Dynamic modeling of non-Boussinesq subgrid-scale models for large-eddy simulations

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1. Motivation and objectives

As the Reynolds number of a turbulent flow increases, the feasibility of direct numerical simulations (DNS) becomes impractical. As a result, large-eddy simulations (LES) have been widely used for analysis of turbulent flows (Bose & Moin 2014; Germano et al. 1991; Goc et al. 2020b).

Smagorinsky (1963) developed a subgrid-scale (SGS) stress closure model using the strain rates of large-scale eddies to model the isotropic eddies in homogeneous isotropic turbulence. The subgrid stress from this model does not vanish in laminar regions or near the walls, making it unsuitable for simulating transitional or wall-bounded flows. Germano et al. (1991) developed a dynamic procedure for the Smagorinsky model (DSM) in which the model coefficient is dependent on the local flow characteristics, rendering LES as a more predictive approach. However, for numerical stability reasons, ad hoc clipping of the model coefficient is done to prevent backscatter of energy. Later, Vreman (2004) developed a constant-coefficient model with vanishing behavior in laminar and transitional regions. This model was shown to perform as well as DSM for mixing layers and channel flows up to $Re_{\tau} = 360$. The absence of test filtering and a clipping procedure made this model appealing for LES of engineering flows.

Recently, LES of high Reynolds number flows of both canonical and complex flows have been attempted. At these high Reynolds numbers, grid requirements, especially near the wall, become restrictive unless wall models are employed. Wall-modeled LES (WMLES) models the near-wall turbulence with input from outer-LES variables. Multiple such wall models have been developed and extensively tested in canonical and complex flows (Goc et al. 2020b; Bose & Moin 2014; Lozano-Durán & Bae 2019). For canonical flows, classical SGS models have performed reasonably well in predicting mean velocity and intensities accurately (Germano et al. 1991; Lozano-Durán & Bae 2019; Moin et al. 1991).

For complex flows, the grids are often very coarse and the turbulence is anisotropic. As a result, the role of the SGS model potentially increases in accurately capturing the effect of small scales on large-scale motions. Additionally, for LES involving highly anisotropic grids, the assumption of a scalar model coefficient as used in classical Boussinesq eddy viscosity closures is potentially overly restrictive. Advancements in dynamic SGS modeling procedures are hence an important building block in the efforts to accurately simulate flow over complex engineering configurations. In this brief we propose novel dynamic formulations of advanced SGS models, going beyond the classical Boussinesq eddy viscosity closures to include effects arising from flow anisotropy and rotation rate of large-scale eddies.

The next sections of this brief are organized as follows. We revisit the existing SGS formulations in Section 2, and then present our modeling approach in Section 3. A-priori results from these models are presented in Section 4. Detailed a-posteriori analysis of
2. Governing equations and existing SGS modeling procedures

The governing equations for LES of incompressible turbulent flows (of constant density $\rho$) are

$$\frac{\partial \rho_i}{\partial x_i} = 0 \quad (2.1)$$

and

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial \rho_j \rho_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \rho_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j}, \quad (2.2)$$

where $\tau_{ij}^{sgs}$ is the modeled SGS stress. The eddy-viscosity-based SGS closure models take the form

$$\tau_{ij}^{sgs} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\nu \overline{S}_{ij}, \quad \text{where} \quad \overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \rho_i}{\partial x_j} + \frac{\partial \rho_j}{\partial x_i} \right). \quad (2.3)$$

The isotropic component of the SGS stress is often absorbed into pressure, which leads to a pseudo-pressure field. One of the more commonly used Boussinesq models is the Smagorinsky model, which is described in detail below.

### 2.1. Smagorinsky model

Smagorinsky (1963) provided an eddy viscosity model based on the assumption of the balance of the production and dissipation of turbulent kinetic energy for small scales. This model is based on a length scale similar to the LES-grid-resolution scale and a time scale based on the strain-rate tensor. With these assumptions, the eddy viscosity is given as

$$\nu_t = (C_s \Delta)^2 |S|, \quad (2.4)$$

where $|S| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}$ and $\Delta$ is the grid filter width. Later, Lilly (1970) showed that for isotropic turbulence with spatial resolution that lies in the inertial subrange, $C_s \sim 0.17$. Deardorff (1970) recommended $C_s \sim 0.1$ in turbulent shear flows. The applicability of this model is limited, especially in the near-wall region of wall-bounded flows in part because the model coefficient does not asymptotically reach a value of zero. Consequently, previous studies (Moin & Kim 1982) have used wall-damping functions (Van Driest 1956) to correct for the behavior of eddy viscosity in the viscous sublayer.

### 2.2. Dynamic Smagorinsky model

Germano et al. (1991) introduced the notion of test filtering of the LES governing equations. Through the use of these ideas, the Leonard stress tensor (Leonard 1975), $L_{ij} = -\overline{u}_i \overline{u}_j + \overline{u}_i \overline{u}_j \left( \int \right)$ (denotes test-filter operation) can be related to the resolved stress as

$$L_{ij} = 2(C_s \Delta)^2 \left( \frac{\Delta^2}{\Delta^2} |S| S_{ij} - \overline{|S|S_{ij}} \right) = 2(C_s \Delta)^2 M_{ij}, \quad (2.5)$$

where $\tilde{\Delta}$ and $\Delta$ denote test-level and grid-level filter widths, respectively. Lilly (1992) proposed a least-squares solution of this system, leading to the model coefficient being
Owing to numerical instability issues, and to avoid excessive backscatter of energy, the numerator and denominator of this equation are further averaged in space to finally give its working form

\[(C_s \Delta)^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle 2M_{ij} M_{ij} \rangle},\]  

(2.7)

where \(\langle \cdot \rangle\) is the spatiotemporal averaging operator.

3. Modeling framework

While the dynamic procedure improves the predictive capability of the constant-coefficient Smagorinsky model, it does not resolve the model-form error that is inherent to all Boussinesq SGS models (that the SGS stress is not necessarily aligned with the strain-rate tensor). In this brief, we propose novel dynamic formulations to the tensor-coefficient Smagorinsky model (Moin 1993), and a non-linear model characterized by the full velocity gradient tensor (Lund & Novikov 1992). Both models contain non-Boussinesq terms that do not lead to dissipation but would potentially improve the local alignment between modeled and exact subgrid stresses.

3.1. Dynamic tensor coefficient Smagorinsky model (DTCSM)

Moin (1993) proposed the following tensor-coefficient-based Smagorinsky model to account for misalignment in DNS between filtered resolved stresses and mean strain rates,

\[\tau_{s_{ij}} - \frac{\tau_{s_{k}}}{3} \delta_{ij} = -(C_{ik} S_{kj} + C_{jk} S_{ki})|S|\Delta^2.\]  

(3.1)

This model contains nine independent coefficients, thus providing more degrees of freedom in determining alignment of the stress tensor in terms of strain-rate tensor. However, in its current form, the rotational invariance of the model, which is a requirement satisfied by the governing equations, is not guaranteed. To treat this, we put the following constraints on the coefficients

\[C_{11} = C_{22} = C_{33}\]  

(3.2)

and

\[C_{ij} = -C_{ji} \quad (j \neq i).\]  

(3.3)

As shown in Appendix A, with these constraints, the model obeys rotational invariance, a necessary condition for realizability, as required by the Navier-Stokes equations.

The realizability constraints also limit the number of independent coefficients from nine to four. Incorporating this reduction, we invoke the Germano identity for this model to arrive at

\[L_{ij} = (C_{ik} \Delta^2 M_{kj} + C_{jk} \Delta^2 M_{ki}).\]  

(3.4)

For an incompressible flow, this system of five independent equations with four coefficients is solved using the least-squares solution method (Lilly 1992) to obtain the coefficients dynamically. It is noteworthy that only \(C_{11}\) contributes to dissipating energy from the large scales. As a consequence, the spatial averaging, along with a non-negativity constraint on \(C_{11}\), can be applied to remove any backscatter of energy for numerical stability.
purposes. Note that for the flows considered in this brief, the non-negativity constraint was not applied. The non-dissipative coefficients are local in space and not clipped.

3.2. Dynamic Lund-Novikov II-term model (DLN2M)

Lund & Novikov (1992) argued that the omission of the rotation-rate tensor from the SGS model is unjustified, as the vorticity stretching leads to production of 3D turbulence. As a result, using the Cayley-Hamilton theorem, they proposed a non-linear subgrid-stress model based on the expansion of the velocity gradient tensor (Pope 1975). A-priori analysis of decaying isotropic turbulence has shown (Lund & Novikov 1992) that the addition of more terms to the two-term model produced smaller improvements in the tensor-level correlations of exact and modeled SGS stresses. As a result, the proposed model in this brief is limited to the two-term expansion. The model form is given as

$$\tau_{ij}^{sgs} = \tau_{kk}^{sgs} \delta_{ij} = -2C_s \Delta^2 S_{ij}|S| - C_{rs} \Delta^2 (S_{ik} R_{kj} - R_{ik} S_{kj}).$$

(3.5)

Applying the Germano identity on this model yields

$$L_{ij} = 2C_s \Delta^2 M_{kj} + 2C_{rs} \Delta^2 N_{ij},$$

(3.6)

where $N_{ij}$ is equal to

$$N_{ij} = \frac{1}{2} \left[ \frac{\Delta^2}{\Delta^2} (\hat{S}_{kj} \hat{R}_{ki} - \hat{R}_{ik} \hat{S}_{kj}) - (S_{kj} \hat{R}_{ki} - \hat{R}_{ik} S_{kj}) \right].$$

(3.7)

Equation (3.6) is also solved using the least-squares approach to compute $C_s$ and $C_{rs}$ dynamically. For this model, only the Boussinesq-type term contributes to energy dissipation from the large scales. Similar to DTCSM, only an averaging procedure on $C_s$ is applied.

It should be noted that the proposed modeling approach can be easily extended to using the full five-term expansion of the velocity gradient tensor (Lund & Novikov 1992) to solve for a system of five independent equations and five model coefficients.

The reader is directed to Appendices B and C for more details on the dynamic procedures for both DTCSM and DLN2M and a brief discussion of how the two model forms can be reconciled analytically.

4. A-priori tests

In this section, we compare a-priori performance of DSM, DTCSM and DLN2M at tensor and scalar levels with respect to filtered-DNS data for a channel flow at $Re_\tau = 395$. In the presence of flow anisotropy, an improved SGS model is expected to produce higher tensor-level correlations and provide more realistic representation of the small scales. The correlations at tensor level are defined as

$$\rho = \frac{1}{6} \sum_{k=1}^{6} \frac{\text{cov}(\tau_{model,k}, \tau_{exact,k})}{\sigma(\tau_{models,k}) \sigma(\tau_{exact,k})}.$$  

(4.1)

where $k = 1, 2, ..., 6$ are the six components of exact ($\tau_{exact}$) and modeled ($\tau_{model}$) SGS stress tensors. Note that $\text{cov}(X, Y)$ denotes the covariance between quantities $X$ and $Y$ and $\sigma(X)$ is the standard deviation of the distribution of the quantity $X$. The scalar-level correlations are similarly defined by contracting the stress tensor with the large-scale strain-rate tensor.
Figure 1 shows that DTCSM and DLN2M produce higher correlations than the Boussinesq-type Smagorinsky model at the tensor level. It is encouraging that the correlations are most improved near the wall, which is the region of high anisotropy and, in practical calculations, the limiting region in terms of resolution requirements. *A-priori* calculations, however, are not completely reflective of the model performance in simulations. The model by Bardina *et al.* (1980) showed much-improved tensor-level correlations than even DTCSM and DLN2M; however, it was shown to be significantly under-dissipative in simulations and required ad hoc supplementary dissipation from a Smagorinsky term. At the *a-priori* level, DTCSM and DLN2M have exactly the same scalar-level correlation (see Figure 2) as DSM across the entire channel height. This is indeed expected since the only terms in DTCSM and DLN2M that contribute to dissipation are Smagorinsky-type terms. A verification of the dissipative nature of these models in LES is presented next in the *a-posteriori* results section.
5. A-posteriori calculations

LES is performed for both homogeneous isotropic turbulence (HIT) and turbulent channel flow to verify the a-posteriori performance of the proposed models. For comparison, these results are compared with DNS and LES, employing DSM closure.

5.1. Decaying homogeneous isotropic turbulence

We perform DNS and LES of decaying HIT at \( Re_\lambda = u_{rms} \lambda / \nu = 70 \) (Comte-Bellot & Corrsin 1971). The initial turbulent field follows the spectrum in Passot & Pouquet (1987), with \( u_{rms} = 1 \). For a triply-periodic box of size \((2\pi)^3\), our DNS is performed on a grid of \( 128^3 \) resolution while LES is performed using a coarser grid containing \( 32^3 \) points.

For HIT, we define the turbulent kinetic energy \((tke)\) and its dissipation rate \((\epsilon)\) as

\[
\text{tke}^t = \langle \frac{1}{2} u_i u_i \rangle \quad \text{and} \quad \epsilon^t = \langle 2\nu \Sigma_{ij} \Sigma_{ij} - \tau_{ij}^{\text{sgs}} \Sigma_{ij} \rangle,
\]

where \( \langle \cdot \rangle \) is the volumetric-averaging operator. In Figures 3 and 4 we compare the evolution of kinetic energy and its dissipation rate in LES and filtered DNS. Since the calculation without an SGS model does not dissipate enough kinetic energy, it is apparent that the SGS models are active and needed to properly dissipate turbulent kinetic energy. The time evolution of both \( \text{tke} \) and \( \epsilon \) with all of the LES models are in excellent agreement with the filtered DNS after the initial transient. It is then agreeable that DTCSM and DLN2M dissipate energy as well as DSM, unlike the existing constant-coefficient non-Boussinesq SGS models (Bardina et al. 1980; Clark et al. 1979).

5.2. Forced homogeneous isotropic turbulence

The results for decaying HIT at a low Reynolds number provides quantitative information about the dissipative nature of the SGS models but limited information about the transfer of energy between the resolved large scales as the Reynolds number decreases with time. For these reasons, we now compare LES of forced HIT at \( Re_\lambda = 315 \) with \( 128^3 \) grid
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Figure 4. Evolution of the turbulent kinetic energy dissipation rate for decaying isotropic turbulence.

Figure 5. Comparison of kinetic energy spectra, $E(\kappa)$, in forced isotropic turbulence between filtered-DNS and SGS models. The resolution of the filtered-DNS is at $1024^3$ compared to the LES resolution of $128^3$.

points with the filtered DNS of Cardesa et al. (2017) performed with $1024^3$ grid points. A linear momentum forcing is applied to maintain constant turbulent kinetic energy in the system (Bassenne et al. 2016).

At high Reynolds numbers, Kolmogorov (1941) hypothesized the presence of $\kappa^{-5/3}$ scaling in the kinetic energy spectrum (defined next) for incompressible turbulence. In three dimensions, the energy content in a shell between the wavenumbers $\kappa$ to $\kappa + d\kappa$ is

$$E(k) = \sum_{k=\kappa}^{\kappa+d\kappa} \frac{1}{2} \bar{u}_i(k) \bar{u}_i^*(k),$$

where $\tilde{X}$ is the Fourier transform of quantity $X$, and $\tilde{X}^*$ denotes its complex conjugate.

Three-dimensional energy spectra are compared in Figure 5, where the $\kappa^{-5/3}$ scaling is well recovered by both DTCSM and DLN2M. The energy spectra for LES also compare
Figure 6. Comparison of kinetic energy spectra, $E(\kappa)$, between filtered-DNS and SGS models as $Re_{\lambda} \to \infty$. The LES resolution considered here is $128^3$.

Table 1. Simulation parameters for turbulent channel flow at $Re_{\tau} = 4200$

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$L_x$</th>
<th>$L_y$</th>
<th>$L_z$</th>
<th>$N_x$</th>
<th>$N_y$</th>
<th>$N_z$</th>
<th>$\Delta x^+$</th>
<th>$\Delta y_{\text{min}}^+$</th>
<th>$\Delta y_{\text{center}}^+$</th>
<th>$\Delta z^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNS</td>
<td>$2\pi \delta$</td>
<td>$2\delta$</td>
<td>$\pi \delta$</td>
<td>3072</td>
<td>1081</td>
<td>3072</td>
<td>12.8</td>
<td>0.31</td>
<td>10.7</td>
<td>6.4</td>
</tr>
<tr>
<td>WMLES</td>
<td>$2\pi \delta$</td>
<td>$2\delta$</td>
<td>$\pi \delta$</td>
<td>128</td>
<td>40</td>
<td>64</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
</tr>
</tbody>
</table>

very well with the filtered DNS (evaluated using a box filter of filter width equal to LES grid size). This agreement suggests that the proposed models transfer energy from the largest scales to the inertial subrange as expected and hence on average do not show any scale-to-scale spurious energy transfer. Since the flow does not have large-scale global anisotropy, it is also expected that the performance of DSM would be similar to that of DTCSM and DLN2M, which is consistent with our results.

5.3. Homogeneous isotropic turbulence in the limit $Re_{\lambda} \to \infty$

In the limit of $Re_{\lambda} \to \infty$, i.e., in the limit of no viscous dissipation, the $K41$ scaling (i.e., $E \sim \kappa^{-5/3}$) is expected at all scales. From Figure 6, it is evident that the $K41$ scaling is well recovered with DTCSM and DLN2M (as well as DSM), further confirming both their dissipative nature and interscale energy transfer properties. The $\kappa^2$ scaling in the absence of an SGS model is observed inline with the principle of equipartition of energy.

5.4. Wall-modeled LES of channel flow

In this section, we investigate the performance of DTCSM and DLN2M for a channel flow at $Re_{\tau} = u_{\tau} \delta / \nu = 4200$, where $u_{\tau}$ is the friction velocity and $\delta$ is channel half-height. Lozano-Durán & Jiménez (2014) performed DNS of this flow with grids as refined as $\Delta x^+ = 12.8$, $\Delta y_{\text{min}}^+ = 0.31$ and $\Delta z^+ = 6.4$ in inner units. For practical WMLES calculations, the grid resolutions are fixed in outer units, and grid resolutions of 20 – 60 points ($\Delta y^+ \sim 60 – 200$) across the boundary layer have been previously used (Lozano-Durán & Bae 2019). In this brief, we use 20 points per half-height of the channel.
Table 1 summarizes the simulation parameters used in the DNS reference and the present WMLES. Since in the vicinity of the wall the flow is heavily underresolved, the equilibrium wall model by Cabot & Moin (2000) with second point matching (Kawai & Larsson 2013) ($y^+ \sim 300$) is used in conjunction with the SGS model.

Since the grids are much coarser than the grids in DNS, in the bulk of the flow, the SGS model is supposed to capture a large fraction of the turbulence. From Figure 7, it is clear that DTCSM and DLN2M are slightly better than DSM at predicting the mean streamwise velocity profile. Specifically, in the log layer, the prediction of the Kármán constant (a measure of the slope of mean profile in the log layer, $\kappa = 0.38$) is as much as 10% off with DSM compared with a 4% error with DTCSM and DLN2M.

Since WMLES is expected to match filtered DNS, the overprediction of the mean streamwise component of intensity with respect to DNS in LES of channel flows has been a concern. Figure 8 depicts the lowering of all turbulent intensities with DLN2M compared with DSM near the wall. The near-wall, wall-normal and spanwise components of turbulent intensities with DLN2M are also lower than those with the DSM, which is a qualitative indicator of improved predictions when compared to turbulence fluctuations based on filtered DNS (Figure 10 in Lozano-Durán & Bae (2019) compares the WMLES intensities to filtered DNS for DSM).

5.4.1. Subgrid scale shear stress

For a turbulent channel flow driven at $Re_\tau$ as low as 395, Morinishi & Vasilyev (2002) observed that DSM requires ad hoc clipping in the near-wall region. A similar trend is observed at $Re_\tau = 4200$ in our simulations (Figure 9), where the subgrid stresses in the second off-wall point are clipped. On the other hand, DTCSM and DLN2M produce non-zero mean stresses across the channel (except the centerline).

6. Conclusions

In this brief, we have developed and validated two new non-Boussinesq-type dynamic SGS closure formulations for the tensor-coefficient Smagorinsky model (DTCSM) and a non-linear model (DLN2M) including both large-scale strain and rotation rates. A-priori calculations have confirmed improved tensor-level correlations with exact SGS stresses with these models. We have compared the model performances for canonical flows such as decaying and forced HIT at $Re_\lambda = 70, 315$ and $Re_\lambda \to \infty$. Both DTCSM and DLN2M perform well in HIT at all Reynolds numbers considered, providing evidence...
Figure 8. Wall-normal profiles of turbulent intensities for DSM, DTCSM and DLN2M in turbulent channel flow, $Re_{τ} = 4200$. The curves without symbols represent the mean intensities from DNS.

Figure 9. Wall-normal profiles of mean SGS shear stress for DSM, DTCSM and DLN2M in WMLES of turbulent channel flow at $Re_{τ} = 4200$. Note that a Neumann boundary condition ($dτ_{sgs}/dy = 0$) at the wall is used to determine the SGS stress there.

of accurate subgrid dissipation from these models. Improvements in mean-velocity and turbulent intensities profiles and Kármán constant predictions are observed in WMLES of turbulent channel flow at $Re_{τ} = 4200$, with the proposed models especially near wall. The performance of these models will now be tested in complex flows where grid resolutions are significantly coarser.

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Appendix A. Proof of rotational invariance of DTCSM

In this appendix, we prove in two dimensions the rotational invariance of DTCSM using the model constraints imposed in Eqs. (3.2) - (3.3). Recall that the model formulation for DTCSM is

\[ \tau_{ij}^{\text{sgs}} - \frac{\tau_{kk}^{\text{sgs}}}{3}\delta_{ij} = -(C_{ik}S_{kj} + C_{jk}S_{ki})|S|\Delta^2. \]  

(A 1)

Let \( M \) be the rotation matrix in two dimensions; then for an anticlockwise rotation of the coordinate axes by angle \( \theta \), \( M \) is given as

\[ M = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}. \]  

(A 2)

This gives 

\[ [S]^{\text{rot}} = M^T[S]M, \]

where \([S]^{\text{rot}}\) and \([S]\) are the strain-rate tensors in rotated and original coordinates, respectively. Now, we impose the constraint of the required invariance on the deviatoric part of the model stress as follows

\[ \tau_{\text{dev, sgs}}([S]^{\text{rot}}) = M^T[\tau_{\text{dev, sgs}}]M. \]  

(A 3)

Imposing incompressibility (\( tr[S] = 0 \)) and simplifying Eq. (A 3) with Eq. (A 1), we get

\[ C_{11} = C_{22} ; \quad C_{12} = -C_{21}. \]  

(A 4)

This approach can be extended to three dimensions to pose the final constraints in Eqs. (3.2)-(3.3).

Appendix B. Dynamic procedures for DTCSM and DLN2M

B.1. DTCSM

Recall for DTCSM,

\[ L_{ij} = (C_{ik}\Delta^2M_{kj} + C_{jk}\Delta^2M_{ki}). \]  

(B 1)

This can be rewritten as

\[
\begin{pmatrix}
L_{11} \\
L_{22} \\
L_{33} \\
L_{12} \\
L_{13} \\
L_{23}
\end{pmatrix} = \begin{pmatrix}
2M_{11} & 2M_{12} & 2M_{13} & 0 \\
2M_{22} & -2M_{12} & 0 & 2M_{23} \\
2M_{33} & 0 & -2M_{13} & -2M_{23} \\
2M_{12} & M_{22} - M_{11} & M_{23} & M_{13} \\
2M_{13} & M_{23} & M_{33} - M_{11} & -M_{12} \\
2M_{23} & -M_{13} & -M_{12} & M_{33} - M_{22}
\end{pmatrix} \begin{pmatrix}
C_{11}\Delta^2 \\
C_{12}\Delta^2 \\
C_{13}\Delta^2 \\
C_{23}\Delta^2
\end{pmatrix}
\]  

(B 2)

and can be condensed as

\[ \{L\} = [M_{\text{mat}}]\{C\}. \]  

(B 3)

Using the least-squares solutions approach, we get

\[ [M_{\text{mat}}]^T\{L\} = [M_{\text{mat}}]^T[M_{\text{mat}}]\{C\}. \]  

(B 4)

Finally, Eq. (B 4) is solved directly to dynamically evaluate the four model coefficients.

B.2. DLN2M

The model equation is written as

\[ L_{ij} = 2C_s\Delta^2M_{kj} + 2C_{rs}\Delta^2N_{ij}. \]  

(B 5)
Expressed in matrix form, we have

\[
\begin{pmatrix}
L_{11} & L_{22} & L_{33} & L_{12} & L_{13} & L_{23}
\end{pmatrix} = \begin{pmatrix}
2M_{11} & 2N_{11} \\
2M_{22} & 2N_{22} \\
2M_{33} & 2N_{33} \\
2M_{12} & 2N_{12} \\
2M_{13} & 2N_{13} \\
2M_{23} & 2N_{23}
\end{pmatrix} \begin{pmatrix}
C_s \Delta^2 \\
C_{rs} \Delta^2
\end{pmatrix},
\]  

(B6)

which can be condensed as

\[
\{ L \} = [M_{\text{mat},2}] \{ C \}.
\]  

(B7)

Using the least-squares solutions approach, we get the following equation, which can be solved to find \( C_s \) and \( C_{rs} \),

\[
[M_{\text{mat},2}]^T \{ L \} = [M_{\text{mat},2}]^T [M_{\text{mat},2}] \{ C \}.
\]  

(B8)

**Appendix C. A connection between DTCSM and DLN2M**

In this appendix, we provide a connection between DTCSM and DLN2M closures by comparing the two model forms under a special case. In general, the stresses from DTCSM and DLN2M are expressed as

\[
\tau_{ij}^{\text{DTCSM}} = -(C_{ik} \Delta^2 S_{kj})|S| + C_{jk} \Delta^2 S_{ki}|S|, \\
\tau_{ij}^{\text{DLN2M}} = -2C_s \Delta^2 S_{ij}|S| - C_{rs} \Delta^2 (S_{ik} R_{kj} - R_{ik} S_{kj}).
\]  

(C1)

(C2)

Using the realizability constraints on DTCSM, and decomposing the model coefficient matrix, \([C]\), into isotropic and deviatoric parts as \([C] = C_{11} I + [C^d]\), where \( I \) is an identity matrix, we write

\[
[\tau^{\text{DTCSM}}] = -(C_{11} I \Delta^2 + [C^d])|S||S|\Delta^2 - ((C_{11} I \Delta^2 + [C^d])|S||S|\Delta^2)^T.
\]  

(C3)

Since \([C^d]\) is a deviatoric component of the model coefficient matrix, which is also a property of the rotation-rate tensor, on setting \(|S||C^d| = -\Lambda |R|\), Eq. (C3) can be simplified to give

\[
[\tau^{\text{DTCSM}}] = -2C_{11} \Delta^2 |S||S| - \Lambda \Delta^2 (|S||R| - |R||S|),
\]  

(C4)

which for \( C_{rs} = \Lambda \) is the same model form as for DLN2M. Hence, DLN2M is a special case of DTCSM when the deviatoric model coefficients of DTCSM satisfy \([C^d] = -C_{rs} |R|/|S|\).

**REFERENCES**


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