mathcal{D}_{ij}^{ab}, \quad \mathcal{D}_{ij}^{ab} := \frac{1}{6} \left(4\delta_{ij} - \frac{r_i^a r_j^a}{(r^{ab})^2} \right), \quad (77)$$

where C represents a universal constant with approximate value $C \approx 2$. Substituting (77) in (76) gives

$$\begin{aligned} B_{ij,kj}^{ab} &= -\frac{11}{18} u'^2 C (\varepsilon_{\text{mol}} r^{ab})^{2/3} \delta_{ik} \\ &+ \left[-\frac{5}{3} u'^2 C (\varepsilon_{\text{mol}} r^{ab})^{2/3} + \frac{11}{6} C^2 (\varepsilon_{\text{mol}} r^{ab})^{4/3} \right] \mathcal{D}_{ik}^{ab} \\ &+ C^2 (\varepsilon_{\text{mol}} r^{ab})^{4/3} \mathcal{D}_{ij}^{ab} \mathcal{D}_{jk}^{ab}. \end{aligned} \quad (78)$$

Taking into account that for isotropic turbulence the r.m.s velocity is related to the lengthscale L characterizing the large eddies and to molecular dissipation through (see e.g., [36])

$$u' \sim (\epsilon_{\text{mol}} L)^{1/3}, \tag{79}$$

we get after substitution in (78)

$$B_{ij,kj}^{ab} = C \epsilon_{\text{mol}}^{4/3} \left\{ -\frac{11}{18} L^{2/3} (r^{ab})^{2/3} \delta_{ik} + \left[-\frac{5}{3} L^{2/3} (r^{ab})^{2/3} + \frac{11}{6} C (r^{ab})^{4/3} \right] \mathcal{D}_{ik}^{ab} + C (r^{ab})^{4/3} \mathcal{D}_{ij}^{ab} \mathcal{D}_{jk}^{ab} \right\} =: \epsilon_{\text{mol}}^{4/3} \mathcal{K}_{ik}^{ab}, \tag{80}$$

where \mathcal{K}_{ik}^{ab} has been defined in the last line of (80).

In view of (80), Eq. (60) for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU}$ can be rewritten as

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{UU} = \frac{1}{V_e} \epsilon_{\text{mol}}^{4/3} \sum_{a,b} \mathcal{K}_{ik}^{ab} \left(I_{ik}^{ab} - G_{ik}^{ab} \right). \tag{81}$$

4.2. Two point triple-order velocity–pressure correlations for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$

It is our aim now to find an expression analogous to (81) but relating the two point triple-order velocity–pressure correlation $B_{p,ij}^{ab}$ with the rate of physical dissipation ϵ_{mol} . To do so we will closely follow [32] although with some particularities. We will abuse of notation and use $B_{p,ij}^{ab}$ to denote the triple-order velocity–pressure correlations of either the exact velocity field or the finite element approximated one. Whether equations are valid for one or the other, or for both of them, can be easily determined by the context. Likewise, we will identify $r \equiv r^{ab}$, being clear that this is the distance between nodes \mathbf{x}^a and \mathbf{x}^b .

The tensor of second rank $B_{p,kl}^{ab}$ for the isotropic case can be written as

$$B_{p,kl}^{ab} = P_1(r) r_k r_l + P_2(r) \delta_{kl}, \tag{82}$$

where

$$P_1(r) = \frac{1}{r^2} \left[B_{p,LL}^{ab} - B_{p,NN}^{ab} \right], \quad P_2(r) = B_{p,NN}^{ab}, \tag{83}$$

with the subscript L standing for *longitudinal* and designating the direction of the vector \mathbf{r}^{ab} and N standing for *normal* and designating any perpendicular direction to it.

Consider the Poisson equation for the pressure at node a

$$\Delta p = -\partial_r \partial_r \left(u_i^a u_i^a \right) \tag{84}$$

where Δ is the Laplacian operator that for functions only depending on r becomes

$$\Delta = \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}. \tag{85}$$

Multiplying both sides of (84) by $u_k^b u_l^b$ and performing an ensemble average of the results yields

$$\Delta B_{p,kl}^{ab} = -\partial_r \partial_r \left(B_{ij,kl}^{ab} \right). \tag{86}$$

In the case of homogeneous isotropic turbulence, the tensor in the r.h.s of (86) is an isotropic symmetric tensor of second rank that can be expressed as

$$\partial_r \partial_r \left(B_{ij,kl}^{ab} \right) = Q_1(r) r_k r_l + Q_2(r) \delta_{kl}. \tag{87}$$

Inserting (82) and (87) in (86) and equating the coefficients of $r_k r_l$ and δ_{kl} on both sides yields two differential equations for the unknowns P_1 and P_2 :

$$\frac{d^2 P_1}{dr^2} + \frac{6}{r} \frac{dP_1}{dr} = -Q_1. \tag{88}$$

$$\frac{d^2 P_2}{dr^2} + \frac{2}{r} \frac{dP_2}{dr} + 2P_1 = -Q_2. \tag{89}$$

These equations can be uncoupled defining a new function P_3 such that

$$P_3(r) = r^2 P_1(r) + 3P_2(r) = B_{p,LL}^{ab} + 2B_{p,NN}^{ab}. \tag{90}$$

Multiplying (88) by r^2 and adding the result to three times (89) gives the following equation for P_3 :

$$\frac{d^2 P_3}{dr^2} + \frac{2}{r} \frac{dP_3}{dr} = -Q_3, \tag{91}$$

where

$$Q_3(r) = r^2 Q_1(r) + 3Q_2(r). \tag{92}$$

Eq. (88) can be solved following a standard Green function approach, taking into account that 1 and r^{-5} are solutions of the homogeneous equation. Imposing the boundary conditions $P_1(0) < \infty$ and $\lim_{r \rightarrow \infty} P_1(r) \rightarrow 0$ results in

$$P_1(r) = -\frac{1}{5r^5} \int_0^r r_0^6 Q_1(r_0) dr_0 - \frac{1}{5} \int_r^\infty r_0 Q_1(r_0) dr_0. \tag{93}$$

Analogously, for (91) we get (1 and $1/r$ are the homogeneous solutions in this case)

$$P_3(r) = -\frac{1}{r} \int_0^r r_0^2 Q_3(r_0) dr_0 - \int_r^\infty r_0 Q_3(r_0) dr_0. \tag{94}$$

From (93) and (94) we can obtain P_2 using (90) and insert it in (82), together with P_1 , to obtain the two point triple-order velocity–pressure correlation $B_{p,kl}^{ab}$. Therefore, the remaining step to proceed accordingly is to find a value for the inhomogeneous terms Q_1 and Q_3 . To do so, the use of the quasi-normal approximation and of Kolmogorov’s similarity hypotheses will prove very useful again. We remind that our interest is in finding the results for $r \equiv r^{ab}$ assumed to be in the inertial subrange i.e., $r \in [l_D, l_E]$.

Making use of the quasi-normal approximation (72) in (87) and taking into account that due to the incompressibility constraint $\partial_r \partial_r B_{ij}^{ab} = \partial_r \partial_r B_{ij}^{ab} = 0$ (see [32]), it follows that

$$Q_1(r) r_k r_l + Q_1(r) \delta_{kl} = \partial_r \partial_r \left(B_{ij,kl}^{ab} \right) = 2 \partial_r \partial_r B_{ik}^{ab} \partial_r B_{jl}^{ab} \tag{95}$$

and given that the second-order velocity correlation tensor B_{ij}^{ab} for homogeneous isotropic turbulence can be expressed as [32]

$$B_{ij}^{ab} = -\partial_r B_{LL}^{ab}(r) \frac{r_i r_j}{r} + \left[B_{LL}^{ab}(r) + \frac{r}{2} \partial_r B_{LL}^{ab}(r) \right], \tag{96}$$

we can obtain the following expressions for Q_1 , Q_2 and Q_3 solely in terms of the longitudinal second-order velocity correlation B_{LL}^{ab} :

$$Q_1(r) = \frac{6}{r^2} \left[\frac{d}{dr} B_{LL}^{ab}(r) \right]^2 + \frac{1}{r} \frac{d}{dr} B_{LL}^{ab}(r) \frac{d^2}{dr^2} B_{LL}^{ab}(r), \tag{97}$$

$$Q_2(r) = -3 \left[\frac{d}{dr} B_{LL}^{ab}(r) \right]^2 - r \frac{d}{dr} B_{LL}^{ab}(r) \frac{d^2}{dr^2} B_{LL}^{ab}(r), \tag{98}$$

$$Q_3(r) = -\frac{1}{r^2} \frac{d}{dr} \left\{ r^3 \left[\frac{d}{dr} B_{LL}^{ab}(r) \right]^2 \right\}, \tag{99}$$

where use has been made of (92) to obtain the expression for Q_3 .

We can next use (75) to relate B_{LL}^{ab} with the longitudinal velocity structure function D_{LL}^{ab} and the rate of dissipation ϵ_{mol} ,

$$B_{LL}^{ab} = B_{LL}^{aa} - \frac{1}{2} D_{LL}^{ab} = B_{LL}^{aa} - \frac{C}{2} (\epsilon_{\text{mol}} r)^{2/3}. \tag{100}$$

Substituting (100) in (97) and (99) yields

$$Q_1(r) = \frac{17}{27} C^2 \epsilon_{\text{mol}}^{4/3} r^{-8/3}, \tag{101}$$

$$Q_3(r) = -\frac{7}{27} C^2 \epsilon_{\text{mol}}^{4/3} r^{-2/3}, \tag{102}$$

which are to be inserted respectively in Eqs. (93) and (94). Note that (88) and (91) are only needed for $r \equiv r^{ab}$, which is of order h . Therefore, we may extend the source terms Q_1 and Q_3 in these equations by zero outside this range, so that we finally get

$$P_1(r) = F_1 \varepsilon_{\text{mol}}^{4/3} r^{-2/3}, \quad (103)$$

$$P_3(r) = F_3 \varepsilon_{\text{mol}}^{4/3} r^{4/3}, \quad (104)$$

with F_i $i = 1, 2, 3$ generic constants being redefined where appropriate. We can next obtain $P_2(r) = B_{p,NN}^{ab}(r)$ substituting (103) and (104) into (90):

$$P_2(r) := \frac{F_3}{3} \varepsilon_{\text{mol}}^{4/3} r^{4/3} - r^2 F_1 \varepsilon_{\text{mol}}^{4/3} r^{-2/3} =: F_2 \varepsilon_{\text{mol}}^{4/3} r^{4/3}. \quad (105)$$

Inserting (103) and (105) in (82) we find the expression for the two-point triple order velocity–pressure correlation $B_{p,ij}^{ab}$ we were looking for:

$$B_{p,ij}^{ab} = P_1(r) r_i r_j + P_2(r) \delta_{ij} = F_1 \varepsilon_{\text{mol}}^{4/3} r^{-2/3} r_i r_j + F_2 \varepsilon_{\text{mol}}^{4/3} r^{4/3} \delta_{ij} =: \varepsilon_{\text{mol}}^{4/3} \mathcal{F}_{ij}^{ab}(r), \quad (106)$$

$\mathcal{F}_{ij}^{ab}(r)$ being defined in the last line.

Finally, we can find an expression for the numerical kinetic energy transfer term $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU}$ in Eq. (64). Substituting (106) in (64) yields

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PU} = \frac{1}{V_e} \varepsilon_{\text{mol}}^{4/3} \sum_{a,b} \mathcal{F}_{ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}). \quad (107)$$

4.3. Two point second-order pressure correlations for $\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP}$

Let us next relate the two point second-order pressure correlation B_{pp}^{ab} with the rate of physical dissipation ε_{mol} . We will first express B_{pp}^{ab} in terms of the second-order pressure structure function D_{pp}^{ab} given by

$$D_{pp}^{ab} = \langle (P^b - P^a)^2 \rangle. \quad (108)$$

Assuming homogeneous isotropic turbulence so that $B_{pp}^{aa} \approx B_{pp}^{bb} \equiv P^2$, with P^2 representing the ensemble average of the squared pressure field either at nodes a or b , we get

$$B_{pp}^{ab} = P^2 - \frac{1}{2} D_{pp}^{ab}. \quad (109)$$

The first term in (109) can be neglected as it was done for the ensemble average of the velocity in (76), because it will vanish once integrated. Again, this is so because this term can be factorized out of the summation on nodes and the shape functions form a partition of unity. Consequently, terms of the type $\partial_i (\sum_a N^a)$ will be zero. On the other hand, the second-order pressure structure function in the second term of (109) can be related to the molecular dissipation for the flow in the inertial subrange (see e.g., [48,32]):

$$D_{pp}^{ab} = C_p \rho^2 (\varepsilon_{\text{mol}} r^{ab})^{4/3}. \quad (110)$$

Defining $\tilde{D}_{pp}^{ab} := -(1/2) C_p \rho^2 (r^{ab})^{4/3}$ and substituting in (66) results in

$$\langle \mathcal{P}_{r,e}^{h\tau_1} \rangle_{PP} = \frac{\varepsilon_{\text{mol}}^{4/3}}{V_e} \sum_{a,b} \tilde{D}_{pp}^{ab} (I_{ii}^{ab} - G_{ii}^{ab}). \quad (111)$$

4.4. Two point second-order velocity correlations for $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$

The last term that has to be dealt with is $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$ in (68) arising from the pressure subscales stabilization. As seen, (68) only involves the second-order velocity correlation tensor B_{ij}^{ab} . From (75)

and (77) it can readily be checked that the expression analogous to (81), (107) or (111) for the term $\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle$ in (68) is given by

$$\langle \mathcal{P}_{r,e}^{h\tau_2} \rangle = \frac{2C}{V_e} \varepsilon_{\text{mol}}^{2/3} \sum_{a,b} r^{2/3} \mathcal{D}_{ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}) =: \frac{1}{V_e} \varepsilon_{\text{mol}}^{2/3} \sum_{a,b} \tilde{\mathcal{D}}_{ij}^{ab} (I_{ij}^{ab} - G_{ij}^{ab}), \quad (112)$$

with $\tilde{\mathcal{D}}_{ij}^{ab} := 2Cr^{2/3} \mathcal{D}_{ij}^{ab}$.

4.5. Relation between $\langle \mathcal{P}_{r,e}^{h\tau} \rangle$ and the physical rate of dissipation ε_{mol}

From Eqs. (81), (107), (111) and (112) substituted in (69) we get

$$\langle \mathcal{P}_{r,e}^{h\tau} \rangle = \left\{ \frac{1}{V_e} \sum_{a,b} \left[\underbrace{\tau_1 \varepsilon_{\text{mol}}^{4/3} (\mathcal{K}_{ik}^{ab} + 2\mathcal{F}_{ik}^{ab} + \tilde{D}_{pp}^{ab} \delta_{ik})}_2 + \underbrace{\tau_2 \varepsilon_{\text{mol}}^{2/3} \tilde{\mathcal{D}}_{ik}^{ab}}_3 \right] \right\} \underbrace{(I_{ik}^{ab} - G_{ik}^{ab})}_4. \quad (113)$$

It next has to be shown that Eq. (113) yields the expected result $\langle \mathcal{P}_{r,e}^{h\tau} \rangle \sim \varepsilon_{\text{mol}}$, for a fine enough computational mesh so that its size h lies in the inertial subrange of an isotropic turbulent flow. That is to say, we need to find expressions for the stabilization parameters τ_1 and τ_2 that guarantee such behavior for $h/L \ll 1$ (i.e., large eddies much larger than the computational mesh size). Prior to doing so, let us check the dependence of the various terms in (113) with h . The first factor $1/V_e$ in (113) goes as h^{-3} whereas it can be observed from Eqs. (56) and (57) that the fourth factor behaves as h . If we now focus on the second factor we can see from (80) that $\mathcal{K}_{ik}^{ab} \sim L^{2/3} h^{2/3} + Ch^{4/3}$, C standing again for a generic constant to be redefined where appropriate, from (106) that $\mathcal{F}_{ik}^{ab} \sim Ch^{4/3}$ and from (110) that $\tilde{D}_{pp}^{ab} \sim Ch^{4/3}$. Finally, it can be observed from (112) and (77) that $\tilde{\mathcal{D}}_{ik}^{ab} \sim Ch^{2/3}$. Grouping together these results brings the following behavior for Eq. (113)

$$\langle \mathcal{P}_{r,e}^{h\tau} \rangle \sim \tau_1 \varepsilon_{\text{mol}}^{4/3} [L^{2/3} h^{-4/3} + Ch^{-2/3}] + \tau_2 \varepsilon_{\text{mol}}^{2/3} h^{-4/3}. \quad (114)$$

In the case of convection dominated flows, the viscosity term in expression (25) for the stabilization parameter τ_1 can be neglected yielding

$$\tau_1 \approx \frac{h}{c_2 U_{1e}} \quad (115)$$

and using (115) in the expression for the parameter τ_2 in (26) we get

$$\tau_2 \approx \frac{c_2}{c_1} h U_{2e}. \quad (116)$$

The key step that will allow the OSS formulation to exhibit the correct behavior for isotropic turbulence precisely relies in choosing appropriate values for the elemental velocities U_{1e} and U_{2e} . It is proposed to take

$$U_{1e} = \frac{\langle |\mathbf{u}_h| \rangle}{\xi}, \quad (117)$$

$$U_{2e} = \xi \langle |\mathbf{u}_h| \rangle, \quad (118)$$

with

$$\xi = 1 + \chi \left[\left(\frac{h}{L} \right)^{\frac{1}{3}} - 1 \right], \quad (119)$$

$$\chi = \min \left\{ 1, \beta \frac{u'}{\langle |\mathbf{u}_h| \rangle} \right\}. \quad (120)$$

$\langle |\mathbf{u}_h| \rangle$ in the above expressions denotes the mean of the modulus of the nodal velocities at each element (note that the mean of the

nodal velocity vectors would be zero for isotropic turbulence, but not the mean of the velocity vector moduli, whereas u' is the r.m.s velocity. β stands for a positive constant. In the case of a convection dominated laminar flow u' turns to be very small so that $\chi = 0$ and thus $\xi = 1$. The expressions already used in the standard OSS formulation [33] for τ_1 and τ_2 are then recovered. In the case of isotropic turbulence, it follows from (79) that the r.m.s velocity scales as $u' \sim \varepsilon_{\text{mol}}^{1/3} L^{1/3}$ and the same behavior is encountered for $\langle |\mathbf{u}_h| \rangle$. If β is chosen large enough, it will follow that $\chi = 1$ and thus $\xi = (h/L)^{1/3}$. Making use of these expressions for $\langle |\mathbf{u}_h| \rangle$ and ξ in (117), (118) results in $U_{1e} \sim \varepsilon_{\text{mol}}^{1/3} L^{2/3} h^{-1/3}$ and $U_{2e} \sim \varepsilon_{\text{mol}}^{1/3} h^{1/3}$, which once inserted in (115) and (116) yield the following behavior for the stabilization parameters τ_1 and τ_2 ,

$$\tau_1 \sim \frac{h^{4/3}}{\varepsilon_{\text{mol}}^{1/3} L^{2/3}}, \quad (121)$$

$$\tau_2 \sim \varepsilon_{\text{mol}}^{1/3} h^{4/3}. \quad (122)$$

Finally, substitution in Eq. (114) provides the expected result

$$\langle \mathcal{P}_{r,e}^{h\tau} \rangle \sim \varepsilon_{\text{mol}} \left[1 + \mathcal{O}\left(\frac{h}{L}\right)^{2/3} \right]. \quad (123)$$

Consequently, the average of the rate of production of residual kinetic energy will be proportional to the molecular dissipation, the first correction being of the order $(h/L)^{2/3}$, which will be clearly negligible if the mesh size h lies in the inertial subrange of a turbulent flow.

5. Discussion and remarks

5.1. General comments

In Section 2.3.3 we wondered about the possibility that some terms in $\mathcal{P}_r^{h\tau}$ integrated over the whole computational domain equated the overall physical dissipation in the energy balance equation. It was argued that this should not necessarily be the case for all the stabilization terms in $\mathcal{P}_r^{h\tau}$, given that they arise from purely numerical considerations rather than physical ones. However, we have found in (123) that when using appropriate values for the stabilization parameters in the OSS formulation, the leading terms in the ensemble average of $\mathcal{P}_r^{h\tau}$ are effectively proportional to the dissipation ε_{mol} .

As observed from (113) the proportionality factor between $\langle \mathcal{P}_{r,e}^{h\tau} \rangle$ and ε_{mol} is a rather complicated function depending on the element and mesh geometry, as well on the chosen finite element interpolation spaces. Although one could be tempted to think that its optimum value should equal unity in order to have the desired physical behavior, we have no basis to assess this point given that, as stated, the terms in (113) have to account not only for appropriate physical behavior, but also for circumventing purely numerical difficulties (e.g., to allow the use of equal interpolation spaces for the velocity and the pressure). In any case, setting the proportionality factor equal to one would amount to fix the algorithmic constants in (116) and (117).

What seems to follow from the above analysis is that it makes somehow redundant the use of physical LES models. Effectively, should we have done the above analysis for the energy balance Eq. (34), a result of the type $\overline{\mathcal{P}}_r^{h\tau} = \alpha \varepsilon_{\text{mol}}$ (with α being a proportionality function analogous to the one that would appear in (123)) would have been obtained. On the other hand, the term arising from the LES model should also behave as $\overline{\mathcal{P}}_r^h = \beta \varepsilon_{\text{mol}}$ so that its additional effects, if any, could be included in the $\overline{\mathcal{P}}_r^{h\tau}$ term with appropriate redefinition of the proportionality factor. Hence, if a good enough discretization of the Navier–Stokes equations is performed, filtering and modeling at the continuous level might turn unnecessary.

5.2. Other numerical approaches

As it has been mentioned in the Introduction of the paper, the purely numerical strategy to simulate turbulent flows is not new, and can be traced back (at least) to the MILES approach. Sometimes, these type of models are referred to as *implicit LES* models. Some examples of them can be found in [1]. In these type of methods, the subgrid-scale stress tensor is modeled depending on the numerical procedure. For example, in [49] the model proposed is based on the parallel solution of the truncated Navier–Stokes equations on a mesh twice smaller in each Cartesian direction than the one used to compute the resolved quantities. In this method, the subgrid velocity is computed at each time step, without accounting for its time evolution, and its expression is used to evaluate the subgrid-scale stress tensor. One of the conclusions that can be drawn from the numerical results presented is that the method does not have enough dissipation. In an attempt to overcome this misbehavior, the parameters on which the formulation depends could be adjusted so as to follow the correct dissipation structure, as proposed in [50], where the spectra of the numerical solution and the physical one are forced to match for isotropic turbulence.

A fundamental difference between the approaches described and the one we have analyzed here is that *we do not model neither the subgrid scale stress tensor nor its effect*. Rather, we simply add terms based on the effect of the subscales onto the finite element component of the solution. As we have shown, the overall effect is a dissipation that mimics the physical one. In this sense, our approach has to be considered *residual based*, as the one proposed in [19] and also in [27,28]. In this case, the terms added to the Galerkin formulation of the problem depend on the residual of the finite element solution, which is thus considered the resolved scale. In contrast to our approach with *orthogonal* subscales, in the references mentioned the subscales are considered directly proportional to the finite element residual. This implies that the orthogonal projection is dropped in (23) and (24). This fact has an important consequence in the energy balance Eq. (28). First, the time derivative of the velocity, when weighted by the Navier–Stokes operator applied to the unknown, will yield a modification of the coefficient of the kinetic energy. It could be related to dissipation, but as far as the authors know there are no results of statistical fluid mechanics that allow to correlate these terms with the molecular dissipation. Second, for the body force term the situation is different, since it does not contribute to a dissipation term, but changes the effective external power exerted on the fluid and therefore the statistical analysis does not even make sense.

5.3. Numerical evidence

The starting assumption of our analysis is that the finite element mesh is able to capture velocity fields that lay in the inertial range and for which the results of statistical fluid mechanics can be applied. This condition should not be considered particularly stringent, as it is in fact analogous to what is assumed for the filtered velocity in classical LES models for which the filter width is proportional to (if not directly equal) the mesh size.

Although our analysis is restricted to isotropic turbulence, recent works seem to indicate that pure numerical approaches to LES turn to be valid not only for this case but also for a large variety of turbulent flows. A relevant numerical study of a residual based formulation modeling turbulent flows is [19]. The formulation is tested for isotropic forced turbulence and turbulent channel flows and the results are extremely good, in the sense that they clearly display the numerical convergence towards results from direct numerical simulation (DNS). Both mesh refinement and polynomial order increase (using NURBS) are tested. In the case of

isotropic turbulence, for coarse discretizations the numerical spectra match the DNS results only for small wave numbers, whereas the matching improves as the discretization is also improved. The important point, however, is that even for coarse discretizations *there is part of the inertial range which is captured* and, of course, with the correct slope, a characteristic feature of turbulent flows. For channel flows it is also shown that the boundary layers that are created have the regions corresponding to turbulence.

Further simulations on turbulent channel flows can be found in [29]. Moreover, in this work the case of turbulent flow on an asymmetric diffuser is also addressed. Again, excellent matching is found between all computed mean flow data and results from DNS and experiments. Besides, the case of turbulent flow over cuboid shaped surfaces is considered in [27] and in [30]. In the second work, the OSS approach with transient subscales is implemented [23] and it is shown capable to predict backscatter, as for dynamic LES closures. The OSS method is also used in [51] to simulate the flow over a circular plate. The expected slope for the pressure spectrum at the center of the plate is correctly recovered, in accordance with experiments. Finally, the variational multiscale turbulence modeling approach has also proved to yield very accurate results even for demanding rotating flows, such as the well-known Taylor–Couette turbulent flow between two concentric rotating cylinders [52].

In summary, there seems to be sound numerical evidence that it is in fact possible to model turbulence flows by means of residual based numerical formulations, without having to resort to physical LES modeling.

6. Conclusions

For a fine enough computational mesh, it has been proved that the contribution to the energy balance equation of the stabilization terms of the Orthogonal Subgrid Scale finite element method can be made proportional to the physical dissipation rate, if an appropriate redesign of the original OSS stabilization parameters is carried out. This has been done with the sole use of the quasi-normal approximation for two point fourth-order velocity correlations and using Kolmogorov's first and second similarity hypotheses. It has been also assumed that several statistical fluid mechanics results, which are valid for the exact velocity field, hold true for the approximated finite element velocity field.

Taking into account that the stabilization terms in the OSS method arise from pure numerical necessities it is a noteworthy fact that they have the correct physical behavior in the inertial sub-range of a turbulent flow. This somehow provides additional support to the idea that pure numerical LES through appropriate discretization of the Navier–Stokes equations could suffice to simulate turbulent flows, without having to resort to extra physical LES modeling at the continuum level.

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