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A minimum-relaxation model for large-eddy simulation

Roel Verstappen

Abstract This paper is about a relaxation model for large-eddy simulation of turbulent flow that truncates 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 relaxation parameter is determined in such a way that the production of too small, box-fitting, scales is counteracted by the modeled dissipation. This dissipation-production balance is worked out with the help of Poincaré’s inequality, which results in a relaxation model that depends on the invariants of the velocity gradient. This model is discretized and equipped with a Schumann filter. It is successfully tested for isotropic turbulence as well as for turbulent channel flow.

1 Large-eddy simulation of turbulence

As usual, a spatial filter is applied to the (incompressible) Navier-Stokes (NS) equations to obtain a model for the larger eddies. The filtered NS-equations read

$$\partial_t \pi + \nabla \cdot (\pi \otimes \pi) - \nu \nabla \cdot \nabla \pi + \nabla \tilde{p} = \nabla \cdot (\pi \otimes \pi - \pi \otimes \pi)$$

(1)

where $\pi$ 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.(1). So, at the discrete level, the effective filter is not so clear, unless we use the Schumann filter [1]. Therefore we adopt the Schumann filter, i.e., we take

$$\bar{u} = \frac{1}{|\Omega_h|} \int_{\Omega_h} u(x,t) \, dx,$$
where \( \Omega_h \) denotes a computational cell that is used in the finite-volume discretization, see [2], e.g. Replacing the right-hand side by a ‘model’ yields

\[
\frac{\partial}{\partial t} v + \nabla \cdot (v \otimes v) - v \nabla v + \nabla \pi = -\nabla \cdot \tau(v)
\]  

(2)

where the variable name is changed from \( \bar{u} \) to \( v \) (and \( \bar{p} \) to \( \pi \)) to stress that the solution of Eq. (2) differs from that of Eq. (1), because the model is not exact.

### 1.1 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 \( \tau \). To determine that condition, we consider an arbitrary part of the flow domain with diameter \( \delta \). With the aid of the associated box filter,

\[
\bar{v} = \frac{1}{|\Omega_{\delta}|} \int_{\Omega_{\delta}} v(x,t) \, dx,
\]  

(3)

the undesirable small scales in the LES solution \( v \) are defined by \( v' = v - \bar{v} \); here \( \Omega_{\delta} \) is to selected by the user. It may be emphasized that the filter box \( \Omega_{\delta} \) will generally differ from the grid box \( \Omega_h \) that was used to filter the NS-equations; here it is assumed that \(|\Omega_{\delta}| \geq |\Omega_h|\).

The residual of the box filter, \( v' = v - \bar{v} \), consist of the scales of size smaller than \( \delta \). The closure model must be designed so that these small scales are dynamically insignificant. By applying the residual operator to Eq. (2) we find the equation for \( v' \) and from that we obtain the evolution of it’s \( L^2(\Omega_{\delta}) \) norm:

\[
\frac{d}{dt} \int_{\Omega_{\delta}} \frac{1}{2} ||v'||^2 \, dx = \int_{\Omega_{\delta}} (v \nabla \cdot \nabla v' - \nabla \pi') \cdot v' \, dx - \int_{\Omega_{\delta}} (\nabla \cdot (v \otimes v) + \nabla \cdot \tau') \cdot v' \, dx
\]  

(4)

The two contributions to the last integral represent the energy that is transferred from the box-filtered velocity field \( \bar{v} \) to the residual field \( v' \) and the eddy dissipation resulting from the closure model, respectively. Eq. (2) does not produce residual scales if the eddy dissipation balances the energy transfer at the scale set by the box filter. Now if the closure model is taken so that the production and eddy dissipation terms in Eq.(5) cancel each other out, then

\[
\frac{d}{dt} \int_{\Omega_{\delta}} \frac{1}{2} ||v'||^2 \, dx = \int_{\Omega_{\delta}} (v \nabla \cdot \nabla v' - \nabla \pi') \cdot v' \, dx
\]  

(5)

and the evolution of the energy of \( v' \) does not depend on \( \bar{v} \). Stated otherwise, the energy of residual scales dissipates at a natural rate, without any forcing mechanism involving \( \bar{v} \). In this way, the scales \(< \delta \) are separated from scales \( \geq \delta \).
2 A scale-truncation condition based on Poincaré’s inequality

The closure model must keep the residual field \( \nu' = \nu - \tilde{\nu} \) from becoming dynamically significant. 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 it to be balanced by the modelled dissipation:

\[
\int_{\Omega_\delta} \nu' \cdot (\nabla \cdot \tau') \, dx = - \int_{\Omega_\delta} \nu' \cdot (\nabla \cdot (\nu \otimes \nu')) \, dx
\]  

(6)

Of course, we can verify whether this condition is met during a LES. But that is not very attractive, because it requires a fair approximation of \( \nu' \), which is quite expensive to compute. The more so since the user has chosen the filter length \( \delta \) in such a way that the residual field \( \nu' \) is not of interest to him. Alternatively, \( \nu' \) 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. Therefore, we will make use of Poincaré’s inequality to get a scale-truncation condition which does not refer to the residual field \( \nu' \), see also [3]-[4].

Poincaré’s inequality

\[
\int_{\Omega_\delta} ||\nu - \tilde{\nu}||^2 \, dx \leq C \int_{\Omega_\delta} ||\nabla \nu||^2 \, dx
\]  

(7)

shows that the \( L^2(\Omega_\delta) \) norm of the residual field \( \nu' \) is bounded by a constant (independent of \( \nu \)) times the \( L^2(\Omega_\delta) \) norm of \( \nabla \nu \). Payne and Weinberger [5] have shown that the Poincaré constant is given by \( C_\delta = (\delta / \pi)^2 \) for convex (bounded, Lipschitz) domains \( \Omega_\delta \). This is the best possible estimate in terms of the diameter alone. In case the filter box \( \Omega_\delta \) is quite anisotropic, the diameter does not provide a sufficiently detailed description of it’s geometry. This problem can be sidestepped by using a modified Poincaré inequality, see [6]. For simplicity, it is assumed that the filter box \( \Omega_\delta \) is rectangular with (very different) dimensions \( \delta x_1, \delta x_2 \) and \( \delta x_3 \). The energy of the sub-filter scales can then be confined using the modified Poincaré inequality:

\[
\int_{\Omega_\delta} ||\nu - \tilde{\nu}||^2 \, dx \leq C \int_{\Omega_\delta} (\delta x_i \partial_i v_j)^2 \, dx
\]

where \( C \) is a constant independent of \( \delta x_i \). Thus, whereas the original Poincaré inequality (7) incorporates the dependence on the size of the filter box in the Poincaré constant \( C_\delta \), the modified Poincaré inequality incorporates the dependence on the size of the filter box by scaling the velocity gradient \( \partial_i v_j \) with \( \delta x_i \). Further details can be found in Ref. [6]. In this paper, we will assume that the dimensions \( \delta x_i \) are similar, so that the Poincaré inequality need not be scaled. We aim to convert the balance condition (6) to the upper limit set by the Poincaré inequality (7).

Poincaré’s inequality (7) shows that the residual field \( \nu' \) can be suppressed by controlling the velocity gradient. According to Eq. (2), we have
\[
\frac{d}{dt} \int_{\Omega_\delta} \frac{1}{2} |\nabla v|^2 \, dx = \int_{\Omega_\delta} \nabla (v \nabla \cdot \nabla v - \nabla \pi - \nabla \cdot (v \otimes v) - \nabla \cdot \tau) : \nabla v \, dx \tag{8}
\]

Once again, the latter two terms in the right-hand side represent the nonlinear production and eddy-dissipation, respectively. Thus expressed in terms of the velocity gradient the production-dissipation balance (6) reads

\[
\int_{\Omega_\delta} \nabla \cdot \tau(v) : \nabla v \, dx = -\int_{\Omega_\delta} \nabla \cdot (v \otimes v) : \nabla v \, dx \tag{9}
\]

Stated differently, if the model \(\tau\) satisfies Eq. (9), Eq. (8) shows that the Poincaré upperbound of the residual field \(v'\) - that is, the \(L^2(\Omega_\delta)\)-norm of \(\nabla v\) - dissipates at it’s natural rate (which is set by the fluid viscosity \(\nu\)). Moreover, if the flow is initialized such that the \(L^2(\Omega_\delta)\) norm of \(\nabla v\) vanishes then (8)-(9) and (7) ensure that the \(L^2(\Omega_\delta)\) norm of the residual field \(v'\) equals zero for all times. For incompressible flows, the Cayley-Hamilton theorem states that

\[
\nabla v^3 - Q \nabla v + R = 0,
\]

where the second and third invariant of the velocity-gradient tensor are \(Q(v) = \frac{1}{2} \nabla \cdot \nabla v\) and \(R(v) = -\frac{1}{3} \nabla \cdot \nabla v \nabla v = -\det \nabla v\), respectively. The right-hand side of Eq. (9) can be written in terms of these invariants. Indeed, since \(\partial_k v_k = 0\), we have

\[
\int_{\Omega_\delta} \partial_k (\partial_k v_j) \partial_i v_j \, dx = \int_{\Omega_\delta} \partial_k v_k \partial_i v_j + \frac{1}{2} \partial_k (\partial_i v_j)^2 \, dx
\]

\[
= -\int_{\Omega_\delta} 3R(v) \, dx + \int_{\partial \Omega_\delta} Q(v) v \cdot n \, ds
\]

where \(n\) is the outward-pointing normal vector to the boundary \(\partial \Omega_\delta\) of \(\Omega_\delta\).

In conclusion, the convective contribution to the evolution of the \(L^2(\Omega_\delta)\) norm of \(\nabla v\) is properly balanced by the closure model if

\[
\int_{\Omega_\delta} \nabla \cdot \tau(v) : \nabla v \, dx = 3 \int_{\Omega_\delta} R(v) \, dx - \int_{\partial \Omega_\delta} Q(v) v \cdot n \, ds \tag{10}
\]

### 3 Relaxation model

The basic idea of LES is that the large scales of motion remain virtually unchanged, whereas the tail of the modulated spectrum (the spectrum of \(v\)) falls of much faster than the spectrum of the NS-solution \(u\). In the present setting, the model \(\tau\) is chosen properly if the associated box-filtered solution \(\bar{v}\) approximates the box-filtered NS-solution \(\bar{u}\). The residual velocity field \(v - \bar{v}\) does not have any physical significance; it is only used to shorten the energy spectrum. The right-hand side of Eq. (1) does not dissipate energy, but transfers it (on average) towards smaller scales of motion that can dissipate energy at a higher rate. Here, we do not try to model the transport itself, but only just the net effect thereof. So the model should strengthen the dissipation (without producing smaller scales of motion, of course). To that end, we study the relaxation model introduced by Stolz et al. [3]. They used the relaxation
\[ \nabla \cdot \tau(v) = \chi(v - \bar{v}) \] (11)

to truncate the small scales of motion by dissipating their energy. The attractive feature of their relaxation method is that no (explicit) use is made of a differential operator; hence a relaxation model can be discretized accurately near/at the grid cut-off as well as on "awkward" (unstructured, e.g.) grids.

The relaxation parameter \( \chi \) is determined from the requirement that the production of any fine flow details of size smaller than \( \delta \) by the convective nonlinearity is counteracted by the dissipation resulting from the relaxation model. The production-dissipation balance associated with the relaxation model is obtained by substituting (11) in (10). This yields

\[
\chi = \frac{3 \int_{\Omega_\delta} R \, dx - \int_{\partial\Omega_\delta} Q \cdot n \, ds}{\int_{\Omega_\delta} \nabla (v - \bar{v}) : \nabla v \, dx} 
\] (12)

where the relaxation parameter is taken constant in \( \Omega_\delta \) i.e., \( \delta \) is assumed to by the smallest scale at which \( \chi \) varies. If \( \chi \) is negative, the small box-fitting scales transfer energy to the larger eddies. Since these small scales of motion have no physical significance, \( \chi \) is set to zero if Eq. (12) yields a negative value (i.e, \( \chi \) is clipped).

As in Schumann’s approach, the spatial discretization of the convective term defines the grid-filter. In one spatial dimension, the convective derivative is approximated to second-order accuracy by

\[
\partial_x \phi_i \approx (\phi_{i+1} - \phi_{i-1})/2h; \quad \text{hence effectively we have } \partial_x \phi_i \approx (\phi_{i+1} - \phi_{i-1})/(2h). 
\]

The diffusive term is approximated using

\[
\partial^2_x v_i \approx (v_{i+1} - 2v_i + v_{i-1})/h^2. 
\]

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. Therefore we take \( \delta = 2h \), see also [6]. In 1D the box filter (3) is approximated by

\[
\bar{v}_i = \frac{1}{2} v_i + \frac{1}{4} (v_{i+1} + v_{i-1}) 
\] (13)

This discretization rule is also applied to the \( \Omega_\delta \)-integrals in Eq. (12). Here it is to be stressed that we approximate all integrals using the trapezoidal rule with constant coefficients, even if the grid is non-uniform, since the point-to-point mode must be an integral part of the residue of the discrete box filter. Moreover, the model is evaluated directly, i.e., without applying any form of deconvolution to the grid-filter; so any difficulties associated with the deconvolution procedure are circumvented. The invariants \( Q(v) \) and \( R(v) \) are computed from the discrete velocity gradient, where the gradient is discretized as in the convective term.

The performance of the resulting discrete relaxation model has been investigated for isotropic turbulence and turbulent channel flow. As an example results for turbulent channel flow (Re_\tau = 590) are shown in Fig.1. As is customary in this test-case, the computational grid for the LES consists of \( 64^3 \) points. Details about the numerical method can be found in Ref. [2].
Fig. 1 Results for turbulent channel flow (Re_τ = 590): mean velocity (upper figure) and root-mean-square velocities.

References