AUTONOMIC SUBGRID-SCALE CLOSURE FOR LARGE EDDY SIMULATIONS

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Abstract Motivated by advances in constrained optimization methods, a fundamentally new *autonomic* closure for LES is presented that invokes a self-optimization method for the subgrid-scale stresses instead of a predefined turbulence model. This autonomic closure uses the most general dimensionally-consistent expression for the local subgrid-scale stresses in terms of all resolved-scale variables and their products at all spatial locations and times, thereby also incorporating all possible gradients of all resolved variables and products. In so doing, the approach addresses all possible nonlinear, nonlocal, and nonequilibrium turbulence effects without requiring any direct specification of a subgrid-scale model. Instead it uses an optimization procedure with a test filter to find the best local relation between subgrid stresses and resolved-scale variables at every point and time. We describe this autonomic closure approach, discuss truncation, regularization, and sampling in the optimization procedure, and present results from *a priori* tests using DNS data for homogeneous isotropic and sheared turbulence. Even for the simplest 2$^{\text{nd}}$-order truncation of the general formulation, substantial improvements over the dynamic Smagorinsky model are obtained with this new autonomic approach to turbulence closure.

INTRODUCTION

The primary challenge in large eddy simulations (LES) is to formulate a physically accurate closure model for the SGS stresses, $\tau_{ij}(\mathbf{x}, t)$, and many such closure models have been proposed (e.g., see [4] for a review). To date, however, no SGS model has been found that in *a priori* tests produces accurate values of $\tau_{ij}(\mathbf{x}, t)$ to ensure the correct space- and time-varying momentum and energy exchange between the resolved and subgrid scales at each location and time. This is essential for accurate LES, since errors in the modeled $\tau_{ij}(\mathbf{x}, t)$ field propagate up through the resolved scales. Here we avoid this by presenting a fundamentally new *autonomic* approach to LES closure that does not presume any predefined constitutive model of the SGS stresses in terms of resolved-scale quantities. Instead, the approach allows the simulation itself to determine the best local relation between the subgrid stresses and all resolved state variables at a test filter scale, and then projects the resulting local relation to evaluate the local subgrid stresses at the LES filter scale. This new autonomic turbulence closure shows significant improvements over the dynamic Smagorinsky model in *a priori* tests.

THE AUTONOMIC SUBGRID-SCALE CLOSURE

Fundamentally, the search for any subgrid-scale closure amounts to formulating a suitable expression for τ_{ij} in terms of the primitive state variables in the governing equations – for incompressible flow these are the resolved-scale velocities $\widetilde{u}_i$ and pressure $\widetilde{p}$. Moreover, in order to account for nonlocal and nonequilibrium effects the closure expression should not preclude the possibility that τ_{ij} at a particular point and time depends on the primitive variables at other points and times. We can write the local subgrid stresses in this fully general way via the most general dimensionally-consistent expression involving all resolved-scale variables $\widetilde{u}_i$ and pressure $\widetilde{p}$ and their products at all spatial locations and times, namely

$$\tau_{ij}(\mathbf{x}, t) = \mathcal{F}\left[\widetilde{\mathbf{u}}(\mathbf{x}', t'), \widetilde{p}(\mathbf{x}', t'), \mathbf{x}', t', \mathcal{L}, \mathcal{T}\right] , \tag{1}$$

in which the function $\mathcal{F}$ denotes the closure model, and where $\mathbf{x}'$ denotes the entire spatial domain, t' denotes all times, $\mathcal{L}$ is a characteristic length scale (e.g., the filter width Δ), and $\mathcal{T}$ is a characteristic time scale (e.g., the resolved strain rate magnitude). All prior SGS models assume some highly restrictive chosen functional form for $\mathcal{F}$. By contrast, here we allow $\mathcal{F}$ to include all linear and nonlinear combinations of all resolved-scale variables and all possible products among them at all spatial locations and times. This thereby also indirectly includes a wide range of mathematical operations among all resolved-scale variables and their products, including temporal and spatial derivatives, filters, multi-point differences, and multi-point products. Moreover, since Eq. (1) incorporates the entire spatial and temporal domains, it includes not only nonlinear effects but also nonlocal and nonequilibrium effects [5, 1, 2].

Specifically, we can express $\mathcal{F}$ in this fully general manner, including all linear and nonlinear combinations of $\widetilde{u}_i$ and $\widetilde{p}$ at all points and times, and using $\mathcal{T}$ and $\mathcal{L}$ to ensure dimensional consistency of each term, via the relation

$$\tau_{ij}(\mathbf{x}, t) = \frac{\mathcal{L}^2}{\mathcal{T}^2}\left[\alpha_{ij}^{k_1 n_1 m_1}\left(\frac{\mathcal{T}}{\mathcal{L}}\widetilde{v}_{k_1 n_1 m_1}\right) + \beta_{ij}^{k_1 n_1 m_1 k_2 n_2 m_2}\left(\frac{\mathcal{T}^2}{\mathcal{L}^2}\widetilde{v}_{k_1 n_1 m_1}\widetilde{v}_{k_2 n_2 m_2}\right)\right.$$
$$\left. + \gamma_{ij}^{k_1 n_1 m_1 k_2 n_2 m_2 k_3 n_3 m_3}\left(\frac{\mathcal{T}^3}{\mathcal{L}^3}\widetilde{v}_{k_1 n_1 m_1}\widetilde{v}_{k_2 n_2 m_2}\widetilde{v}_{k_3 n_3 m_3}\right) + \left(\frac{\mathcal{T}^4}{\mathcal{L}^4}\right)(\text{4th order terms}) + \ldots\right] , \tag{2}$$

where $m = [1, M]$ spans all discrete time steps, $n = [1, N]$ spans all discrete spatial locations in the three-dimensional domain, and where the primitive variables are $\widetilde{v}_{knm} = [\widetilde{u}_1(\mathbf{x}_n, t_m), \widetilde{u}_2(\mathbf{x}_n, t_m), \widetilde{u}_3(\mathbf{x}_n, t_m), \widetilde{p}(\mathbf{x}_n, t_m)]$ with $k = [1, 4]$, with summation implied over repeated indices. Note that this general relation involves a very large set of unknown coefficients, namely all the α's, β's, γ's, etc., which in general can be expected to vary from point-to-point and with time as the local subgrid stress dynamics adapt to local changes in the turbulence state. Since the coefficients are unspecified, there is no predefined turbulence model imposed in this autonomic approach, and no assumptions are made as to how the subgrid stresses are related to the resolved primitive variables beyond the fundamental assumption underlying all LES that the subgrid stresses are functions of the resolved-scale fields $\widetilde{u}(\mathbf{x}, t)$ and $\widetilde{p}(\mathbf{x}, t)$ and characteristic time and length scales. The coefficient matrices $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ in Eq. (2) at each point and time can then be found using standard inverse modeling and optimization techniques based on known SGS stresses at a test filter scale. An objective function based on scale similarity and a test filter is used to drive the optimization process and determine the coefficients, which are then used to formulate SGS stresses at the grid scale. Since the coefficient values are determined *autonomically* via this local self-optimization within the simulation, we avoid any need to specify a subgrid-scale model, and the simulation instead finds the best local relation between subgrid stresses and resolved-scale variables at every point and time.

TEST RESULTS FROM THE AUTONOMIC CLOSURE

We present results from *a priori* tests of this new autonomic LES closure method (termed ALES closure) using DNS data for homogeneous isotropic turbulence [6]. Spectrally sharp filters were applied at Δ_{LES} and Δ_1 to respectively generate LES and test filtered fields. To show a minimal working example of ALES closure, we include in $\mathcal{F}$ only terms up to 2nd order in $\widetilde{u}_i$, neglect $\widetilde{p}$, use only the current time, and limit the spatial information to a $3 \times 3 \times 3$ stencil. At the test filter scale Figure 1 shows the true stresses τ_{11}, τ_{13}, and τ_{23}, the ALES stresses, and corresponding stresses from the dynamic Smagorinsky model [3]. Since Δ_1 is where the ALES coefficients are optimized, the new closure accurately captures the structure and magnitudes of these stress fields. The real test of the ALES closure and scale invariance of the ALES coefficients is in Figure 2, showing the same stress components as in Figure 1 but at Δ_{LES}. Here structures in the stress fields are sharper and more intermittent than at the test filter scale, but the ALES closure correctly captures nearly all of these features. This agreement is remarkable considering the severe truncation applied in these initial tests of the ALES approach. The final paper will present full details on the ALES closure and more extensive demonstration results.

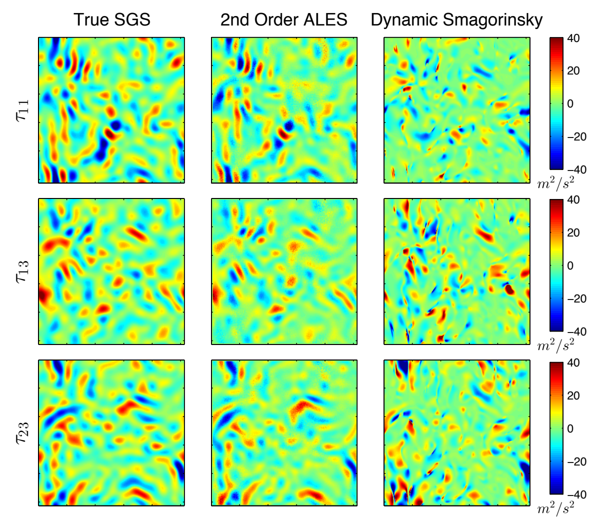

Figure 1. True SGS fields, 2nd order ALES, and Dynamic Smagorinsky [3] predictions at the test filter scale Δ_1 for homogeneous isotropic turbulence (HIT).

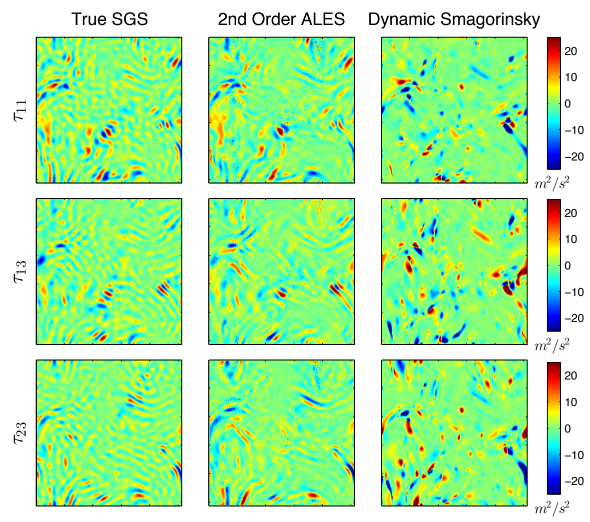

Figure 2. True SGS fields, 2nd order ALES, and Dynamic Smagorinsky [3] predictions at the LES filter scale Δ_{LES} for homogeneous isotropic turbulence (HIT).

References

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