Lagrangian dynamics of the tensor diffusivity model for turbulent subfilter stresses

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1. Motivation and objectives

Large-eddy simulations (LES) are most often considered attempts to numerically approximate the solution to the filtered Navier-Stokes equations (Leonard 1974; Meneveau & Katz 2000; Sagaut 2006). LES provides significant advantages over simulation approaches based on Reynold-Averaged Navier-Stokes (RANS) because less is asked or expected of the closure model for the unknown turbulent stresses. As a result, LES models for the subfilter stress (also called the subgrid stress) are typically simpler in form than RANS models. Many of the most popular LES stress models are algebraic, introducing no additional transport equations. The reason for this is that it is generally more advantageous to invest computational power in finer meshes to resolve more of the turbulent fluctuations than to invest in more expensive turbulence models which will remain approximate anyway.

The most popular LES stress model, the Smagorinsky model (Smagorinsky 1963), is part of a larger class of eddy viscosity models which assume that the subfilter stress instantaneously aligned with the filtered rate-of-strain tensor. This assumption is demonstrably false (Borue & Orszag 1998; Ballouz & Ouellette 2018), although the Smagorinsky model has achieved considerable success in practice. The physical reason that the Smagorinsky model fails is that the subfilter stress contains significant memory, particularly of the previous flow along its Lagrangian path (Ballouz *et al.* 2020). This Lagrangian memory is significant for filtered turbulent flows because of the lack of scale separation between resolved and subfilter scales, particularly in terms of the active timescales. Some stress models have attempted to include Lagrangian history information, via Lagrangian averaging during the dynamic procedure for the Smagorinsky coefficient (Meneveau *et al.* 1996), or by making a recent deformation approximation (Li *et al.* 2009). However, in the spirit of developing models with minimal computational cost and complexity, this report explores the extent to which Lagrangian history effect may be implicitly included in a subfilter stress model, particularly the tensor diffusivity model of Clark *et al.* (1979). (Note that Clark *et al.* (1979) introduced the tensor diffusivity model for the Leonard & cross-stresses, such that is should be supplemented with an eddy viscosity term for the Reynolds stress component.)

2. The Lagrangian memory of the subfilter stress tensor

The velocity field, $\mathbf{u}(\mathbf{x}, t)$, of an incompressible fluid flow is assumed to follow the Navier-Stokes equations,

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \nu \nabla^2 u_i, \tag{2.1}$$

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where the pressure (divided by density), p, enforces a zero-divergence condition on the velocity field, $\partial_k u_k = 0$.

The goal of a large eddy simulation is often assumed to be the calculation of a spatially-filtered version of a given flow (Leonard 1974),

$$\overline{\mathbf{u}}^{\ell} = G_{\ell} \star \mathbf{u}, \qquad \mathcal{F}\{\overline{\mathbf{u}}^{\ell}\} = \mathcal{F}\{G_{\ell}\}\mathcal{F}\{\mathbf{u}\}, \tag{2.2}$$

where ℓ is the filter width and $\mathcal{F}$ denotes a Fourier transform when the simulation domain is triply periodic. Applying this spatial filtering operation to the incompressible Navier-Stokes equations yields

$$\partial_t \overline{u}_i + \overline{u}_j \partial_j \overline{u}_i = -\partial_i \overline{p} + \nu \nabla^2 \overline{u}_i - \partial_j \tau(u_i, u_j) \tag{2.3}$$

where the divergence-free condition, $\partial_k \overline{u}_k = 0$, can be used to form a Poisson equation for the filtered pressure, $\overline{p}$. The final term on the right of Eq. (2.3) is a generalized second-moment of the form (Germano 1992)

$$\tau(a, b) = \overline{ab} - \overline{a}\overline{b} \tag{2.4}$$

so

$$\tau_{ij} \equiv \tau(u_i, u_j) = \overline{u_i u_j} - \overline{u_i}\ \overline{u_j} \tag{2.5}$$

is the subfilter stress tensor representing the unresolved flux of filtered momentum due to small-scale velocity fluctuations.

Making direct use of Eqs. (2.1) and (2.3), along with the definition of the subfilter stress tensor, Eq. (2.5), one may write an evolution equation for the subfilter stress which has the form

$$\partial_t \tau_{ij} + \overline{u}_k \partial_k \tau_{ij} = -\overline{A}_{ik} \tau_{jk} - \tau_{ik} \overline{A}_{jk} + \text{other terms}, \tag{2.6}$$

where $\overline{A}_{ij} = \partial \overline{u}_i / \partial x_j$ is the filtered velocity gradient tensor. The other terms will be discussed in more detail below. If they are neglected, then a formal solution is available for the evolution of the subfilter stress tensor along a Lagrangian path following the filtered velocity field (Li *et al.* 2009),

$$\tau_{ij}(t) = H_{im}(t, t_0) \tau_{mn}(t_0) H_{jm}(t, t_0), \tag{2.7}$$

where the mapping tensor $\mathbf{H}(t, t_0)$ evolves with the equation

$$\partial_t H_{ij} + \overline{u}_k \partial_k H_{ij} = -\overline{A}_{ik} H_{kj} \tag{2.8}$$

and its formal solution is given as a time-ordered exponential along the (filtered) Lagrangian path

$$H_{ij}(t, t_0) = \exp^{+}\left(\int_{t_0}^{t} -\overline{A}_{ij}(t') dt' \right). \tag{2.9}$$

(The + denotes that this is the time-ordered matrix exponential.) This highlights an important physical behavior that the subfilter stress has a memory of the past filtered velocity gradients along its (filtered) Lagrangian path, even if it becomes distorted in practice by the other terms in Eq. (2.6).

To give some intuitive appreciation, an analogy may be drawn with the behavior of viscoelastic fluids. The Cauchy stress tensor for viscoelastic fluids typically includes a stress proportional to a configuration tensor, $\mathbf{C}$. For example, in fluids with dissolved polymers, the symmetric configuration tensor describes the orientation of the polymers as a function of space and time in the flow (White & Mungal 2008). A typical evolution equation for the configuration tensor is

$$\partial_t C_{ij} + u_k \partial_k C_{ij} = A_{ik} C_{jk} + C_{ik} A_{jk} + \text{relaxation terms}, \tag{2.10}$$

which bears a direct resemblance with the evolution of the subfilter stress evolution, Eq. (2.6). Neglecting relaxation terms, the formal solution is

$$C_{ij}(t) = F_{im}(t, t_0) C_{mn}(t_0) F_{jn}, \tag{2.11}$$

where

$$F_{ij} = \exp^+ \left(\int_{t_0}^{t} \overline{A}_{ij}(t') dt' \right) \tag{2.12}$$

is the Finger tensor of fundamental importance in elementary continuum mechanics. The difference in Lagrangian memory between polymer and turbulent stresses is the negative sign, which symbolizes that turbulent stresses are enhanced by compressive strain rates rather than extensional ones.

Turbulent flows of Newtonian fluids, when observed at a scale coarser than the Kolmogorov scale, have a behavior that may be qualitatively compared with viscoelastic fluids. This was discussed in some detail for RANS by Crow (1968). Indeed, Tennekes and Lumley remark in the first chapter of their celebrated textbook (Tennekes & Lumley 1972):

> *"We may, for analytical reasons, speak of a turbulent fluid rather than of a turbulent flow. Turbulent 'fluids,' however, are non-Newtonian: they exhibit viscoelasticity and suffer memory effects."*

This Lagrangian memory directly contradicts the eddy viscosity hypothesis that forms the basis for the most popular LES closures, namely, those of the Smagorinsky family. The significance of the memory is tied to the lack of scale separation when the broadband activity of turbulence is filtered at an arbitrary scale. There will always be significant residual motions that are only slightly smaller than the resolved scales and hence evolve on similar timescales at the resolved dynamics.

A simple way to account for Lagrangian memory, which has turned out to have significant empirical success, is to average over Lagrangian trajectories with exponentially fading memory when performing the dynamic procedure for determining the eddy viscosity (Meneveau *et al.* 1996). This approach only partially accounts for the memory in that it still assumes the eddy viscosity form in which the instantaneous subfilter stress tensor is proportional to the instantaneous filtered strain-rate tensor. Lagrangian memory will also cause misalignment between these two tensors, which has been found to be quite significant even in stationary homogeneous isotropic turbulence (Ballouz & Ouellette 2018).

A better representation of Lagrangian memory effects may be obtained following the approach of Li *et al.* (2009) to define a matrix exponential-based closure inspired by the recent fluid deformation approximation (Chevillard & Meneveau 2006; Chevillard *et al.* 2008). This approach still involves some (uncontrolled) assumptions about the other terms in Eq. (2.6) as well as approximating the history integral using only the current filtered velocity gradient. Furthermore, the numerical calculation of a matrix exponential involves additional challenges that are undesirable, though not prohibitive.

However, there is a much simpler way to encapsulate the Lagrangian history into a closure for the subfilter stress tensor. The basic idea is that the closure model should have an evolution equation with the same form as Eq. (2.6). It turns out that this is quite simple. Consider the tensor diffusivity model of Clark *et al.* (1979),

$$\tau_{ij}^{m} = c\ell^2 \overline{A}_{ik}\overline{A}_{jk}. \tag{2.13}$$

This model form may be justified as follows. Johnson (2020) showed that, for a Gaussian filter, the generalized second-order moment satisfies the following diffusion equation

$$\frac{\partial \tau^{\ell}(a,b)}{\partial(\ell^2)} = \frac{1}{2}\nabla^2\tau^{\ell}(a,b) + \partial_k\overline{a}^{\ell}\partial_k\overline{b}^{\ell}, \tag{2.14}$$

where ℓ^2 serves as a time-like variable. As a result, one may write

$$\tau^{\ell}(a,b) = \ell^2\partial_k\overline{a}\partial_k\overline{b} + \int_0^{\ell^2} d\alpha\ \tau^{\beta}\left(\partial_k\overline{a}^{\sqrt{\alpha}}, \partial_k\overline{b}^{\sqrt{\alpha}}\right) \tag{2.15}$$

where $\beta = \sqrt{\ell^2 - \alpha}$. For a broader class of filter shapes, one may show via Taylor expansion that

$$\tau^{\ell}(a,b) = c\ell^2\partial_k\overline{a}\partial_k\overline{b} + \text{higher-order terms}, \tag{2.16}$$

where $c = 1$ for a Gaussian filter. The tensor diffusivity model may be constructed from either of these expressions by neglecting everything beyond the first term. The tensor diffusivity model typically performs very well in *a priori* studies of the subfiltered stress tensor (Borue & Orszag 1998).

The Lagrangian evolution of this model stress tensor is determined by the Lagrangian evolution of the filtered velocity gradient tensor. To this end, the gradient of Eq. (2.3) gives

$$\partial_t\overline{A}_{ij} + u_k\partial_k\overline{A}_{ij} = -\overline{A}_{ik}\overline{A}_{kj} + \text{other terms}. \tag{2.17}$$

This shows that the filtered velocity gradient amplifies itself in a manner similar to the subfilter stress, Eq. (2.6). Differentiating Eq. (2.13) and substituting Eq. (2.17), it may be shown that

$$\partial_t\tau_{ij}^{m} + \overline{u}_k\partial_k\tau_{ij}^{m} = -\overline{A}_{ik}\tau_{jk}^{m} - \tau_{ik}^{m}\overline{A}_{jk} + \text{other terms}. \tag{2.18}$$

The tensor diffusivity model, through the precise form of its dependence on the filtered velocity gradient, has a Lagrangian memory that mimics that of the true subfilter stress tensor. Thus, a closure of the form given in Eq. (2.13) provides a simple, effective way to encapsulate accurate Lagrangian history into a subfilter stress model without Lagrangian averaging or matrix exponentials.

3. Transport equation for the tensor diffusivity model

For a more detailed understanding of the behavior of the tensor diffusivity model, the full evolution equation of the tensor diffusivity model must be considered in comparison with the full evolution equation for the subfilter stress tensor. These are constructed following the same procedure as above, but now explicitly writing all terms previously grouped as other terms.

The full evolution equation for the subfilter stress tensor is (Germano 1992)

$$\partial_t\tau_{ij} + u_k\partial_k\tau_{ij} = -\overline{A}_{ik}\tau_{jk} - \tau_{ik}\overline{A}_{jk} - \partial_k T_{ijk} + 2\tau(p, S_{ij}) - 2\nu\tau\left(A_{ik}, A_{jk}\right), \tag{3.1}$$

where the spatial transport term is

$$T_{ijk} = \tau(u_i, u_j, u_k) + \tau(p, u_i)\delta_{jk} + \tau(p, u_j)\delta_{ik} - \nu\partial_k\tau_{ij}. \tag{3.2}$$

The generalized second moment from Eq. (2.4) is used here along with the generalized third moment (Germano 1992),

$$\tau(a,b,c) = \overline{abc} - \overline{a}\tau(b,c) - \overline{b}\tau(a,c) - \overline{c}\tau(a,b) - \overline{a}\overline{b}\overline{c}. \tag{3.3}$$

The full evolution equation for the tensor diffusivity model is

$$\partial_t \tau^m_{ij} + \overline{u}_k \partial_k \tau^m_{ij} = -\overline{A}_{ik}\tau^m_{jk} - \tau^m_{ik}\overline{A}_{jk} - \partial_k T^m_{ijk} + 2c\ell^2 \partial_k \overline{p}\ \partial_k \overline{S}_{ij} - 2\nu c\ell^2 \partial_l \overline{A}_{ik} \partial_l \overline{A}_{jk} + \Phi_{ij}, \tag{3.4}$$

where the flux is given by

$$T^m_{ijk} = c\ell^2 \partial_l \overline{u}_i\ \partial_l \tau_{jk} + c\ell^2 \partial_l \overline{u}_j\ \partial_l \tau_{ik} + c\ell^2 \partial_l \overline{p}\ \partial_l \overline{u}_i \delta_{jk} + c\ell^2 \partial_l \overline{p}\ \partial_l \overline{u}_j \delta_{ik} - \nu \partial_k \tau^m_{ij} \tag{3.5}$$

and the source term

$$\Phi_{ij} = c\ell^2 \partial_l \overline{A}_{ik} \partial_l \tau_{jk} + c\ell^2 \partial_l \overline{A}_{jk} \partial_l \tau_{ik}, \tag{3.6}$$

appears without any apparent or intuitive justification. Comparing Eqs. (3.1) and (3.4), one may deduce models for the unclosed terms in the subfilter stress evolution equation implied by the tensor diffusivity model.

The implied model for the pressure-strain-rate is

$$\tau(p, S_{ij})^m = c\ell^2 \partial_k \overline{p}\ \partial_k \overline{S}_{ij}, \tag{3.7}$$

which may be obtained by the same Taylor expansion procedure used to obtain the tensor diffusivity model for $\tau(u_i, u_j)$. However, this does not necessarily make this a good closure. The tensor diffusivity closure for the subfilter stress enjoys (a-priori) success because it is primarily due to scales near the filter scale. The pressure-strain-rate, however, is more reliant on the smallest scales in the flow because the strain-rate is primarily organized at small scales.

The implied pressure transport model is

$$\tau(p, u_i)^m = c\ell^2 \partial_k \overline{p}\ \partial_k \overline{u}_i, \tag{3.8}$$

which, again, can be formed following the same procedure leading to the tensor diffusivity model for $\tau(u_i, u_j)$. At first glance, this model seems more promising that the pressure-strain-rate model above, since both the residual velocity and pressure are dominated near the filter scale. However, the subfilter stress evolution is likely less sensitive to pressure transport models.

The implied subfilter transport model is

$$\tau(u_i, u_j, u_k)^m = c\ell^2 \partial_l \overline{u}_i\ \partial_l \tau_{jk} + c\ell^2 \partial_l \overline{u}_j\ \partial_l \tau_{ik}. \tag{3.9}$$

The Gaussian filter has the following exact relationship for the generalized third-order moment,

$$\frac{\partial \tau^\ell(a,b,c)}{\partial(\ell^2)} = \frac{1}{2}\nabla^2 \tau^\ell(a,b,c) + \ell^2 \partial_l \overline{u}_i\ \partial_l \tau_{jk} + \ell^2 \partial_l \overline{u}_j\ \partial_l \tau_{ik} + \ell^2 \partial_l \overline{u}_k\ \partial_l \tau_{ij}, \tag{3.10}$$

so that we see the implied transport model above lacks the final term, $\ell^2 \partial_l \overline{u}_k\ \partial_l \tau_{ij}$, to be an appropriate approximation. In fact, the implied model does not satisfy the proper symmetries on the indices i, j, k. Otherwise, however, it is the model consistent with the procedure for how the tensor diffusivity model is formed.

The implied model for the viscous destruction is

$$-2\nu\tau\left(A_{ik}, A_{jk}\right) = -2\nu c\ell^2 \partial_l \overline{A}_{ik} \partial_l \overline{A}_{jk} + \Phi_{ij}, \tag{3.11}$$

so that the first part is exactly formed by the tensor diffusivity model procedure, but the second term Φ_{ij} does not appear to have a straightforward interpretation. Certainly, the first term is not expected to be accurate because the viscous destruction occurs primarily at the smallest scales.

Overall, the similarities between the evolution equation for the subfilter stress, Eq. (3.1) and the tensor diffusivity model for the stress, Eq. (3.4), are numerous and compelling. However, some of the implied models for the unclosed terms in the stress evolution equation have important deficiencies that one would want to address if designing a six-equation transport model for the subfilter stress. A priori testing of the implied models could be used illuminate the performance of each implied model.

4. Conclusions

It is shown in this report that the tensor diffusivity model for the subfilter stress tensor efficiently encodes the Lagrangian history effect of the filtered velocity gradient tensor along the pathline. This provides a particularly easy way to include the viscoelastic-like effects of subfilter turbulence when performing large-eddy simulations (LES). However, consideration of the full evolution equations shows apparent deficiencies for most of the implied models for unclosed terms if a six-equation stress transport model were to be constructed consistent with the tensor diffusivity model. These shortcomings aside, from a certain theoretical point of view, the tensor diffusivity model enjoys significant advantages over other (more expensive) procedures for including Lagrangian history effects in subfilter stress models.

As a caveat, note that the tensor diffusivity model is usually under-dissipative in practice, so steps should be taken to address this deficiency. One possible solution is to adjust the value of the coefficient $c > 1/12$. For LES, this choice theoretically depends on the assumed filter shape and the filter width to grid ratio. In other words, one may assume the filter width to be somewhat larger than the grid and hence obtain a more dissipative tensor diffusivity model. On the other hand, the Gaussian relation developed by Johnson (2020) provides a promising way to supplement the tensor diffusivity model with a model for the multiscale vortex stretching and strain self-amplification effects. These multiscale terms may turn out to be well-approximated by a Smagorinsky-like term, resulting in further physics-based support for a mixed model (Clark *et al.* 1979; Vreman *et al.* 1996) for subfilter stresses.

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