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How much eddy dissipation is needed to counterbalance the nonlinear production of small, unresolved scales in a large-eddy simulation of turbulence?

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ABSTRACT

This paper is about models for large-eddy simulation of turbulent flow that truncate the small scales of motion for which numerical resolution is not available by making sure that they do not get energy from the larger, resolved, eddies. The resolved scales are defined with the help of a box filter. The eddy dissipation is determined in such a way that the production of too small, box-fitting, scales is counteracted. This dissipation-production balance is worked out with the help of Poincaré's inequality, which results in a condition that depends on the invariants of the velocity gradient. If the filter box is anisotropic the truncation condition is to be scaled in order to account for the anisotropy in the right way. The scaled truncation condition is applied to an eddy-viscosity model. This model is discretized and equipped with a Schumann filter. It is successfully tested for homogeneous turbulence as well as for turbulent channel flow.

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1. Larger eddies in turbulent flow

1.1. Navier–Stokes equations and turbulence

The Navier–Stokes (NS) equations provide a model for turbulent flow. In the absence of compressibility ($\nabla \cdot u = 0$), the NS-equations are

$$\partial_t u + \nabla \cdot (u \otimes u) - \nu \nabla \cdot \nabla u + \nabla p = 0, \quad (1)$$

where u denotes the fluid velocity, p stands for the pressure and ν is the viscosity.

Turbulence is generally visualized as a cascade of kinetic energy, see [1], e.g. Since the large scales of motion cannot reach an equilibrium between the rate at which energy is supplied and the rate at which energy is dissipated (by the action of viscosity), they break up, convecting energy to somewhat smaller scales (through the nonlinear term). The smaller scales undergo a similar process, and thus energy is transferred to yet smaller scales. The energy cascade continues until the scale is so small that dissipation becomes dominant. The entire spectrum - ranging from the scales where the flow is driven to the smallest, dissipative scales - is to be resolved numerically when turbulence is computed from the NS-equations. In most applications, however, the available computing power is inadequate to resolve the small scales where the dissipation takes

place. In other words, the NS-equations do not provide a tractable model for turbulent flow. Therefore, finding a coarse-grained description is one of the main challenges to turbulence research. A most promising methodology for that is large-eddy simulation [2].

1.2. Large-eddy simulation

Large eddy simulation (LES) seeks to predict the dynamics of spatially filtered turbulent flows. Usually a spatial filter is applied to the NS-equations to obtain a model for the larger eddies. The filtered NS-equations read

$$\partial_t \bar{u} + \nabla \cdot (\bar{u} \otimes \bar{u}) - \nu \nabla \cdot \nabla \bar{u} + \nabla \bar{p} = \nabla \cdot (\bar{u} \otimes \bar{u} - \bar{u} \otimes \bar{u}) \quad (2)$$

where $\bar{u}$ denotes the filtered velocity field. When the NS-equations are discretized in space, the low-pass characteristics of the discrete operators effectively act as a filter. This numeric filter will inevitably interact with the explicit filter in Eq. (2). So, at the discrete level, the effective filter is not so clear, unless we use the Schumann filter [3]. Therefore we adopt the Schumann filter, i.e., we take

$$\bar{u} = \frac{1}{|\Omega_h|} \int_{\Omega_h} u(x, t) dx,$$

where Ω_h denotes a computational cell that is used in the finite-volume discretization. Eq. (2) is derived assuming that the filter $u \mapsto \bar{u}$ commutes with linear differential operators in the NS-equations. The main problem is that the filter does not commute

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with the nonlinear term $u \otimes u$. The right-hand side represents the effects of the residual scales on the ‘larger eddies’. It depends on both u and $\bar{u}$. To remove the dependence on u the commutator of $u \otimes u$ and the filter is replaced by a closure model. This yields

$$\partial_t v + \nabla \cdot (v \otimes v) - \nu \nabla \cdot \nabla v + \nabla \pi = -\nabla \cdot \tau(v) \quad (3)$$

where the variable name is changed from $\bar{u}$ to v (and $\bar{p}$ to π) to stress that the solution of Eq. (3) differs from that of Eq. (2), because the closure model τ is not exact [4].

1.3. Introduction to closure models

In large-eddy simulation, the effects of the small-scale motions on the large scales (eddies) have to be modeled. Many closure models have been proposed and successfully applied to the simulation of a wide range of turbulent flows (see, e.g., [2] for an overview). Some models have been derived such that properties of the exact closure (resulting from the Navier–Stokes equations) are built in. Vreman [5], for example, proposed a model that vanishes for a class of laminar flows. Razafindralandy et al. [6] designed models that preserve the symmetries of the Navier–Stokes equations. Nicoud et al. [7] introduced models having the proper near-wall scaling. Clark et al. [8] considered the leading-order term of a formal series expansion of the commutator of $u \otimes u$ and an box filter. Germano et al. [9] introduced the so-called dynamic procedure that enforces the Jacobi identity. This identity applies to every commutator; in the present context it is often called the Germano identity. Verstappen [10] proposed an eddy-viscosity model where the eddy-viscosity is determined such that the production of small scales of motion is counterbalanced by the eddy-dissipation. The resulting eddy-viscosity was expressed in term of the invariants Q_s and R_s of S , the symmetric part of the velocity gradient. However, simulations with the $Q_s R_s$ model produced mixed results on anisotropic grids [11,12]. Rozema et al. [13,14] argued that the $Q_s R_s$ model gives wrong predictions on anisotropic grids, because a sufficiently accurate approximation of the filter width - on anisotropic grids - could not be found. They reformulated the minimum dissipation condition in such a way that the geometry of the filter box is explicitly taken into account, thus avoiding the need to prescribe the width of an anisotropic filter. Their anisotropic minimum dissipation (AMD) eddy-viscosity model gave good results for decaying isotropic turbulence, a turbulent mixing layer and a turbulent channel flow [13]. However, the AMD model does not express the eddy viscosity in terms of invariants of the velocity gradient; hence, it is not frame-invariant. In this paper, we reuse the reasoning underlying the AMD model, but deviate thereof (i.e., treat the anisotropy of the filter differently) in order to derive a closure model depending on the invariants and of the velocity gradient. Furthermore, we generalize the approach, that is the eddy-viscosity model becomes a realization of a more general principle. Besides, the resulting closure model is discussed in a discrete setting.

The outline of this paper is as follows. In Section 2 we introduce the basic idea: the production of undesirable small scales of motion is to be counterbalanced by the eddy dissipation, i.e., the dissipation resulting from the closure model. Next, we make use of Poincaré’s inequality to develop the production-dissipation balance without explicitly referring to the small scales of motion. Section 3 is dedicated to the Poincaré inequality. The key point in this section is the scaling of the Poincaré inequality on (highly) anisotropic grids. The production-dissipation balance is worked out in Section 4 with the help of the scaled Poincaré inequality. In Section 5 we consider eddy-viscosity models. Section 6 discusses the spatial discretization; in particular it illustrates the entanglement of the discretization error and the closure model. On isotropic grids, the proposed closure model is identical to the

AMD model [13]. Therefore, the model is only tested on anisotropic grids, details can be found in Section 7. Finally, Section 8 consists of a summary of the current work and an outlook.

2. Truncation of scales

The very essence of large-eddy simulation (LES) is that the (explicit) calculation of all small-scale turbulence - for which numerical resolution is not available - is avoided. This sets a condition to the closure model [10]. To determine this condition, we consider an arbitrary part of the flow domain with diameter δ . With the aid of the associated box filter,

$$\tilde{v} = \frac{1}{|\Omega_\delta|} \int_{\Omega_\delta} v(x, t) dx, \quad (4)$$

the undesirable small scales in the velocity field v are defined by $v' = v - \tilde{v}$. It may be remarked that the size of the filter box Ω_δ is to be selected by the user. The filter box will generally differ from the grid box Ω_h that was used to filter the NS-equations; here it is assumed that $|\Omega_\delta| \geq |\Omega_h|$.

The residual of the box filter, v' , consist of scales of size smaller than δ . The closure model τ must be designed so that these small scales are decoupled from the larger eddies; here defined as eddies having a diameter larger than δ . If this decoupling is achieved the small-scale field v' need not be calculated and we can suffice with a simulation of the larger eddies only. Therefore the nonlinear coupling between the velocity fields $\tilde{v}$ and v' must be broken. To develop this further, we consider the coupling from the side of the residue v' . By applying the residual operator to Eq. (3) we find the governing equation for v' and from that we obtain the evolution of its $L^2(\Omega_\delta)$ norm:

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |v'|^2 dx &= \nu \int_{\Omega_\delta} (\nabla \cdot \nabla v)' \cdot v' dx \\ &\quad - \int_{\Omega_\delta} (\nabla \cdot (\pi I + v \otimes v + \tau))' \cdot v' dx \end{aligned} \quad (5)$$

The first term in the right-hand side above is the result of a linear process, the diffusion caused by the fluid viscosity. The other terms in the right-hand of Eq. (5) represent the nonlinear processes that modify the energy of the small scales of motion. Here it may be noted that the nonlinearity of the pressure-velocity relation becomes apparent when the divergence of Eq. (3) is taken; indeed this gives $\nabla \cdot \nabla \pi = -\nabla \cdot (v \otimes v + \tau)$. Only nonlinear processes can transfer energy from the box-filtered velocity field $\tilde{v}$ to the residual field v' and vice versa. Consequently, if the closure model is taken so that the nonlinear terms in Eq. (5) cancel each other out, then

$$\frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |v'|^2 dx = \nu \int_{\Omega_\delta} (\nabla \cdot \nabla v)' \cdot v' dx \quad (6)$$

and the evolution of the energy of v' does not depend on $\tilde{v}$. Stated otherwise, the energy of residual scales dissipates at its natural rate, without any forcing mechanism involving $\tilde{v}$. In this way, all scales of size smaller than δ are separated from those larger than δ .

To further illustrate the scale-separation condition (6) we assume that the flow domain is covered by a large number of non-overlapping filter boxes. Integrating Eq. (6) by parts gives

$$\frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |v'|^2 dx = -\nu \int_{\Omega_\delta} |\nabla v'|^2 dx + \nu \int_{\partial\Omega_\delta} v' \cdot \partial_n v' ds \quad (7)$$

where n is the outward-pointing normal vector to the boundary $\partial\Omega_\delta$ of Ω_δ . Because the volume integral in the right-hand side is non-positive, only the surface integral can result into an increase of the $L^2(\Omega_\delta)$ norm of v' . The sign of the boundary integral in (7) poses an intricate unsettled question, since the box filter is not

equipped with boundary conditions. However, the natural initial condition for a large-eddy simulation is given by $v' = 0$ in every filter box. So, initially, there is no difference between the v' 's on the two sides of the interface between adjacent filter boxes. Consequently, the diffusive flux through this face is zero. In case the consider face coincides with a part of the boundary of the flow domain, we further assume that the boundary condition are $v' = 0$ or $\partial_n v' = 0$, i.e., the boundary conditions do not generate a sub-filter contribution to the velocity field. Therefore, with $v' = 0$ initially and passive boundary conditions Eq. (7) leads to the conclusion that the $L^2(\Omega_\delta)$ norm of v' remains zero for all times $t > 0$. It may be noted that this implies that v' vanishes pointwise. Finally, $v' = 0$ is a stable solution, meaning that any disturbance decays exponentially fast. Indeed if a disturbance is introduced in one of the filter boxes then it diffuses through the faces of the boxes and thus spreads through the flow domain whereby it disappears eventually due to action of the viscosity. Here energy can not be accumulated in one filter box, because of the diffusive character of Eq. (7). Again it may be emphasized that Eq. (7) contains no external forces; hence, if the energy increases in a certain filter box due to a disturbance in an adjacent box, it is at the expense of the disturbance.

The closure model must keep the residual field v' from becoming dynamically significant for the 'larger eddies', i.e., the part of the motion consisting of scales of size larger than the filter length δ . Our guiding principle is that the residual part of the motion is removed by the action of viscosity, as described by Eq. (5). Therefore the production of small scales of motion is to be balanced by the modeled dissipation:

$$\begin{aligned} \int_{\Omega_\delta} (\nabla \cdot \tau)' \cdot v' dx &= - \int_{\Omega_\delta} (\nabla \cdot (v \otimes v + \pi I))' \cdot v' dx \\ &= - \int_{\Omega_\delta} (\nabla \cdot (v \otimes v))' \cdot v' dx \\ &\quad - \int_{\partial\Omega_\delta} \pi' v' \cdot n ds \end{aligned} \quad (8)$$

where use is made of $\nabla \cdot v' = 0$ and n is the outward-pointing normal vector to the boundary $\partial\Omega_\delta$ of Ω_δ . In principle, we could verify whether this condition is met during a LES. But that is not very attractive, because it requires a fair approximation of v' , which is quite expensive to compute. The more so since the user has chosen the filter length δ in such a way that the residual field v' is not of interest to him or her. Alternatively, v' might be expressed in terms of the resolved field by means of an approximate deconvolution procedure. However, such a procedure is not attractive either, since it is inherently ill-conditioned. In short, we are caught in the following dilemma: we do not want to compute the small details, but in order to verify that they need not be computed, we have to compute them.

3. Poincaré's inequality

We make use of Poincaré's inequality to develop the dissipation-production balance (8) without explicitly referring to the residual field v' , see also [10]–[14]. Poincaré's inequality bounds the norm of a function in terms of the norm of its derivative and the geometry of the domain of definition, see [15], e.g. There are different versions of Poincaré's inequality. Here we use the variant which is also called Poincaré–Wirtinger inequality. It states that there exists a constant C_δ depending only on the domain Ω_δ such that

$$\int_{\Omega_\delta} |v - \tilde{v}|^2 dx \leq C_\delta \int_{\Omega_\delta} |\nabla v|^2 dx \quad (9)$$

That is, the $L^2(\Omega_\delta)$ norm of the residual field v' is bounded by a constant (independent of v) times the $L^2(\Omega_\delta)$ norm of ∇v . Payne

and Weinberger [16] have shown that the Poincaré constant is given by $C_\delta = (\delta/\pi)^2$ for convex (bounded, Lipschitz) domains Ω_δ . This is the best possible estimate in terms of the diameter alone.

The Poincaré inequality provides an upper bound for the energy of the unwanted subfilter scales of motion using bounds on the velocity gradient and the geometry of the filter box. The Poincaré constant C_δ provides the bound for the geometry. In case the filter box is quite anisotropic, however, the diameter δ does not provide a sufficiently detailed description of the geometry of the filter box. Consequently, the Poincaré upperbound systematically overestimates a portion of the contributions to $L^2(\Omega_\delta)$ norm of the sub-filter velocity v' . This issue can be solved by scaling Poincaré's inequality properly, see also [13].

3.1. Need to scale Poincaré's inequality

To illustrate the basic problem, we consider a rectangular box with (very different) dimensions δ_1 , δ_2 and δ_3 , respectively. The velocity field is made up of waves with length $\lambda_j = \delta_j/n_j$, i.e., the wave number is $k_j = 2\pi n_j/\delta_j$, where $j = 1, 2, 3$. Further we consider the following scalar velocity

$$v(x) = e^{ik_j x_j}$$

where it may be noted that the Einstein summation convention applies again, i.e., the right-hand side represents a summation over the terms indexed by j . The 3D filter box Ω_δ consists of all ξ_j that satisfy $x_j - \delta_j/2 \leq \xi_j \leq x_j + \delta_j/2$, where $j = 1, 2, 3$. For any j we have,

$$\frac{1}{\delta_j} \int_{x_j - \delta_j/2}^{x_j + \delta_j/2} e^{ik_j \xi_j} d\xi_j = G(n_j) e^{ik_j x_j} \quad \text{with} \quad G(n_j) = \frac{\sin(\pi n_j)}{\pi n_j} \quad (10)$$

and $\pi n_j = k_j \delta_j/2$. Thus the box-filtered velocity is given by

$$\tilde{v}(x) = G(n_j) e^{ik_j x_j}$$

In other words, the accuracy with which the filtered velocity $\tilde{v}$ can represent the full velocity v depends on the number of filter lengths per wave length, that is n_j , and is not an explicit function of the filter length δ_j . Here it may be noted that G is the well-known box filter kernel in the spectral space. The residue v' is given by a combination of Fourier-modes wherein the weights $1 - G_j$ are functions of n_j . If the filter box is centered around the origin $x_j = 0$, Eq. (10) shows that the application of the filter to an arbitrary Fourier-mode results into an expression that depends only on n_j . Hence, applying the box filter to $(v')^2$ leads to an expression of the form

$$\frac{1}{|\Omega_\delta|} \int_{\Omega_\delta} (v - \tilde{v})^2 dx = \text{function}(n_1, n_2, n_3) \quad (11)$$

where again the position x drops out because the filter box is centered around $x = 0$. Thus, the $L^2(\Omega_\delta)$ -norm of the fluctuating velocity v' depends on the ratio n_j of wave length λ_j to the box size δ_j ; it does not depend directly on the filter length δ_j . However, a straightforward calculation shows that

$$\begin{aligned} \frac{C_\delta}{|\Omega_\delta|} \int_{\Omega_\delta} |\nabla v|^2 dx &= \frac{C_\delta}{|\Omega_\delta|} \int_{\Omega_\delta} (\partial_j v)^2 dx \\ &= -\frac{C_\delta}{\delta_j^2} (2\pi n_j)^2 \sin(2\pi n_j) \end{aligned} \quad (12)$$

where we have again taken $x = 0$. Hence, the Poincaré upperbound depends in this case on both the ratio n_j and filter length δ_j , unless the filter box is a cube ($\delta_j = \delta = \text{constant}$). So, in conclusion, although for fixed n_j the filter length δ_j does not affect the $L^2(\Omega_\delta)$ norm of the fluctuating velocity, see Eq. (11), the Poincaré upperbound (12) does inevitably depend explicitly on δ_j if the filter box is not a cube; that is, if the filter is anisotropic. Eq. (12) shows

that (again for fixed n_j) the $L^2(\Omega_\delta)$ norm of the velocity gradient is dominated by contributions associated with the direction in which the filter length is smallest. Consequently, a scale-truncation model based on that Poincaré upperbound gets a bias in the direction of the smallest filter length. To remove that dominant direction, Poincaré's inequality is to be scaled.

3.2. Scaling of Poincaré's inequality

The example in the previous section illustrates the need to scale Poincaré's inequality. Of course, mathematically there is nothing wrong with Poincaré's inequality; the problem in question is that Poincaré's upperbound is physically not tight enough if the filter box differs significantly from a cube. This problem finds its origin in an erroneous functional dependence on the filter lengths: seen physically, it is too imprecise to condense all geometrical data into one number, the Poincaré constant C_δ , if the filter box has (very) different length scales δ_j .

We can tighten Poincaré's upperbound by scaling the velocity gradient with the filter length. To that end the derivative in the i th direction is multiplied by the corresponding filter length δ_{i_k} i.e., the scaled partial derivative with respect to x_i is defined by $\hat{\partial}_i = \delta_i \partial_i$. The components of the scaled velocity gradient are then described by

$$(\hat{\nabla} v)_{ij} = \delta_i \partial_i v_j \quad (13)$$

It may be remarked that $\hat{\nabla}$ can be viewed as the gradient operator in an isotropic computational space that is defined through the map $x_j \mapsto \hat{x}_j = x_j/\delta_j$.

If we now consider the (scalar) example from the previous section, we find

$$\begin{aligned} \frac{1}{|\Omega_\delta|} \int_{\Omega_\delta} |\hat{\nabla} v|^2 dx &= \frac{1}{|\Omega_\delta|} \int_{\Omega_\delta} \delta_j^2 (\partial_j v)^2 dx \\ &= -(2\pi n_j)^2 \sin(2\pi n_j) \end{aligned}$$

So the box-averaged norm of the scaled velocity gradient depends only on the ratio n_j of the box length δ_j to the wave length λ_j of the velocity, just like the box-averaged norm of the fluctuating velocity. Therefore, the scaled gradient provides a better starting-point for bounding the small-scale details than the unscaled gradient. Therefore Rozema et al. [13] proposed the modified Poincaré inequality

$$\int_{\Omega_\delta} |v - \tilde{v}|^2 dx \leq C \int_{\Omega_\delta} |\hat{\nabla} v|^2 dx \quad (14)$$

where C is a constant independent of δ_j . Thus, whereas the original Poincaré inequality (9) incorporates the dependence on the size of the filter box in the Poincaré constant C_δ , the modified Poincaré inequality incorporates the dependence on the size of the filter box by scaling the velocity gradient $\partial_j v$ with δ_j .

3.3. Anisotropic Poincaré inequality

Thus far the scaling of Poincaré's inequality was considered for a scalar velocity only. The resulting scaling (14) is identical to that proposed in Ref. [13]. If the filter box is highly anisotropic, however, we will have to consider the scaling of the components of the velocity vector too. This part of the scaling is missing in Ref. [13]. Here, we choose the scaling of the velocity components in such a way that both the convective term and closure remain invariant under the scaling of the velocity vector. Therefore, we introduced the scalings

$$\hat{x}_i = \frac{x_i}{\delta_i} \quad \text{and} \quad \hat{v}_i(\hat{x}, t) = \frac{v_i(x, t)}{\delta_i}$$

Thus, the incompressibility constraint becomes $\hat{\nabla} \cdot \hat{v} = 0$, and the momentum equation transforms in

$$\partial_t \hat{v} + \hat{\nabla} \cdot (\hat{v} \otimes \hat{v}) - \nu \nabla \cdot \nabla \hat{v} + \hat{\nabla} \cdot \hat{\pi} = -\hat{\nabla} \cdot \hat{\tau} \quad (15)$$

where $\hat{\pi} = \text{diag}(\delta_i^{-2}) \pi$ and $\hat{\tau}_{ij} = \tau_{ij}/(\delta_i \delta_j)$. So, in conclusion, we apply the modified Poincaré inequality to $\hat{v}$, that is we make use of

$$\int_{\Omega_\delta} |\hat{v}'|^2 dx \leq C \int_{\Omega_\delta} |\hat{\nabla} \hat{v}|^2 dx \quad (16)$$

to bound the residual velocity field.

4. Balancing the production of small scales of motion

Poincaré's inequality (16) shows that the residual field $\hat{v}'$ can be suppressed by controlling the velocity gradient $\hat{\nabla} \hat{v}$. In other words, the flow can be confined to the larger eddies by introducing a suitable amount of eddy dissipation in the dynamics of the velocity gradient. In this section we aim to convert the dissipative condition (6) to the upper bound set by the Poincaré inequality (16). According to Eq. (15) the $L^2(\Omega_\delta)$ norm of ∇v is governed by

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |\hat{\nabla} \hat{v}|^2 dx &= \int_{\Omega_\delta} \hat{\nabla} (\nu \nabla \cdot \nabla \hat{v} - \hat{\nabla} \cdot \hat{\pi} \\ &\quad - \hat{\nabla} \cdot (\hat{v} \otimes \hat{v}) - \hat{\nabla} \cdot \hat{\tau}) : \hat{\nabla} \hat{v} dx \end{aligned} \quad (17)$$

Here it may be remarked that we use the notation $a : b = \sum_{ij} a_{ij} b_{ij}$. As in Eq. (5), the latter three terms in the right-hand side represent the nonlinear production as a result of the pressure, convection and the modeled eddy-dissipation, respectively. Thus expressed in terms of the velocity gradient the production-dissipation balance (8) reads

$$\begin{aligned} \int_{\Omega_\delta} \hat{\nabla} \hat{\nabla} \cdot \hat{\tau} : \hat{\nabla} \hat{v} dx &= - \int_{\Omega_\delta} \hat{\nabla} \hat{\nabla} \cdot (\hat{v} \otimes \hat{v}) : \hat{\nabla} \hat{v} dx \\ &\quad - \int_{\partial \Omega_\delta} (\hat{\nabla} \cdot \hat{\pi}) \cdot \hat{\nabla} \hat{v} \hat{n} ds \end{aligned} \quad (18)$$

It may be noted that the part of volume integral in Eq. (17) which contains the pressure gradient can be written as a surface integral because $\hat{\partial}_j \hat{v}_j = 0$:

$$\begin{aligned} \int_{\Omega_\delta} (\hat{\partial}_i \hat{\partial}_j \hat{\pi}) (\hat{\partial}_i \hat{v}_j) dx &= \int_{\Omega_\delta} \hat{\partial}_j (\hat{\partial}_i \hat{\pi} \hat{\partial}_i \hat{v}_j) dx \\ &= \int_{\partial \Omega_\delta} (\hat{\partial}_i \hat{\pi}) (\hat{\partial}_i \hat{v}_j \hat{n}_j) ds \end{aligned}$$

where the Einstein summation convention applies, i.e., the above formula represents a summation over the terms indexed by i and j . In the sequel we will implicitly use Einsteins notation too. Thus if the model $\hat{\tau}$ satisfies Eq. (18) then Eq. (17) shows that the Poincaré upperbound of the residual field $\hat{v}'$ - that is, the $L^2(\Omega_\delta)$ -norm of $\hat{\nabla} \hat{v}$ - dissipates at its natural rate (which is set by the fluid viscosity ν).

For incompressible flows, the Cayley-Hamilton theorem states that $\hat{\nabla}^3 - \hat{Q} \hat{\nabla} + \hat{R} = 0$, where the second and third invariant of the velocity-gradient tensor are $\hat{Q}(\hat{v}) = \frac{1}{2} \hat{\nabla} \hat{v} : \hat{\nabla} \hat{v}$ and $\hat{R}(\hat{v}) = -\frac{1}{3} \hat{\nabla} \hat{v} \hat{\nabla} \hat{v} : \hat{\nabla} \hat{v} = -\det \hat{\nabla} \hat{v}$, respectively. The right-hand side of Eq. (18) can be written in terms of these invariants. Indeed, since $\hat{\partial}_k \hat{v}_k = 0$, we have

$$\begin{aligned} \int_{\Omega_\delta} \hat{\partial}_i \hat{\partial}_k (\hat{v}_k \hat{v}_j) \hat{\partial}_i \hat{v}_j dx &= \int_{\Omega_\delta} \hat{\partial}_i \hat{v}_k \hat{\partial}_k \hat{v}_j \hat{\partial}_i \hat{v}_j + \frac{1}{2} \hat{\partial}_k (\hat{v}_k (\hat{\partial}_i \hat{v}_j)^2) dx \\ &= - \int_{\Omega_\delta} 3 \hat{R}(\hat{v}) dx + \int_{\partial \Omega_\delta} \hat{Q}(\hat{v}) \hat{v} \cdot \hat{n} ds \end{aligned}$$

where $\hat{n}$ is the outward-pointing normal vector to the boundary $\partial \Omega_\delta$ of Ω_δ and $\hat{n}_i = n_i/\delta_i$. It may be recalled that the entries of $\hat{\nabla} \hat{v}$ are given by $(\hat{\nabla} \hat{v})_{ij} = \delta_i \partial_i v_j/\delta_j$.

In conclusion, the nonlinear contributions to the evolution of the $L^2(\Omega_\delta)$ norm of $\widehat{\nabla}\widehat{v}$ are balanced by the closure model if

$$\int_{\Omega_\delta} \widehat{\nabla}\widehat{v} \cdot \widehat{\tau} : \widehat{\nabla}\widehat{v} dx = 3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx - \int_{\partial\Omega_\delta} \widehat{Q}(\widehat{v}) \widehat{v} \cdot \widehat{n} ds - \int_{\partial\Omega_\delta} \widehat{\nabla}\widehat{\pi} \cdot \widehat{\nabla}\widehat{v} \widehat{n} ds \quad (19)$$

Here it may be noted that the volume integral in the right-hand side of Eq. (19) represents the production of $\widehat{Q} = \frac{1}{2} \|\widehat{\nabla}\widehat{v}\|^2$ inside the box Ω_δ , whereas the first surface integral represents the flux of $\widehat{Q}$ through the boundary of the box; the negative sign occurs because the normal is taken in the outward direction. The second surface integral in (19) represents the contribution that is related to the pressure $\widehat{\pi}$, i.e., it can be seen as the consequence of the incompressibility condition which states that the first invariant of the velocity-gradient vanishes: $\widehat{\nabla}\widehat{v} : I = 0$.

Eq. (19) ensures that the $L^2(\Omega_\delta)$ norm of $\widehat{\nabla}\widehat{v}$ is governed by

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |\widehat{\nabla}\widehat{v}|^2 dx &= \nu \int_{\Omega_\delta} \widehat{\nabla}(\nabla \cdot \nabla \widehat{v}) : \widehat{\nabla}\widehat{v} dx \\ &= -\nu \int_{\Omega_\delta} \nabla \widehat{\nabla}\widehat{v} : \nabla \widehat{\nabla}\widehat{v} dx \\ &\quad + \nu \int_{\partial\Omega_\delta} \widehat{\nabla}\widehat{v} : \partial_n \widehat{\nabla}\widehat{v} ds \end{aligned} \quad (20)$$

Note that Eq. (20) follows from Eqs. (17)–(19). We can now try to copy and paste the reasoning that followed after Eq. (7), with $\widehat{v}'$ replaced by $\widehat{\nabla}\widehat{v}$, and thus show that Eq. (20) ensures that the sub-filter velocity $\widehat{v}'$ does not increase if the large-eddy simulation is started with $\widehat{v}' = 0$ and the boundary conditions create no $\widehat{v}'$. As in Eq. (7), only the surface integral in Eq. (20) need be considered here, since the volume term cannot increase the $L^2(\Omega_\delta)$ norm of $\widehat{\nabla}\widehat{v}$. Here, the filter boxes are non-overlapping and cover the entire flow domain. The initial condition is given by $\widehat{v}' = 0$ in every filter box, i.e., $\widehat{v}$ is constant; hence, we have $\widehat{\nabla}\widehat{v} = 0$ initially. It may be stressed that this applies to all filter boxes. Therefore, $\widehat{\nabla}\widehat{v}$ has initially the same value on both sides of an interface between adjacent filter boxes and as a result, the diffusive flux through the face is zero. This holds for all faces $\partial\Omega_\delta$, except for those parts that are also part of the boundary Γ of the flow domain. There we have $\widehat{v}' = 0$ or $\partial_n \widehat{v}' = 0$. Yet, these passive boundary conditions cannot be translated easily to $\widehat{\nabla}\widehat{v}$. In general it is not clear what boundary condition are imposed to $\widehat{\nabla}\widehat{v}$. To begin with, we can ensure that $\widehat{\nabla}\widehat{v}$ remains zero for all times by moving all contributions resulting from the boundary of the flow domain from Eq. (20) to the production-dissipation balance (19). Thus we arrive at

$$\begin{aligned} \int_{\Omega_\delta} \widehat{\nabla}\widehat{v} \cdot (\widehat{\tau} + \widehat{\pi}I) : \widehat{\nabla}\widehat{v} dx &= 3 \int_{\Omega_\delta} \widehat{R} dx - \int_{\partial\Omega_\delta} \widehat{Q} \widehat{v} \cdot \widehat{n} ds \\ &\quad + \nu \int_{\Gamma_\delta} \partial_n \widehat{Q} ds \end{aligned} \quad (21)$$

where Γ_δ denotes the (possibly empty) intersection of the boundary Γ of the fluid domain and the boundary $\partial\Omega_\delta$ of the filter box. Now, the boundary integral in Eq. (20) is to be taken over the part of $\partial\Omega_\delta$ that is not part of the boundary of the flow domain, i.e. over $\partial\Omega_\delta \setminus \Gamma_\delta$. Because any non-passive boundary conditions are removed from Eq. (20), there is nothing left that can result in an increase in $\widehat{\nabla}\widehat{v}$ and, therefore, $\widehat{\nabla}\widehat{v}$ remains zero for all times $t > 0$. Moreover, $\widehat{\nabla}\widehat{v} = 0$ is a stable solution of the diffusive process governed by Eq. (20). Since $\widehat{\nabla}\widehat{v} = 0$ implies that $\widehat{v}$ is constant in Ω_δ , we can conclude that $\widehat{v}' = 0$ for all $t > 0$.

The last term in Eq. (21) is introduced solely to mathematically guarantee that $\widehat{v}' = 0$, for all possible boundary conditions on (the second invariant $\widehat{Q}$ of) $\widehat{\nabla}\widehat{v}$. Obviously, the last term in Eq. (21) can be dropped if it is assumed that $\partial_n \widehat{Q} \approx 0$ at the boundary Γ of the flow domain. This assumption is very reasonable. In-

deed, if $\partial_n \widehat{Q} \neq 0$ at the boundary Γ , then $\widehat{Q} = \frac{1}{2} |\widehat{\nabla}\widehat{v}|^2$ is forced in the adjacent filter box. As a result $\widehat{\nabla}\widehat{v}$ will not remain zero there. This implies that $\widehat{v} \neq 0$ in the filter box adjacent to Γ . Therefore a boundary condition of the form $\partial_n \widehat{Q} \neq 0$ is not passive meaning that it introduces a mechanism that can produce $\widehat{v}'$. Therefore $\partial_n \widehat{Q} \neq 0$ at Γ is not really suitable as a boundary condition in a large-eddy simulation. For that reason, we assume that $\partial_n \widehat{Q} \approx 0$ at Γ . Under that assumption the conditions (19) and (21) coincide, and therefore, we can conclude that if the flow is initialized such that $\widehat{v}' = 0$ and the boundary conditions create no $\widehat{v}'$ (i.e., $\partial_n \widehat{Q} \approx 0$) then Eq. (19) ensures that the residual field $\widehat{v}'$ remains zero for all times. So, Eq. (19) represents a scale-truncation condition which does not involve the subfilter velocity $\widehat{v}'$.

Finally it may be remarked that condition (19) ensures that the modeled dissipation (that is, $\int_{\Omega_\delta} \widehat{\nabla}\widehat{v} \cdot \widehat{\tau} : \widehat{\nabla}\widehat{v} dx$) counterbalances the nonlinear production of scales that are so small that they fit in the box Ω_δ . But this balance is achieved just as well if energy is transferred from the small, box-fitting scales to the larger eddies. In this case the modeled dissipation is negative. The problem here is that the small box-fitting scales of motion do not have any physical significance; actually, their dynamics is swept under the carpet, because it is too expensive to compute. Hence, data transferred from the small, box-fitting scales to the larger eddies is mostly incorrect. Therefore, the closure model is set to zero if Eq. (19) yields a negative value for the eddy dissipation, i.e., the closure model is clipped just as in the dynamical procedure. As such we have a good truncation model, but it may be noted that is not completely leakproof. Since only the model is disabled if the small, sub-filter scales transfer energy to the larger eddies, the transfer itself continues, i.e., the convective term in Eq. (19) can still send erroneous data from the small, sub-filter scales to the larger eddies. We touch here the subtle difference between scale truncation and scale separation. To provide a complete separation the model has to stop the effect of the little ones on the larger eddies too. This may be accomplished by removing the amount of energy that would otherwise be transferred; the adagio would then be: if it is taken away nothing is left to transfer. To dissipate energy also in case it is transferred towards the larger eddies, the clipping method is to be replaced by taking the absolute value. However, we expect this will make no significant difference to the clipping method, because the truncation model is so designed that the subfilter scales are not made, so if they also not initialized, their magnitude, and hence also their impact, will be negligible.

By definition, $\widehat{Q}$ and $\widehat{R}$ are the second and third invariant of the scaled velocity-gradient $\widehat{\nabla}\widehat{v}$. To give an interpretation to $\widehat{R}$, we note that the surface terms in Eq. (19) represent the influx of $\widehat{Q}$ and the impact of a pressure difference on $\widehat{Q}$, respectively. Thus the volume integral of $\widehat{R}$ can be seen as the term which describes the production of $\widehat{Q}$. To see how the production of $\widehat{Q}$ is related to the production of the small-scale energy $\frac{1}{2} |\widehat{v}'|^2$, we split off a divergence term from the volume term in Eq. (19), i.e., the volume integral is written as

$$\begin{aligned} & - \int_{\Omega_\delta} \widehat{\partial}_i ((\nabla \cdot (\mathbf{v} \otimes \mathbf{v}))_j \widehat{\partial}_i v_j) dx + \int_{\Omega_\delta} (\nabla \cdot (\mathbf{v} \otimes \mathbf{v}))_j \widehat{\partial}_i \widehat{\partial}_i v_j dx \\ \text{Note: } \widehat{\nabla}\widehat{v} \cdot (\widehat{v} \otimes \widehat{v}) : \widehat{\nabla}\widehat{v} &= \widehat{\nabla}\widehat{v} \cdot (\mathbf{v} \otimes \mathbf{v}) : \widehat{\nabla}\widehat{v}. \text{ Thus with the help of Gauss divergence theorem, we get} \\ & - \int_{\Omega_\delta} \widehat{\nabla}\widehat{v} \cdot (\widehat{v} \otimes \widehat{v}) : \widehat{\nabla}\widehat{v} dx = - \int_{\partial\Omega_\delta} (\nabla \cdot (\mathbf{v} \otimes \mathbf{v})) \cdot (\widehat{\nabla}\widehat{v})^T \widehat{n} ds \\ & \quad + \int_{\Omega_\delta} (\nabla \cdot (\mathbf{v} \otimes \mathbf{v})) \cdot (\widehat{\nabla}\widehat{v}) dx \end{aligned} \quad (22)$$

where $\widehat{n}_i = \delta_i n_i$ and $(\widehat{\nabla}\widehat{v})^T \widehat{n} = \widehat{\partial}_i v_j \widehat{n}_i$. The volume integral in the right-hand side of Eq. (22) can be seen as the component of the convective term $\nabla \cdot (\mathbf{v} \otimes \mathbf{v})$ in the direction of $\widehat{\nabla}\widehat{v}$. To interpret this direction, we relate the residue of the box filter

to the error in the midpoint rule for numerical integration. In one spatial dimension, the error ϵ in the midpoint rule is given by $\int_0^\delta v(x) dx = \delta v(\delta/2) + \epsilon$ with $\epsilon = \frac{1}{24} \delta^3 \partial_x^2 v(c)$ where c lies somewhere between 0 and δ . An expression for the residue of the one-dimensional box filter is obtained by dividing this error by $-\delta$. Thus we get in lowest order: $v'(x) = -\frac{1}{24} \partial_x^2 v(x) + \mathcal{O}(\delta^3)$ for any x in the one-dimensional “box” $0 \leq x \leq \delta$. The above approximation of the residue can be extended to more spatial dimensions. This yields (cf. [8])

$$v' = -\frac{1}{24} \widehat{\nabla} \cdot \widehat{\nabla} v + \mathcal{O}(\delta^3) \quad (23)$$

So, in conclusion, the volume integral in the right-hand side of Eq. (22) is (in lowest order) proportional to the component of the convective, nonlinear term in Eq. (3) in the direction of the residue of the box filter (4). Here the constant of proportionality can be incorporated into the constant C in the scaled Poincaré inequality (14). Notice that $1/24$ corresponds to taking $C = 1/12$ in Eq. (14).

5. Eddy viscosity

The anisotropic scale-truncation condition (19) applies to any closure model τ . The eddy-viscosity model is the most widely used model. For that reason, we consider it here. That is, we adopt the template

$$\tau(v) - \frac{1}{3} \text{tr}(\tau) I = -2 \nu_t S(v) \quad (24)$$

where ν_t denotes the eddy viscosity and $S(v)$ is the symmetric part of the velocity gradient, i.e., $S(v) = \frac{1}{2}(\nabla v + \nabla v^*)$. As usual, the factor -2 is introduced in Eq. (24). Moreover only the deviatoric component of the closure tensor is described here, because the divergence of the volumetric, isotropic component $\frac{1}{3} \text{tr}(\tau) I$ can be incorporated into the pressure gradient; see Eq. (3). The classical Smagorinsky model reads $\nu_t = C_S^2 \delta^2 \sqrt{4q}$, where C_S is the Smagorinsky constant and $q = \frac{1}{2} S : S$ is the second invariant of S .

For the eddy-viscosity model (24) the scale-truncation condition (19) becomes

$$\begin{aligned} - \int_{\Omega_\delta} \widehat{\nabla} \nabla \cdot \nu_t \widehat{\nabla} v : \widehat{\nabla} v dx &= 3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx - \int_{\partial \Omega_\delta} \widehat{Q}(\widehat{v}) \widehat{v} \cdot \widehat{n} ds \\ &\quad - \int_{\partial \Omega_\delta} (\widehat{\nabla} \cdot \widehat{\pi}) \cdot \widehat{\nabla} v \widehat{n} ds \end{aligned} \quad (25)$$

Here the left-hand side represents the eddy-dissipation of scales that are too small to be resolved, the volume integral over $\widehat{R}$ represents the production of these scales, and the surface integrals in the right-hand side describe their transport. Now if we assume that the dissipation balances the production, then there is no net production; so there is nothing to be transported. Therefore we omit the contribution of the transport terms here. Furthermore, we assume that the eddy-viscosity consists of large scales only, i.e., ν_t is taken constant in Ω_δ . Under these assumptions, Eq. (25) simplifies to

$$-\nu_t \int_{\Omega_\delta} \widehat{\nabla} \nabla \cdot \widehat{\nabla} v : \widehat{\nabla} v dx = 3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx$$

If we divide this equation by the $L^2(\Omega_\delta)$ -norm of the scaled velocity gradient $\widehat{\nabla} v$, we get

$$\nu_t \text{Ray}(-\nabla \cdot \nabla, \widehat{\nabla} v) = \frac{3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx}{2 \int_{\Omega_\delta} \widehat{Q}(\widehat{v}) dx} \quad (26)$$

where the Rayleigh quotient is defined by

$$\text{Ray}(-\nabla \cdot \nabla, \widehat{\nabla} v) = \frac{\int_{\Omega_\delta} -\nabla \cdot \nabla \widehat{\nabla} v : \widehat{\nabla} v dx}{\int_{\Omega_\delta} \widehat{\nabla} v : \widehat{\nabla} v dx} \quad (27)$$

So the eddy viscosity ν_t depends on the (scaled) velocity-gradient via $\widehat{Q}$ and $\widehat{R}$ as well as on the Rayleigh quotient of the (negative) Laplacian $-\nabla \cdot \nabla$ in the direction of $\widehat{\nabla} v$. The physical dimension of the right-hand side in Eq. (25) is 1/time; the Rayleigh quotient in (25) has dimension $1/\text{length}^2$. So in this set-up, the ratio of the invariants $\widehat{Q}(\widehat{v})$ and $\widehat{R}(\widehat{v})$ defines the time that is necessary to construct an eddy-viscosity, and the Rayleigh quotient provides the length. In other words, the Rayleigh quotient assigns implicitly a value to the filter length, which is anything but trivial if the filter is anisotropic. We have been able to circumvent this problem in Sect. 4 by scaling the Poincaré inequality, but the eddy-viscosity model re-introduces this problem, since it requires an explicit description of the length of the filter.

Unfortunately, calculating the Rayleigh quotient numerically is not a great option, because a direct numerical computation yields a proper approximation of the spectrum of the Laplacian (i.e., of the Rayleigh quotient) only if the filter length is taken much larger than the grid width, which means in practice that the cost of the simulation becomes too high. Indeed, the (negative) Laplace operator multiplies the amplitude of a mode with wavenumber k by k^2 , which implies that high wavenumbers need be resolved (to calculate the Rayleigh coefficient), even though their amplitude is small. To work around this numerical problem, we bound the Rayleigh quotient analytically (on basis of the smallest eigenvalue of the (negative) Laplacian on Ω_δ). This yields a lower bound of the form

$$\text{Ray}(-\nabla \cdot \nabla, \widehat{\nabla} v) \geq \min_{\widehat{\nabla} v} \text{Ray}(-\nabla \cdot \nabla, \widehat{\nabla} v) \stackrel{\text{def}}{=} (c/\delta)^2$$

where c denotes a constant; details to follow. In this way we arrive at

$$\nu_t \leq (\delta/c)^2 \frac{3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx}{2 \int_{\Omega_\delta} \widehat{Q}(\widehat{v}) dx} \quad (28)$$

where the index ‘+’ denotes the positive part, i.e., $f_+ = \max\{0, f\}$ i.e., negative values are clipped (see also [9]).

Obviously, taking the equality sign in the above expression systematically overestimates the amount of eddy viscosity needed to truncate the dynamics of the unresolved scales of motion, but, nevertheless, it provides a model. Here it may be stressed that δ^2 does not depend on the velocity $\widehat{v}$; hence the description of the length in this eddy-viscosity model does not vary with the velocity, i.e., it is static.

6. Discrete scale truncation

To start, we consider a one-dimensional, finite-volume discretization on a uniform mesh with spacing h . Schumann [3] was one of the first to notice that such a discretization defines a spatial filter that fits within the context of large-eddy simulation. The filtered field is then determined by taking the average over the smallest volume of the computational grid. In one spatial dimension, Schumann’s filter is given by

$$\bar{u}_i = \bar{u}(x_i, t) = \frac{1}{h} \int_{x_i-h/2}^{x_i+h/2} u(\xi, t) d\xi \quad (29)$$

In the context of LES, this is obviously an one-dimensional box filter with length h .

In a finite-volume method, the conservation of momentum is described by

$$h \frac{d\bar{u}_i}{dt} + u_{i+1/2}^2 - u_{i-1/2}^2 = \dots \quad (30)$$

where $u_{i+1/2}$ denotes the velocity at $x_{i+1/2}$, that is exactly midway between the grid points x_i and x_{i+1} . The dots in Eq. (30) stand for the non-convective (diffusive) contributions to the conservation

law. These contributions are omitted because they are not important here. The core problem is that the velocities $u_{i+1/2}$ at the box sides are to be expressed in terms of the box-averaged velocities $\bar{u}_i$. To make that connection, we use a second box filter with filter length δ :

$$\tilde{u}_{i+1/2} = \tilde{u}(x_{i+1/2}, t) = \frac{1}{\delta} \int_{x_{i+1/2}-\delta/2}^{x_{i+1/2}+\delta/2} u(\xi, t) d\xi \quad (31)$$

Note that this filter is half a grid cell shifted relative to the first filter (29). Now by choosing $\delta = 2h$, we obtain the key relation

$$\tilde{u}_{i+1/2} = \frac{1}{2} (\bar{u}_i + \bar{u}_{i+1}) \quad (32)$$

This equation does not contain any error. Thus the conservation law (30) can be written as

$$h \frac{d\bar{u}_i}{dt} + \tilde{u}_{i+1/2}^2 - \tilde{u}_{i-1/2}^2 = -\sigma_{i+1/2} + \sigma_{i-1/2} + \dots \quad (33)$$

where $\sigma_{i+1/2} = \tilde{u}_{i+1/2}^2 - u_{i+1/2}^2$. The left-hand side depends on the spatially filtered velocities $\tilde{u}_{i-1}$, $\bar{u}_i$ and $\bar{u}_{i+1}$, see Eq. (32). In the conventional finite-volume method, Eq. (32) is viewed as the interpolation rule for the fluxes and the right-hand side of (33) represents the discretization error. If, however, Eq. (33) is seen as a closure problem, then the problem reads: express $\sigma_{i+1/2}$ in terms of the mean value $\tilde{u}_{i+1/2}$. So, from the point of view of LES, (the effect) of the residual of the δ -filter (31) is to be modeled to close Eq. (33). These different viewpoints also illustrate the entanglement of the discretization (here: interpolation) error and the closure model. Finally, it can be noted that a natural transition from LES to DNS is obtained within the finite-volume setting, if the closure model disables itself when the grid provides sufficient resolution to compute all scales of motion.

Now, we consider two neighboring volumes, say grid volume i and $i+1$, and take $\delta = 2h$. The two corresponding finite-volume equations (33) can be added together using the identity $\delta d_t \tilde{u}_{i+1/2} = 2h \frac{1}{2} (d_t \bar{u}_i + d_t \bar{u}_{i+1})$. Thus, we obtain from Eq. (33) that

$$\delta \frac{d\bar{u}}{dt} + \tilde{u}_{i+3/2}^2 - \tilde{u}_{i-1/2}^2 = -\sigma_{i+3/2} + \sigma_{i-1/2} + \dots$$

A finite-difference approximation with stepsize $\delta = 2h$ induces a spatial filter too. Indeed,

$$\frac{\phi_{i+3/2} - \phi_{i-1/2}}{\delta} = \frac{1}{\delta} \int_{x_{i-1/2}}^{x_{i+3/2}} \frac{\partial \phi}{\partial x}(\xi) d\xi = \frac{\partial \phi}{\partial x} \Big|_{i+1/2}$$

Hence by combining the two equations above, we obtain

$$\partial_t \bar{u} + \partial_x (\bar{u}^2) = \partial_x (\tilde{u}^2 - u^2) + \dots \quad (34)$$

This is a LES-template wherein the grid-box filter (29) is replaced by the interpolation filter (31) with $\delta = 2h$. This shows once again that the finite-volume template (33) can be closed by modeling the effect of the residue of the interpolation filter (31). This obviously has important consequences for the scale-truncation condition that was developed in Sect. 3. If we view the finite-volume method in this way, we should be borne in mind that the scale-truncation condition is to be imposed at the scale $\delta = 2h$ which is determined by the interpolation rule. This means that there is some space (specifically between h and δ) to evaluate the integrals that occur in the scale-separation condition.

Probably the best discretization of the scale-truncation condition is obtained by taking a discrete Poincaré inequality as a starting point, and by subsequently repeating all the steps in the previous derivation in a discrete setting. This results into a natural discretization of the scale-truncation condition, whereby all the properties of the considered discretization automatically are discounted.

We opt for a simpler approach, i.e., we directly discretize the continuous scale-truncation condition.

To incorporate the effect of the numerical discretization on the scale truncation condition to some degree, we reconsider the continuous derivation, wherein not all gradient operators are exactly the same, because they are often discretized in different ways. In one spatial dimension, for instance, the derivative in the convective term is approximated to second-order accuracy by

$$\partial_x v_i \approx \frac{v_{i+1} - v_{i-1}}{2h} \quad (35)$$

The diffusive term is approximated using

$$\partial_{xx}^2 v_i \approx \frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} \quad (36)$$

Consequently, the discrete convective term does not see a point-to-point oscillation, whereas the discrete diffusive term does see this mode. So the convection-diffusion balance is not approximated correctly at the scale h set by the grid. This argument leads again to the choice $\delta = 2h$, see also [13].

The approximation (36) of the second-order derivative in the diffusive term is not equal to the square of the approximation (35) of the first-order derivative that is used for the convective term. Consequently, it is not clear how the gradients in Eq. (19) should be approximated. They are all based on some approximation of ∇ , but different approximations of the gradient operator are used for the convective and diffusive term. To understand how the different discretizations affect the scale truncation criterion, we denote the gradient operators in Eq. (19) differently. The gradient in the convective term is denoted by ∇^c , the diffusive operator is denoted ∇^d , and the closure model is $\nabla^d \cdot \tau$. Furthermore, the gradient in the Poincaré inequality in Eq. (9) is denoted by ∇^p . By repetition of the derivation that led to Eq. (19), we obtain

$$\int_{\Omega_\delta} \widehat{\nabla}^p \widehat{\nabla}^d \cdot \widehat{\tau} : \widehat{\nabla}^p \widehat{v} dx = - \int_{\Omega_\delta} \widehat{\nabla}^p \widehat{\nabla}^c \widehat{v} : \widehat{\nabla}^p \widehat{v} dx \quad (37)$$

where the boundary (read: transport) terms are omitted. In order to express the scale-truncation condition (37) in terms of one gradient, as in Eq. (19), we have to set $\nabla^p = \nabla^c$. In other words, the gradient in Poincaré's inequality (9) should be approximated exactly as the gradient in the convective term. With this choice, we obtain Eq. (19) again, wherein ∇ is replaced by ∇^c .

The invariants $\widehat{R}(\widehat{v})$ and $\widehat{Q}(\widehat{v})$ are computed from the (scaled) discrete velocity gradient, where the gradient is discretized as in the convective term. Furthermore, the integrals over the filter box Ω_δ are approximated with the help of the mid-point rule. In 1D, for example, we get

$$-3 \int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx \approx \delta (\widehat{v}_{i+1} - \widehat{v}_{i-1})^3 \quad (38)$$

This discretization is straightforwardly extended to three spatial dimensions. The Rayleigh quotient (27) of $-\nabla \cdot \nabla$ (in the direction of $\widehat{\nabla} \widehat{v}$) can be bounded from below with the help of the smallest eigenvalue of the discretization of $-\nabla \cdot \nabla$ on Ω_δ . In 1D the discretization is given by Eq. (36). The lowest frequency that fits within the 1D filter 'box' Ω_δ is described by the mode $-1 \ 0 \ +1 \ 0 \ -1$, i.e., the amplitude is zero in the odd grid points and oscillates between -1 and $+1$ in the even grid point. The associated eigenvalue is given by $4/\delta^2$. Thus in three spatial dimensions, we obtain

$$\min_{\widehat{\nabla} \widehat{v}} \text{Ray}(-\nabla \cdot \nabla, \widehat{\nabla} \widehat{v}) \stackrel{\text{def}}{=} (c/\delta)^2 \approx \frac{4}{\delta_x^2} + \frac{4}{\delta_y^2} + \frac{4}{\delta_z^2}$$

where $\delta_x = x_{i+1} - x_{i-1}$, i.e., δ_x twice the width of the grid in x ; δ_y and δ_z are defined in a similar fashion. Thus with $c = 12$ we have

$$\frac{1}{\delta^2} = \frac{1}{3} \left(\frac{1}{\delta_x^2} + \frac{1}{\delta_y^2} + \frac{1}{\delta_z^2} \right) \quad (39)$$

Combining the above sketched discretizations results into a discrete eddy-viscosity model in which the eddy viscosity is given by

$$\nu_t = \frac{\delta^2}{12} \frac{3(\int_{\Omega_\delta} \widehat{R}(\widehat{v}) dx)_+}{2 \int_{\Omega_\delta} \widehat{Q}(\widehat{v}) dx} \quad (40)$$

where the Ω_δ -integrals are to be replaced by their discretizations (as in Eq. (38), e.g.).

7. Turbulent channel flow

On isotropic meshes, the eddy-viscosity model (40) is identical to the model that was proposed by Rozema et al. [13]. They successfully tested the model for homogenous turbulence by performing large-eddy simulations of an experiment by Comte-Bellot and Corrsin [17]. The energy decay and the energy spectra computed using a 64^3 grid both agreed well with the box-filtered experimental results. Also, the results collapse on results obtained with the dynamic Smagorinsky model. For details the reader is referred to Ref. [13].

On anisotropic meshes, the eddy-viscosity model by Rozema et al. and the present model differ because the scalings and discretizations are performed in different ways. Here, the present model is tested for turbulent channel flow by means of a comparison with direct numerical simulations of turbulent channel flow. This flow forms a prototype for near-wall turbulence: virtually every LES has been tested for it. The results are compared to the DNS data of Moser et al. [18] at $Re_\tau = 590$. The non-dimensionalized dimension of the channel is $2\pi \times 2 \times \pi$. As is customary in this test-case, the computational grid used for the large-eddy simulation consists of 64^3 points. The DNS was performed on a $384 \times 257 \times 384$ grid, i.e., the DNS uses about 144 times more grid points than the present LES. The LES-grid has an uniform spacing in the stream-wise (x) and span-wise (z) directions. In the wall-normal direction the computational grid is stretched. The y -coordinates in the lower half of the channel are given by a hyperbolic sine distribution

$$y_j = \frac{\sinh(\beta j/N_y)}{2 \sinh(\beta/2)}$$

for $j = 0, 1, \dots, N_y/2$, where the stretching parameter β is set equal to 7. The coordinates in the upper half are found by mirroring the mesh in the center plane of the channel. The LES-results are obtained with an incompressible code that uses a fourth-order, symmetry-preserving, finite-volume discretization, see [19] for details. In the large-eddy simulations, the bulk Reynolds number (based on half the height of the channel) is fixed at 11,000 by imposing a constant bulk velocity though a constant pressure gradient in the stream-wise direction. The resulting friction Reynolds number is $Re_\tau = 597$. The mesh spacing of the computational grid in wall units based on the friction Reynolds number are given by $h_x^+ \approx 60$, $h_y^+ \approx 4 - 60$ and $h_z^+ \approx 30$. The mean flow velocity and the turbulent fluctuations normalized by the computed friction velocity are shown in Fig. 1 and Fig. 2, respectively.

The above results demonstrate that the eddy-viscosity model (40) yields accurate results for the considered turbulent channel flow. In fact, only the prediction of the stream-wise fluctuating near the wall differs from the DNS. The near-wall peak in $u'u'$ the LES is about 10% too high in comparison to the reference data. This indicates that the estimation of the filter length with the help of the lower bound of the Rayleigh quotient of $-\nabla \cdot \nabla$ is not sufficiently accurate. According to Eq. (39), the filter width near the wall is dominated by the wall-normal spacing of the grid, that is $\delta \approx \sqrt{3}\delta_y$. The more conventional definition $\delta = (\delta_x \delta_y \delta_z)^{1/3}$ gives $\delta \propto \delta_y^{1/3}$ (near wall). For the considered grid the conventional geometric mean filter width is about three times larger than the

Fig. 1. Mean stream-wise velocity profiles in simulation of turbulent channel flow at $Re_\tau \approx 590$. The markers represent LES data; every symbol corresponds to data in a grid point. The line displays the DNS-result.

Fig. 2. Turbulent fluctuations (in wall coordinates) in simulations of turbulent channel flow at $Re_\tau \approx 590$. The markers represent LES data; every symbol corresponds to data in a grid point. The lines displays the DNS-result. The upper curve corresponds to fluctuating stream-wise velocity, the middle line displays the span-wise fluctuations, the lower curve represents the wall-normal fluctuating velocity.

present definition (39). So, compared to the geometric mean, Eq. (39) provides some near-wall damping, but the near-wall peak in $u'u'$ is still too high; hence a suitable wall damping function is required, that is the estimation of the Rayleigh quotient near-wall is to be adapted.

8. Concluding remarks

We discussed closure models for large-eddy simulation of incompressible turbulent flows. In particular, we aimed to formulate a condition that ensures that the closure model provides sufficient dissipation to counteract the production of any (small) scales for which numerical resolution is not available. Here the resolved scales are defined with the help of Schumann's filter. We used Poincaré's inequality to develop the balance between the production of too small, non-resolved, scales of motion and the dissipation resulting from the closure model, without explicitly referring to the unresolved scales. Poincaré's inequality provides an upper bound for the energy of the unresolved scales of motion using bounds on the velocity gradient and the geometry of the filter. The Poincaré constant provides the bound for the geometry using the diameter alone. In case the filter is anisotropic, however, the diameter does not provide a sufficiently detailed description of the geometry of the filter. Consequently, Poincaré's upper bound systematically overestimates a portion of the small-scale production. Therefore we have looked carefully at ways to incorporate the anisotropy of the filter into Poincaré's inequality. The associate production-dissipation balance is applied within the eddy-viscosity concept. This yields a novel eddy-viscosity model, in which the eddy viscosity is given by a function of the invariants of the scaled velocity-gradient, where the scaling results from the anisotropic Poincaré inequality. This model is discretized and tested for a

turbulent channel flow. The application of the model to turbulent channel flow leads to good results, yet the near-wall stream-wise fluctuations are overpredicted. This is likely due to our rough approximation of the lower bound for the near-wall dissipation. This points out a possible future improvement. Furthermore the present framework can be used to assess other models that are not solely based on an eddy-viscosity assumption.

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