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Verstappen, R.W.C.P.

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ON CLOSING LARGE-EDDY SIMULATIONS

Roel Verstappen

Bernoulli Institute, University of Groningen, Netherlands

Abstract

This paper is about models for large-eddy simulation (LES) 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. To identify the resolved eddies, we apply Schumann's filter to the (incompressible) Navier-Stokes equations, that is the turbulent velocity field is filtered as in a finite-volume method. The spatial discretization effectively act as a filter too; hence we define the resolved eddies for a finite-volume discretization. The interpolation rule for approximating the convective flux through the faces of the finite volumes determines the smallest resolved length scale δ. The resolved length δ is twice as large as the grid spacing for an usual interpolation rule. Thus, the resolved scales are defined with the help of box filter having diameter δ. The closure model describes the nett effect of the unresolved scales on the resolved flow field. The closure model is to be chosen such that the solution of the resulting LES-equations is confined to length scales that have at least the size δ. This condition sets a requirement for every closure model. The direct development of this requirement results into a condition that depends explictly on unresolved scales; hence it is not useable. Therefore, we make use of Poincaré's inequality to determine the amount of dissipation that is to be generated by the closure model in order to counterbalance the nonlinear production of too small, unresolved scales. This dissipation-production balance results into a condition that depends on the invariants of the velocity gradient. This condition is to be scaled properly if the filterbox is anisotropic. In principle, the scaled truncation condition can be applied to any LES-model. Here it is applied to an eddy-viscosity model to illustrate the procedure.

1 Large-eddy simulation

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

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

where u denotes the fluid velocity, p stands for the pressure and ν is the viscosity. 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. The available computing power is often inadequate to resolve the small scales where the dissipation takes place. In that case, the NS-equations do not provide a tractable model. 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 [1].

Large-eddy simulation (LES) seeks to predict the dynamics of spatially filtered turbulent flows. To that end, a spatial filter is applied to the NS-equations:

$$\partial_t\overline{u} + \nabla\cdot(\overline{u}\otimes\overline{u}) - \nu\,\nabla\cdot\nabla\overline{u} + \nabla\overline{p} = \nabla\cdot(\overline{u}\otimes\overline{u} - \overline{u\otimes u})$$

where the filter is denoted by a bar, i.e., $\overline{u}$ denotes the filtered velocity field, and $\overline{p}$ stands for the filtered pressure. Here it may be stressed that it is assumed that the filter commutes with spatial differential operators. The right-hand side represents the effects of the residual scales on the 'larger eddies'. To remove the explicit dependence on the residual scales of motion, the commutator of $u\otimes u$ and the filter is replaced by a closure model. This yields

$$\partial_t v + \nabla\cdot(v\otimes v) - \nu\,\nabla\cdot\nabla v + \nabla\pi = -\nabla\cdot\tau(v) \quad (1)$$

where the variable name is changed from $\overline{u}$ to v (and $\overline{p}$ to π) to stress that the solution of Eq. (1) differs from $\overline{u}$, because the closure model τ is not exact [2].

2 Finite-volume discretization

When the LES-equations are discretized in space, the low-pass characteristics of the discrete operators effectively act as a filter too. This numerical filter will inevitably interact with the filter that is explicitly applied to the Navier-Stokes equations. To try to distinghuish these filters, we apply Schumann's filter to the NS-equations [3]. That is, as in a finite-volume method we take

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

where Ω_h denotes a cell of the computational mesh. To start, we consider an one-dimensional uniform mesh with spacing h. Schumann's filter is then given by

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

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

$$h\,\frac{\mathrm{d}\overline{u}_i}{\mathrm{d}t} + u_{i+1/2}^2 - u_{i-1/2}^2 = \cdots \quad (3)$$

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. (3) stand for the linear (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 faces of the control volume (here in 1D) are to be expressed in terms of the box-filtered velocities $\overline{u}_i$. To make that connection, we introduce a second filter with filter length δ:

$$\widetilde{u}_{i+1/2} = \frac{1}{\delta}\int_{x_{i+1/2}-\delta/2}^{x_{i+1/2}+\delta/2} u(\xi,t)\,d\xi \quad (4)$$

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

$$\widetilde{u}_{i+1/2} \;=\; \tfrac{1}{2}\left(\overline{u}_i \,+\, \overline{u}_{i+1}\right) \tag{5}$$

This equation does not contain any error! Thus the conservation law (Eq. (3)) can also be written as

$$h\,\frac{\mathrm{d}\overline{u}_i}{\mathrm{d}t} \,+\, \widetilde{u}^2_{i+1/2} - \widetilde{u}^2_{i-1/2} \;=\; -\sigma_{i+1/2} + \sigma_{i-1/2} \,+\, \cdots \tag{6}$$

where $\sigma_{i+1/2} = \widetilde{u}^2_{i+1/2} - u^2_{i+1/2}$. According to Eq. (5), the left-hand side depends on the spatially filtered velocities $\overline{u}_{i-1}$, $\overline{u}_i$ and $\overline{u}_{i+1}$. In the conventional finite-volume method, Eq. (5) is viewed as the interpolation rule for the fluxes - the interpolation rule is then given by $u_{i+1/2} \approx \widetilde{u}_{i+1/2}$. Consequently, the right-hand side of Eq. (6) represents the interpolation error. If, however, Eq. (6) is seen as a closure problem, then the problem reads: express $\sigma_{i+1/2}$ in terms of the box-filtered velocity $\widetilde{u}_{i+1/2}$. So from that point of view, (the effect) of the residual of the δ-filter is to be modelled to close Eq. (6). These different points of view illustrate the entanglement of the discretization (here: interpolation) error and the closure model.

Next, we consider two neighboring 'volumes', say $[x_{i-1/2}, x_{i+1/2}]$ and $[x_{i+1/2}, x_{i+3/2}]$, and take $\delta = 2h$. The two corresponding momentum equations (Eq. (6) for $\overline{u}_i$ as well as for $\overline{u}_{i+1}$) can be added together using Eq. (5). Thus, we get

$$\delta\,\frac{\mathrm{d}\widetilde{u}}{\mathrm{d}t}_{i+1/2} \,+\, \widetilde{u}^2_{i+3/2} - \widetilde{u}^2_{i-1/2} \;=\; -\sigma_{i+3/2} \,+\, \sigma_{i-1/2} \,+\, \cdots$$

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

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

Hence by combining the two equations above, we obtain

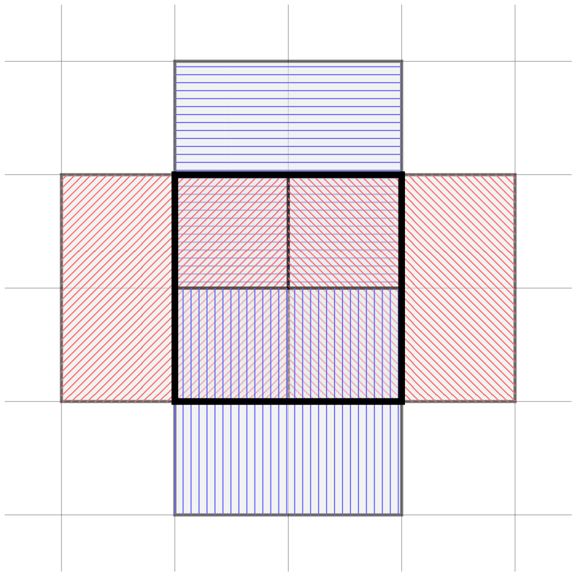
$$\partial_t \widetilde{u} \,+\, \widetilde{\partial_x \widetilde{u}^2} \;=\; \partial_x(\widetilde{\widetilde{u}^2 - u^2}) \;+\; \cdots$$

Once again, it may be stressed that the above momentum equation is exact: it does not contain any error yet. The nonlinear term in the left-hand side is usually not filtered; hence to put it the standard LES-form, we add the residual of $\partial_x \widetilde{u}^2$ to both the left- and right-hand side. Furthermore, we assume as in Sect. 1 that the spatial derivative commutes with the filter. (In fact, this assumption is superfluous here, but because it is always made, we do it too). This yields the common LES-template wherein Schumann's grid-box filter (having filter length h) is replaced by the interpolation filter, i.e., Eq. (4) with filter length $\delta = 2h$:

$$\partial_t \widetilde{u} \,+\, \partial_x \widetilde{u}^2 \;=\; \partial_x(\widetilde{u}^2 - \widetilde{u^2}) \;+\; \cdots \tag{7}$$

So, in a finite-volume setting, we need to model the effects of all scales smaller than $\delta = 2h$, and not just the subgrid contributions. Indeed, the finite-volume template (Eq. (6)) can be closed by modeling the effect of the residue of the interpolation filter (Eq. (4)). If we view the finite-volume method in this way, we should be borne in mind that the closure condition is to be imposed at the scale $\delta = 2h$ which is determined by the interpolation rule. It may be remarked here that the highest frequency that can be represented on the grid (the mode that equals +1 in the even grid points and -1 in the odd grid points) lies in the kernel of the interpolation operator; hence that mode is invisible and therefore it's effect need be modelled.

So far, we have only considered one spatial dimension. The reasoning can simply be extended to more dimensions. In two dimensions, for example, we take volumes of size $(2h)^2$. The figure below shows five of these volumes. To compute the convective flux through the four faces of the central control volume (that is, the volume with the thick edge), we need to to know the velocities at the faces. The velocities at the faces are to be interpolated. For that we use averages over the four $(2h)^2$ volumes that are centred around a face of the central volume. In this way, the interpolation filter can be extended to two and three dimensions.



3 Separation of scales

The very essence of large-eddy simulation 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 [4], [5], [6]. To determine this condition, we consider an arbitrary part of the flow domain with diameter δ. With the aid of the associated box filter,

$$\widetilde{v} = \frac{1}{|\Omega_\delta|}\int_{\Omega_\delta} v(x,t)\,dx, \tag{8}$$

the undesirable small scales in the velocity field v are defined by $v' = v - \widetilde{v}$. It may be remarked that the size of the filter box Ω_δ is to be selected by the user. As argued above, the filter box Ω_δ will generally be larger than the grid box Ω_h.

The residual 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 $\widetilde{v}$ 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. (1) we find the governing equation for v' and from that we obtain the evolution of it's $L^2(\Omega_\delta)$ norm:

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_{\Omega_\delta}\tfrac{1}{2}|v'|^2\,dx \;=\; \nu\int_{\Omega_\delta}(\nabla\cdot\nabla v)'\cdot v'\,dx \qquad (9)$$
$$\qquad -\;\int_{\Omega_\delta}(\nabla\cdot(\pi I+v\otimes v+\tau\,))'\cdot v'\,dx$$

The first term in the right-hand side above is the result of a linear process, the diffusion caused by the fluid viscosity. The second line in Eq. (9) represents 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 apperent when the divergence of Eq. (1) 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 $\widetilde{v}$ to the residual field v' and vice versa. Consequently, if the closure model is taken so that the terms in the second line of Eq. (9) cancel each other out, then

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_{\Omega_\delta}\tfrac{1}{2}|v'|^2\,dx \;=\; \nu\int_{\Omega_\delta}(\nabla\cdot\nabla v)'\cdot v'\,dx \qquad (10)$$

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

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. (10). Therefore, the production of small scales of motion is to be balanced by the modelled dissipation:

$$\int_{\Omega_\delta}(\nabla\cdot\tau\,)'\cdot v'\,dx \;=\; -\int_{\Omega_\delta}(\nabla\cdot(v\otimes v+\pi I)\,)'\cdot v'\,dx \quad (11)$$

In principle, we could verify whether this condition is met during a LES. But that is not very attractive, because verifying Eq. (11) 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. 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 trapped in a catch-22: 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..

4 Poincaré's inequality

We make use of the Poincaré-Wirtinger inequality to develop an alternative for the dissipation-production balance Eq. (11) that does not explicitly refer to the residual field v', see also [4]- [6]. This inequality states that there exists a constant C_δ depending only on the domain Ω_δ such that

$$\int_{\Omega_\delta}|v-\widetilde{v}|^2\,dx \;\leq\; C_\delta\int_{\Omega_\delta}|\nabla v|^2\,dx \qquad (12)$$

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 [7] 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. Basically, we can take the closure model such that $\int_{\Omega_\delta}|\nabla v|^2\,dx = 0$ for all times. Then, $\int_{\Omega_\delta}|v'|^2\,dx = 0$ according to Eq. (12). However, before we elaborate on this reasoning, the Poincaré inequality is to be reconsidered in case the the filter box is quite anisotropic. In that case, 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. This issue can be solved by scaling Poincaré's inequality properly, see also [5].

4.1 Need to scale Poincaré's inequality

To illustrate the scaling 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 $\lambda_j = \delta_j/n_j$, that is, the wave number is $k_j = 2\pi n_j/\delta_j$, where $j = 1,2,3$. To keep the calculations simple, we consider the following scalar velocity $v(x) = \exp(ik_jx_j)$, where the Einstein summation convention applies. A straightforward calculation shows that in this case the left-hand side of the Poincaré inequality Eq. (12) depends only on the ratio n_j of wave length λ_j to the box size δ_j; it does not depend explicitly on the filter length δ_j. Whereas the right-hand side (the upperbound) depends explicitly on both n_j and δ_j, unless the filter box is a cube ($\delta_j = \delta =$ 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, the Poincaré upperbound does inevitably depend explicitly on δ_j if the filter box is not a cube; that is, if the filter is anisotropic. For anisotropic filters the upperbound is proportional to δ_j^{-2}; hence (for fixed n_j) the upperbound is dominated by contributions associated with the direction in which the filter length is smallest. Consequently, the Poincaré upperbound gets a bias in the direction of the smallest filter length. To remove that dominant direction, we introduce a scaling.

4.2 Scaling of 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 δ_i: 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_i. 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; thus, the scaled partial derivative with respect to x_i is defined by $\widehat{\delta}_i = \delta_i\,\partial_i$. The components of the scaled velocity gradient are then described by

$$(\widehat{\nabla}v)_{ij} \;=\; \delta_i\,\partial_i v_j \qquad (13)$$

It may be remarked that $\widehat{\nabla}$ can be viewed as the gradient operator in an isotropic computational space that is defined through the map $x_i \mapsto \widehat{x}_i = x_i/\delta_i$.

If we now consider the (scalar) example from the previous section, we find that the scaled Poincaré upper-bound $\int_{\Omega_\delta} |\widehat{\nabla} v|^2\, dx$ depends only on the ratio n_i of the box length δ_i to the wave length λ_i of the velocity. Hence, the scaled gradient provides a better starting-point for bounding the small-scale details than the unscaled gradient. Therefore Rozema *et al.* [5] proposed the modified Poincaré inequality

$$\int_{\Omega_\delta} |v'|^2\, dx \;\leq\; C \int_{\Omega_\delta} |\widehat{\nabla} v|^2\, dx \qquad (14)$$

where C is a constant independent of δ_j. Thus, whereas the original Poincaré inequality (Eq. (12)) 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 $\partial_i v$ with δ_i.

4.3 Anisotropic Poincaré inequality

Thus far the scaling of Poincaré's inequality was considered for a scalair velocity only. If the filter box is highly anisotropic, we have to considered the scaling of the components of the velocity vector too. 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

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

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

$$\partial_t \widehat{v} + \widehat{\nabla} \cdot (\widehat{v} \otimes \widehat{v}) - \nu\, \nabla \cdot \nabla \widehat{v} + \widehat{\nabla} \cdot \widehat{\pi} \;=\; -\widehat{\nabla} \cdot \widehat{\tau} \qquad (15)$$

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

$$\int_{\Omega_\delta} |\widehat{v}\,'|^2\, dx \;\leq\; C \int_{\Omega_\delta} |\widehat{\nabla} \widehat{v}|^2\, dx \qquad (16)$$

to bound the residual velocity field.

5 Counterbalancing the production of too small scales

Eq. (16) shows that the energy of the too small scales can be bounded by $L^2(\Omega_\delta)$ norm of the velocity gradient $\widehat{\nabla} \widehat{v}$. Thus, the production of too small scales of motion can be counteracted by introducing a suitable amount of eddy dissipation in the dynamics of the velocity gradient. Here we re-use the reasoning that led to the scale-truncation condition Eq. (11), where this time we do not consider the production and dissipation of the small-scale energy. Instead we focus on upper bound given by Eq. (16). According to Eq. (15), we have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{dt}} \int_{\Omega_\delta} \tfrac{1}{2} |\widehat{\nabla} \widehat{v}|^2 dx \;&=\; \int_{\Omega_\delta} \widehat{\nabla} \left(\nu\, \nabla \cdot \nabla \widehat{v}\right) : \widehat{\nabla}\, dx \\ &- \int_{\Omega_\delta} \widehat{\nabla}\, \widehat{\nabla} \cdot (\widehat{\tau} + (\widehat{v} \otimes \widehat{v}) + \widehat{\pi} I) : \widehat{\nabla} \widehat{v}\, dx \end{aligned} \qquad (17)$$

Here it may be remarked that we use the common notation $a : b = \sum_{ij} a_{ij} b_{ij}$. As in Eq. (9), the second line of the right-hand side in Eq. (17) represents the nonlinear production as a result of the pressure, convection and the modelled eddy-dissipation, respectively. Eq. (17) shows that

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_{\Omega_\delta} \tfrac{1}{2} |\widehat{\nabla} \widehat{v}|^2 dx \;=\; -\nu \int_{\Omega_\delta} \widehat{\nabla} \cdot \nabla \widehat{v} : \widehat{\nabla} \cdot \nabla \widehat{v}\, dx \;\leq\; 0 \qquad (18)$$

provided the closure model τ is chosen such that

$$\int_{\Omega_\delta} \widehat{\nabla}\, \widehat{\nabla} \cdot (\widehat{\tau} + (\widehat{v} \otimes \widehat{v}) + \widehat{\pi} I) : \widehat{\nabla} \widehat{v}\, dx = \int_{\partial \Omega_\delta} \nu \widehat{\nabla} \widehat{v} : \partial_n \widehat{\nabla} \widehat{v}\, ds \qquad (19)$$

It goes without saying that we have to initialize the velocity field such that $v' = 0$ at $t = 0$. Then, v is constant in Ω_δ; hence $\nabla v = 0$ in Ω_δ;. Thus, we have $\int_{\Omega_\delta} |\widehat{\nabla} \widehat{v}|^2 dx = 0$ at $t = 0$. If Eq. (18) is supplied with this initial condition we obtain $\int_{\Omega_\delta} |\widehat{\nabla} \widehat{v}|^2 dx = 0$ for all times $t \geq 0$. Now by applying Poincaré's inequality (see Eq. (16)) we arrive at $\int_{\Omega_\delta} |\widehat{v}\,'|^2\, dx = 0$. So, in conclusion, Eq. (19) ensures that all scales of size smaller than δ are insignificant, and hence need not be computed. Stated otherwise, if Eq. (19) is satisfied, the closure model τ properly counterbalances the nonlinear production of small, unresolved scales of motion in a large-eddy simulation of turbulence.

To elaborate on this truncation condition, we use Cayley-Hamilton's theorem. For incompressible flows, Cayley-Hamilton states that $\widehat{\nabla} \widehat{v}^3 - \widehat{Q} \widehat{\nabla} \widehat{v} + \widehat{R} I = 0$, where the second and third invariant of the velocity-gradient tensor are given by $\widehat{Q}(\widehat{v}) = \frac{1}{2} \widehat{\nabla} \widehat{v} : \widehat{\nabla} \widehat{v}$ and $\widehat{R}(\widehat{v}) = -\frac{1}{3} \widehat{\nabla} \widehat{v} \widehat{\nabla} \widehat{v} : \widehat{\nabla} \widehat{v} = -\det \widehat{\nabla} \widehat{v}$, respectively. The convective contribution to the left-hand side of Eq. (19) can be written in terms of these invariants. Indeed, since $\widehat{\partial}_k \widehat{v}_k = 0$, we have

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

where n is the outward-pointing normal vector to the boundary $\partial \Omega_\delta$ of Ω_δ and $\widehat{n}_i = n_i/\delta_i$. It may be noted that he Einstein summation convention applies here, i.e., the above formula represents a summation over the terms indexed by i , j and k. In the sequel we will implicitely use Einsteins notation too.

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

$$\begin{aligned} \int_{\Omega_\delta} \widehat{\nabla} \widehat{\nabla} \cdot (\widehat{\tau} + \widehat{\pi} I) : \widehat{\nabla} \widehat{v}\, dx \;&=\; 3 \int_{\Omega_\delta} \widehat{R}(\widehat{v})\, dx \\ &- \int_{\partial \Omega_\delta} \left(\widehat{Q}(\widehat{v})\, \widehat{v} \cdot \widehat{n} + \nu \partial_n \widehat{Q} \right) ds \end{aligned} \qquad (20)$$

In conclusion, Eq. (20) ensures that the dissipation provided by the closure model is sufficient to damp the production of any scales of size smaller than δ. Thus the model confines the LES-solution to scales having at least length δ. In essence Eq. (20) sets a requirement for every LES-model. It may be noted that the surface integral in Eq. (20) consists of two parts. The first part represents the convective 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 part represents the viscous diffusion of $\widehat{Q}$ through the boundary of the box Ω_δ. The volume integral of describes the production of $\widehat{Q}$; note: $\widehat{R}$ provides a measure for the production.

6 Eddy viscosity

The scale-truncation condition (Eq. (20)) 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

$$\tau(v) - \tfrac{1}{3}\mathrm{tr}(\tau)\mathrm{I} \;=\; -2\,\nu_t\, S(v) \qquad (21)$$

where ν_t denotes the eddy viscosity and $S(v)$ is the symmetric part of the velocity gradient, $S(v) = \frac{1}{2}(\nabla v + \nabla v^*)$. As usual, the factor -2 is introduced in Eq. (21). Moreover only the deviatoric component of the closure tensor is described here, because the divergence of the volumetric, isotropic component $\frac{1}{3}\mathrm{tr}(\tau)I$ can be incorporated into the pressure gradient; see Eq. (1). 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.

The scale-truncation condition can be used to determine the eddy-viscosity in Eq. (21). By substituting the eddy-viscosity model into Eq. (20), we obtain the following expression for the eddy viscosity

$$-\int_{\Omega_\delta} \widehat{\nabla}\nabla\cdot\nu_t\nabla\widehat{v} : \widehat{\nabla}\widehat{v}\,dx \;=\; 3\int_{\Omega_\delta}\widehat{R}(\widehat{v})\,dx \qquad (22)$$
$$-\int_{\partial\Omega_\delta}\left(\widehat{Q}(\widehat{v})\,\widehat{v}\cdot\widehat{n} + \nu\partial_n\widehat{Q}\right)\,ds$$

where we neglected the contribution of the pressure, since we only consider the deviatoric component of the closure model. 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 convective and diffusive transport. Now if we assume that the dissipation balances the production, then there is no nett 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; hence, ν_t is taken constant in Ω_δ. Under these assumptions, Eq. (22) simplifies to

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

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

$$\nu_t\ \mathrm{Ray}\,(-\nabla\cdot\nabla, \widehat{\nabla}\widehat{v}) \;=\; \frac{3\int_{\Omega_\delta}\widehat{R}(\widehat{v})\,dx}{2\int_{\Omega_\delta}\widehat{Q}(\widehat{v})\,dx} \qquad (23)$$

where the Rayleigh quotient is defined by

$$\mathrm{Ray}\,(-\nabla\cdot\nabla, \widehat{\nabla}\widehat{v}) \;=\; \frac{\int_{\Omega_\delta} -\nabla\cdot\nabla\ \widehat{\nabla}\widehat{v} : \widehat{\nabla}\widehat{v}\,dx}{\int_{\Omega_\delta}\widehat{\nabla}\widehat{v} : \widehat{\nabla}\widehat{v}\,dx} \qquad (24)$$

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 $\widehat{\nabla}\widehat{v}$. The physical dimension of the right-hand side in Eq. (23) is 1/time; the Rayleigh quotient in Eq. (24) has dimension 1/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 implicitely 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 scale. A discussion about this issue can be found in Ref. [8] and [9], e.g.

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 (and thus 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. To work around this we first note that the Rayleigh quotient scales with $1/\delta^2$; hence, it can be approximated by $(c/\delta)^2$, where c denotes a constant; details to follow. In this way we arrive at

$$\nu_t \;=\; \frac{3\delta^2}{2c^2}\,\frac{\int_{\Omega_\delta}\widehat{R}(\widehat{v})\,dx_+}{\int_{\Omega_\delta}\widehat{Q}(\widehat{v})\,dx} \qquad (25)$$

where the index '+' denotes the positive part, i.e., $f_+ = \max\{0, f\}$. Thus, negative values are clipped (see also [10]).

Next, we bound the Rayleigh quotient on basis of the smallest eigenvalue of the (negative) Laplacian on Ω_δ. In a numerical simulation, the value of the constant c depends on the discretization of the convective derivative, see [11]. The Rayleigh quotient 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. On an uniform 1D mesh the smallest eigenvalue of a second-order central discretization of the second derivative on an interval of length δ is equal to $4/\delta^2$. The ascociated eigenmode is $-1 \quad 0 \; +1 \quad 0 \; -1$, i.e., the applitude is zero in the odd grid points and oscillates between -1 and +1 in the even grid point. Note: $\delta = 2h$. It may be noted this will be the dominant mode if the closure model functions well, since then all other modes, smaller scales of motion, are effectively dampened by the closure model. Likewise, in 3D, the largest eigenvalue of a second-order central discretization of the Laplacian on Ω_δ is equal to $12/\delta^2$; hence $c^2 = 12$ in that case. For this choice of the discretization (and mesh) the eddy viscosity is given by

$$\nu_t \;=\; \frac{\delta^2}{8}\,\frac{\int_{\Omega_\delta}\widehat{R}(\widehat{v})\,dx_+}{\int_{\Omega_\delta}\widehat{Q}(\widehat{v})\,dx} \qquad (26)$$

To calculate the eddy viscosity from this expression, the invariants $\widehat{R}(\widehat{v})$ and $\widehat{Q}(\widehat{v})$ are to be 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 to be approximated with the help of a quadrature rule, the trapezoidal rule or the midpoint rule, for example. The eddy-viscosity model given by Eq. (26) is successfully tested for homegeneous turbulence as well as for turbulent channel flows; details can be found in Ref [6].

Finally it may be stressed that there are multiple ways to determine an eddy viscosity that meets a scale truncation condition if the mesh is highly nonuniform. In Ref. [5] a minimum-dissipation model was derived by making use of the modified Poincaré inequality Eq. (14) instead of Eq. (16). This yields an expression for the eddy viscosity that differs from Eq. (26) if the grid is (strongly) anisotropic. In Ref. [12] the filterbox Ω_δ was equipped with periodic boundary conditions. If this assumption is adopted, the eddy viscosity depends on the invariants of the symmetric part of the velocity gradient, see [12] for details. In short, the truncation condition does not fully establish the eddy viscosity, leaving room for modelling assumptions, especially about how the grid anisotropy is taken into account. It may be noted that it is even possible to impose the truncation condition on each component of the velocity vector seperately, leading to three eddy viscosities, one for each component. Furthermore, the simplications made here (omitting pressure and convective/diffusive flux) are not strictly necessary and should be invested further.

7 Conclusions

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 interpolation rule for approximating the convective fluxes through the faces of control volumes. We used Poincaré's inequality to develop the balance between the production of too small, non-resolved, scales of motion and the dissipation provided by the closure model, without explicitly refering to the unresolved scales. Poincaré's inequality has a constant that represents the geometry of the filter box 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. A scaled Poincaré inequality is used to determine the amount of dissipation that is to be provided by the closure model in order to counterbalance the nonlinear production of too small, unresolved scales. This dissipation-production balance results into a truncation condition that depends on the invariants of the velocity gradient. It is applied within the eddy-viscosity concept, yielding a novel eddy-viscosity model. Yet, the truncation condition does not fully establish the eddy viscosity, leaving room for modelling assumptions, especially about how the anisotropy is taken into account. This points out a possible future improvement. Finally, it may be stressed that the present framework can be used to assess any LES-models, also models that are not solely based on an eddy-viscosity assumption.

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