A NEW AUTONOMIC CLOSURE FOR LARGE EDDY SIMULATIONS

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ABSTRACT

We present a fundamentally new autonomic subgrid-scale closure for large eddy simulations (LES) that solves a nonlinear, nonparametric system identification problem instead of using a predefined turbulence model. The autonomic approach expresses the local SGS stress tensor as the most general unknown nonlinear function of the resolved-scale primitive variables at all locations and times using a Volterra series. This series is analogous to a Taylor series expansion in both time and space, and incorporates nonlinear, nonlocal, and nonequilibrium turbulence effects. The series introduces a large number of convolution kernel coefficients that are found by solving an inverse problem to minimize the error in representing known subgrid-scale stresses at a test filter scale. The optimized coefficients are then projected to the LES scale by invoking scale similarity in the inertial range and applying appropriate renormalizations. This new closure approach avoids the need to specify a turbulent constitutive model and instead identifies an optimal model on the fly. Here we present the most general formulation of the new autonomic approach and outline an inverse modeling method for optimizing the coefficients. We then explore truncations of the series expansion and demonstrate the effects of regularization and sampling on the optimal coefficients. Finally, we perform *a priori* tests of this approach using data from direct numerical simulations of homogeneous isotropic and sheared turbulence. We find substantial improvements over the Dynamic Smagorinsky model, even for a 2$^{\text{nd}}$ order time-local truncation of the present closure.

INTRODUCTION

Fluid flows of engineering and scientific importance are often turbulent and therefore involve an enormous range of spatial and temporal scales. The computational cost of resolving this full scale range is prohibitive for most applications, so large eddy simulations (LES) are commonly employed to reduce the scale range that must be resolved. Conceptually, the LES equations achieve a scale separation of the original Navier-Stokes equations by convolving the true velocity vector $\mathbf{u}(\mathbf{x},t)$ with a low-pass filter kernel $\mathscr{G}_{\Delta_{LES}}$, where Δ_{LES} is the LES filter scale. The resulting filtered velocity field is denoted $\widetilde{\mathbf{u}}(\mathbf{x},t)$. In practice, the filtering is often done implicitly when discretizing onto a numerical grid, with the consequence that "subfilter" scale quantities become "subgrid" scale quantities.

Making the common assumptions that $\mathscr{G}_{\Delta_{LES}}$ is linear, preserves constants, and commutes with time and space derivatives, the Navier-Stokes equations can be filtered to obtain the incompressible LES equations given by

$$\frac{\partial}{\partial x_i}\widetilde{u}_i = 0 \quad (1)$$

$$\frac{\partial}{\partial t}\widetilde{u}_i + \frac{\partial}{\partial x_j}\left(\widetilde{u}_j\widetilde{u}_i\right) + \frac{\partial}{\partial x_i}\widetilde{p} - \nu\frac{\partial^2}{\partial x_j^2}\widetilde{u}_i = -\frac{\partial}{\partial x_j}\tau_{ij} \quad (2)$$

where $\tau_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j$ is the unclosed subfilter-scale stress and the density has been absorbed into the pressure. When the convolution is implicitly performed by the numerical discretization, filtered variables become resolved variables and the subfilter stress $\tau_{ij}(\mathbf{x},t)$ becomes the subgrid-scale (SGS) stress. This stress must be modeled in terms of resolved quantities to close the LES equations.

The primary challenge in LES is to formulate a physically accurate closure model for the SGS stresses. Many models have been proposed [see Meneveau & Katz (2000) for a review] and the most widely used models invoke principles such as scale similarity (Bardina *et al.*, 1980), the gradient transport hypothesis (Smagorinsky, 1963), and dynamic filtering (Germano *et al.*, 1991). Nearly all such models employ a specific constitutive relation between the SGS stress tensor and one or more resolved-scale physical quantities, such as the strain rate, vorticity, or other quantities derivable from the resolved velocity and pressure. To date, however, no SGS model has been found that in *a priori* tests accurately produces values of $\tau_{ij}(\mathbf{x},t)$ that ensure the correct space- and time-varying momentum and energy exchange between the resolved and subgrid scales.

In this paper a new autonomic closure for LES is outlined that in *a priori* tests correctly reproduces the local instantaneous subgrid stresses $\tau_{ij}(\mathbf{x},t)$. The autonomic closure is outlined in the next section, followed by initial *a priori* tests on data from direct numerical simulations (DNS). Finally, a summary and an outline for future work is provided at the end of the paper.

AUTONOMIC CLOSURE APPROACH

The Autonomic LES closure (abbreviated "ALES") is a fundamentally new approach to closing the LES equations that does not require a predefined constitutive model for the SGS stress. Instead, the approach allows the simulation itself to determine the best local relation between the subgrid stresses and all resolved state variables by solving a system identification problem on the fly. We express the local SGS stresses in terms of the most general nonlinear nonparametric functional, a Volterra series of the resolved state variables. As a nonparametric system identification technique, this approach avoids the need to specify a predefined operator relating the resolved state variables to the SGS stress tensor. The terms in the Volterra series represent convolutions with all possible linear and nonlinear combinations of the state variables at all locations and times, allowing this approach to capture important nonequilibrium, nonlocal, and time lag effects (Hamlington & Dahm, 2008).

The kernel coefficients in the series can be found by posing an inverse modeling problem at a coarser scale where the SGS stresses are known from standard test filtering processes. The state variables are also known at the test scale, and therefore optimal kernel coefficients can be determined. Inverse modeling techniques such as regularization and sampling can be used to control the stability and computational cost of the solution. The resulting kernel coefficients identify the optimal local turbulent constitutive relationship. As long as the test and LES scales are within the inertial range, the relationship between resolved quantities and SGS stresses is approximately scale invariant and coefficients optimized at the test scale can be applied at the LES scale using appropriate renormalizations. The term *autonomic* is applied to the closure because this process is self-optimizing without exogenous inputs or training data, and it allows enormous flexibility in accounting for different physical effects and flow configurations.

Fundamental Closure Assumption

Fundamentally, the search for a subgrid-scale closure amounts to formulating a closed expression for τ_{ij} in terms of primitive state variables obtained from the solution of governing equations. For an incompressible flow governed by the LES equations in Eqs. (1) and (2), the state variables are the resolved-scale velocities $\widetilde{u}_i$ and pressure $\widetilde{p}$. In order to account for nonlocal and nonequilibrium effects the form of the closure should not preclude the possibility that τ_{ij} at a particular point and time depends on primitive variables at other points and times. Additionally, characteristic time and length scales should be included in the closure to help enforce dimensional and scale consistency. The most general SGS closure can thus be written as

$$\tau_{ij}(\mathbf{x},t) = \mathscr{F}\left[\widetilde{\mathbf{u}}(\mathbf{x}',t'), \widetilde{p}(\mathbf{x}',t'), \mathbf{x}', t', \mathscr{L}, \mathscr{T}, \mathscr{M}\right] \qquad (3)$$

where $\mathbf{x}'$ denotes the entire spatial domain, t' denotes all times, $\mathscr{L}$ is a characteristic length scale (e.g., the filter width Δ), $\mathscr{T}$ is a characteristic time scale (e.g., the resolved strain rate magnitude), and $\mathscr{M}$ is a characteristic mass (e.g. $\rho\mathscr{L}^3$). All existing SGS models assume that there is some functional form for $\mathscr{F}$ that can describe the SGS stresses with the inputs listed in Eq. (3). In the ALES approach, we find the optimal functional form for $\mathscr{F}$ by solving a nonlinear nonparametric system identification problem. By allowing any linear or nonlinear combination of the state variables to appear in the function $\mathscr{F}$, it is possible to represent a wide range of mathematical operations, including temporal and spatial derivatives, filters, multi-point differences, and multi-point products. Taking a nonparametric approach means that there is no need to specify *a priori* any particular operator or mathematical structure for $\mathscr{F}$.

Series Expansion for the SGS Stress

The most general nonlinear nonparametric polynomial functional for $\mathscr{F}$ can be expressed using a Volterra series (Schetzen, 2006). This series is analogous to a Taylor series expansion in both time and space, and is an extension of the classical impulse response function for linear systems. The terms in the series are multidimensional convolutions with all possible linear and nonlinear combinations of the input data at all times. For systems with fading memory and bounded inputs, the Stone-Weierstrass theorem guarantees that any continuous function can be uniformly approximated to within arbitrary precision by a Volterra series of sufficient but finite order (Boyd & Chua, 1985). This ensures that the ALES approach is capable of representing the true SGS stresses with arbitrarily high fidelity.

The Volterra series for a continuous system with scalar inputs and outputs $y(t) = f(x(t))$ is a series of multidimensional convolution integrals given by

$$\begin{aligned}
&y(t) = h^{(0)} + \int_{\mathbb{R}} h^{(1)}(\tau_1)\, x(t-\tau_1)\, \mathrm{d}\tau_1 + \\
&\int_{\mathbb{R}^2} h^{(2)}(\tau_1,\tau_2)\, x(t-\tau_1)\, x(t-\tau_2)\, \mathrm{d}\tau_1 \mathrm{d}\tau_2 + \\
&\int_{\mathbb{R}^3} h^{(3)}(\tau_1,\tau_2,\tau_3)\, x(t-\tau_1)\, x(t-\tau_2)\, x(t-\tau_3)\, \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 + \ldots
\end{aligned}$$

where $h^{(n)}$ are Volterra kernels. In operator form, this series is $y(t) = H_0 + H_1 x(t) + H_2 x(t) + \ldots H_n x(t) + \ldots$, and the convolutions comprise the nth order operators $H_n x(t)$ which are characterized by the $h^{(n)}$ kernels. These kernels are formally defined as the partial derivatives of f

$$\begin{aligned}
&h^{(0)} = f(\bar{x}), \quad h^{(1)}(\tau_1) = \left(\frac{\partial f}{\partial x(t-\tau_1)}\right)_{\bar{x}}, \\
&h^{(2)}(\tau_1,\tau_2) = \left(\frac{\partial^2 f}{\partial x(t-\tau_1)\, \partial x(t-\tau_2)}\right)_{\bar{x}}, \quad \ldots
\end{aligned}$$

but with an unknown f they can be found using an optimization procedure. It is worth noting that the expansion is linear in the kernel coefficients despite describing a nonlinear system. Furthermore, a linearization of the expansion returns the impulse response function which completely characterizes the behavior of a dynamical linear system.

A Volterra series can analogously be written for discrete systems with a finite dimensional input vector $\mathbf{x} = [x_1, x_2, \ldots, x_m]^T \in \mathbb{R}^m$ and a scalar output. In the discrete case the nth order operators for $n \geq 1$ are

$$H_n(\mathbf{x}) = \sum_{i_1=1}^{m} \sum_{i_2=1}^{m} \cdots \sum_{i_n=1}^{m} h_{i_n}^{(n)} \prod_{j=1}^{n} x_{i_j} \tag{4}$$

where the operator is composed of m^n coefficients.

In order to apply the Volterra series expansion in the ALES approach, we create an input vector $\widetilde{\mathbf{v}}(t) = \left[\mathrm{vec}\left(\widetilde{u}_1^*(\mathbf{x},t)\right), \mathrm{vec}\left(\widetilde{u}_2^*(\mathbf{x},t)\right), \mathrm{vec}\left(\widetilde{u}_3^*(\mathbf{x},t)\right), \mathrm{vec}\left(\widetilde{p}^*(\mathbf{x},t)\right)\right]^{\mathsf{T}}$ that represents the vectorized form of the nondimensionalized resolved velocity and pressure fields. The series expansion for the SGS stress is then given by

$$\tau_{ij} = \frac{\mathscr{L}^2}{\mathscr{T}^2}\left[h_{ij}^{(0)} + \sum_{n=1}^{L} \sum_{m_1=1}^{M} \cdots \sum_{m_n=1}^{M} h_{m_n,ij}^{(n)} \prod_{k=1}^{n} \widetilde{v}_{m_k}\right] \tag{5}$$

where each unique (i,j) element of the SGS tensor has its own set of kernel coefficients, L is the order of the expansion, and $M = m \times t$ where the "memory" in the series spans t timesteps. We refer to the full set of coefficients as $\mathbf{h}$.

Determination of Kernel Coefficients

The general relation for τ_{ij} in Eq. (5) introduces an exponentially growing number of kernel coefficients. While infinite order and fading memory representations are possible, the representation will be truncated here to finite order and memory to reduce computational cost. The coefficients will be found using inverse modeling and optimization techniques, which are key steps in the ALES approach. This section introduces an objective function based on test filtering that quantifies error in the ALES model and drives the optimization process. We invoke a scale similarity argument to apply ALES coefficients obtained at the test filter scale to the LES scale. Finally, we solve a regularized inverse modeling problem to determine optimal coefficients.

Test Filter Objective Function We introduce a test filter scale, Δ_1, that is larger than the LES filter scale, Δ_{LES}, and characterizes an additional filter, $\mathscr{G}_{\Delta_1}$. This new filter defines the test filtered velocity field $\widehat{\mathbf{u}}(\mathbf{x},t)$. For simplicity, we take both $\mathscr{G}_{\Delta_1}$ and $\mathscr{G}_{\Delta_{LES}}$ to be spectrally sharp filters that are exact projection operators such that $\widehat{\widehat{\mathbf{u}}} = \widehat{\mathbf{u}}$. Additionally, we define scale-specific SGS stresses $\tau_{ij}^{\Delta_{LES}} = \widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j$ and $\tau_{ij}^{\Delta_1} = \widehat{u_i u_j} - \widehat{u}_i\widehat{u}_j$, where $\tau_{ij}^{\Delta_{LES}}$ is sought to close the governing LES equations. Test filtering the LES field $\widetilde{\mathbf{u}}(\mathbf{x},t)$ with $\mathscr{G}_{\Delta_1}$ results in known values for the $\tau_{ij}^{\Delta_1}(\mathbf{x},t)$ and $\widehat{\mathbf{u}}(\mathbf{x},t)$ fields. This is sufficient to define an objective function $\mathscr{J}(\widehat{\mathbf{v}},\mathbf{h}) \in \mathbb{R}$ that measures error in the ALES model results for $\tau_{ij}^{\Delta_1}(\mathbf{x},t)$ as

$$\mathscr{J}(\widehat{\mathbf{v}},\mathbf{h}) = \|\tau_{ij}^{\Delta_1}(\mathbf{x},t) - \tau_{ij,ALES}^{\Delta_1}(\mathbf{x},t;\widehat{\mathbf{v}},\mathbf{h})\|^2 \tag{6}$$

where $\tau_{ij,ALES}^{\Delta_1}(\mathbf{x},t;\widehat{\mathbf{v}},\mathbf{h})$ represents the modeled stresses at scale Δ_1 produced by Eq. (5) for a given order and memory and $\|\cdot\|$ denotes the ℓ^2 norm over all (i,j) elements. The set of kernel coefficients $\mathbf{h}$ that minimizes $\mathscr{J}(\widehat{\mathbf{v}},\mathbf{h})$ identifies the optimal functional representation of $\tau_{ij}^{\Delta_1}(\mathbf{x},t)$ in terms of multidimensional convolutions of the input state vector according to Eq. (5). Since any element of $\mathbf{h}$ can be found to be zero during the optimization for different flows or geometries, there is fundamentally no predefined turbulence model or constitutive equation in this autonomic approach.

Projection to the LES Scale As long as Δ_1 and Δ_{LES} are both in the scale-similar inertial range and the LES filters are spectrally sharp, the functional relationship $\mathscr{F}$ from Eq. (3) and expanded in Eq. (5) should be constant at both scales. The ALES coefficients that parameterize $\mathscr{F}$ must then also be scale invariant throughout the inertial range. Consequently, we use the coefficients optimized at Δ_1 in our ALES expression for $\tau_{ij}^{\Delta_{LES}}$. Although the kernel coefficients parameterizing $\mathscr{F}$ are scale invariant, the actual SGS stresses themselves change as the wavenumber of the filter cutoff changes. We account for this by making our characteristic time and length scales $\mathscr{T}$ and $\mathscr{L}$ scale-specific. We use $\mathscr{L}_{\Delta_1} = \Delta_1$ and $\mathscr{T}_{\Delta_1} = (2\widehat{S}_{ij}\widehat{S}_{ij})^{-1/2}$ in the optimization at our test scale, and $\mathscr{L}_{\Delta_{LES}} = \Delta_{LES}$ and $\mathscr{T}_{\Delta_{LES}} = (2\widetilde{S}_{ij}\widetilde{S}_{ij})^{-1/2}$ at the LES scale. This allows the ALES results for $\tau_{ij}^{\Delta_{LES}}$ to reflect the changes in intensity and scale of the SGS stresses when transitioning from Δ_1 to Δ_{LES}. Furthermore, we apply the coefficients to quantities separated by a normalized length scale. In practice, this means that any stencil applied as part of a spatial truncation must have its grid point spacing nondimensionalized by the filter length scale. This test filtering and scale similarity approach is crucial for the autonomy of ALES. There is thus no need for prior DNS results, training data, or user specified parameters. Instead, the closure leverages scale invariant properties of inertial range turbulence to perform a self-contained optimization. The same scale invariance allows us to apply the test filter-optimized coefficients at the LES scale.

Inverse Modeling The ALES optimization can be posed as the discrete inverse modeling problem

$$\min \quad \mathscr{J} = \|\mathbf{d} - \mathbf{G}\mathbf{h}\|^2 \tag{7}$$

where $\mathscr{J} \in \mathbb{R}$ is the objective function to be minimized, $\mathbf{d}$ is an column vector of known SGS stresses sampled from $\tau_{ij}^{\Delta_1}(\mathbf{x},t)$, $\mathbf{G}$ is a matrix whose rows represent the polynomial arguments to the Volterra convolution integrals at each point where $\tau_{ij}^{\Delta_1}(\mathbf{x},t)$ is sampled, and $\mathbf{h}$ is column vector containing the h kernel coefficients in vector form.

Posing the ALES approach as an inverse modeling problem is a powerful way to reveal insights into the optimization process. First, the cost of the optimization process is driven by the size of the matrix $\mathbf{G}$. The width of $\mathbf{G}$ is determined by the order and memory applied to Eq. (5). The height of $\mathbf{G}$ is determined by the number of samples taken of $\tau_{ij}^{\Delta_1}$. A sparse sampling reduces the computational cost, but also ensures that the observations are statistically independent. The rank of $\mathbf{G}$ reveals how closely a solution vector $\mathbf{h}$ can match the observations $\mathbf{d}$, and the conditioning number of $\mathbf{G}$ determines how stable the solution $\mathbf{h}$ is when there is noise in the observations.

Regularizing the Inverse Problem

Inverse modeling problems are typically ill-posed due to ill-conditioning of $\mathbf{G}$ and consequently exhibit extreme sensitivity to changes in the observation data. As a result, noise or small variations in the test filtered SGS stresses in $\mathbf{d}$ can result in large changes in the inverse solution $\mathbf{h}$. This instability can be seen in the generalized inverse solution $\mathbf{h}_\dagger$ based on the Moore-Penrose pseudoinverse of $\mathbf{G}$, given by

$$\mathbf{h}_\dagger = \underbrace{\mathbf{V}_p \boldsymbol{\Sigma}_p^{-1} \mathbf{U}_p^T}_{\mathbf{G}^\dagger} \mathbf{d} = \sum_{i=1}^{p} \frac{\mathbf{U}_i^T \mathbf{d}}{s_i} \mathbf{V}_i \tag{8}$$

where $\mathbf{G}^\dagger$ is the pseudoinverse, s_i are the singular values of $\mathbf{G}$, the p refers to the compact form of the singular value decomposition of $\mathbf{G}$ with p nonzero singular values, and i refers to the i$^{\text{th}}$ column of $\mathbf{U}$ or $\mathbf{V}$. The columns of $\mathbf{U}$ form a basis spanning the data space and the columns of $\mathbf{V}$ form a basis spanning the model space. The inner product of $\mathbf{U}_i$ and the data vector $\mathbf{d}$ yields a scalar weighting factor for the model space basis vector $\mathbf{V}_i$. The model space basis vectors corresponding to small singular values are typically highly oscillatory and noisy while the basis vectors for large singular values are typically smooth. Random noise in the observations will make $\mathbf{d}$ likely to have a component in the direction $\mathbf{U}_i$ corresponding to a very small s_i singular value. As a result, the $\mathbf{V}_i$ model space basis vector will dominate the solution $\mathbf{h}_\dagger$ and amplify the noise.

Instability in the inverse modeling solution is undesirable because the solution will reflect noise in the data rather than underlying physics. This is often addressed with a regularization technique that adds additional information to prevent overfitting and represents a tradeoff between solution variance and error or bias in the fit. Common regularization techniques include augmenting the objective function with a weighted ℓ^1 or ℓ^2 norm of $\mathbf{h}$ that penalizes large model parameter values.

In this study we employ the truncated singular value decomposition (TSVD) to regularize our solution. In the TSVD regularization we truncate the summation in Eq. (8) at $p' < p$, where p' is chosen based on the discrete Picard condition which seeks a p' where $\mathbf{U}_i^T \mathbf{d}/s_i < 1$. This process reduces the number of model space basis vectors used in $\mathbf{h}_\dagger$, but avoids instabilities due to small singular values. The TSVD procedure thus finds an optimal truncation of the Volterra series based on the numerical properties of its discretized inverse modeling form. This also accelerates the ALES process since $\mathbf{G}^\dagger$ can be found once and used repeatedly in finding $\mathbf{h}_\dagger$ for each unique SGS stress component.

A PRIORI TESTS OF THE ALES CLOSURE

The ALES closure is evaluated here using *a priori* tests on DNS data for homogeneous isotropic turbulence (HIT) and homogeneous sheared turbulence (HST). *A priori* testing is a necessary but not sufficient step in determining whether the closure will succeed in a forward *a posteriori* test. We use de-aliased $256 \times 256 \times 256$ pseudospectral DNS results from a previously published and validated study (Schumacher, 2004) and apply spectrally sharp filters at Δ_{LES} and Δ_1 to synthetically generate the LES and test filtered fields. With these filtered fields and the true DNS fields, the exact SGS stresses can be calculated at any scale and used to evaluate the ALES approach. The ALES results at Δ_{LES} are compared with the exact SGS field and with results from the Dynamic Smagorinsky model outlined by Lilly (1992), which is a commonly used turbulence model that also employs a test filter and least squares optimization.

We first present HIT results for the unregularized objective function in Eq. (7) and then discuss results of the TSVD approach using HST data.

Unregularized HIT Results

To demonstrate a minimal working example of the ALES closure, we truncate Eq. (5) to only include 1$^{\text{st}}$ and 2$^{\text{nd}}$ order terms. We also neglect the pressure field, consider only the final timestep t_f, and limit the spatial extent to a $3 \times 3 \times 3$ stencil around the sampling location. This shortens our input vector to a 81×1 column vector $\widetilde{\mathbf{v}} = \left[\widetilde{u}_1^* (x_1, t_f), \ldots \widetilde{u}_1^* (x_{27}, t_f), \ldots, \widetilde{u}_3^* (x_{27}, t_f)\right]^{\mathsf{T}}$ where x_i refers to a location within the $3 \times 3 \times 3$ stencil. The physical separation between stencil points is also normalized by the filter length scale. We sample $\tau_{ij}^{\Delta_1}$ at every 10$^{\text{th}}$ point when creating $\mathbf{d}$, set $\Delta_1 = 2\Delta_{LES}$, and seek a single solution vector $\mathbf{h}$ for each unique SGS stress component that is optimal over the entire flow domain. One could seek an optimal $\mathbf{h}$ at each location, but the inverse problem would then be underdetermined.

The initial *a priori* tests are performed without any regularization and determine optimal kernel coefficients at the test filter scale Δ_1 using the relation

$$\tau_{ij}^{\Delta_1} = \frac{\mathscr{L}_{\Delta_1}^2}{\mathscr{T}_{\Delta_1}^2} \left[h_{ij}^{(0)} + \sum_{n=1}^{2} \sum_{m_1=1}^{27} \sum_{m_2=1}^{27} h_{m_n,ij}^{(n)} \prod_{k=1}^{n} \widehat{v}_{m_k} \right] \tag{9}$$

corresponding to a Volterra series model of order 2 and with no memory of past inputs. The optimal ALES coefficients are found at Δ_1 by solving the discrete least squares minimization in Eq. (7) for the truncated expression in Eq. (9) using a QR decomposition. The size of the $\mathbf{G}$ matrix created by this sampling frequency is 17576×3403. The optimal coefficients are then applied at every location in the domain at Δ_{LES} using the relation

$$\tau_{ij}^{\Delta_{LES}} = \frac{\mathscr{L}_{\Delta_{LES}}^2}{\mathscr{T}_{\Delta_{LES}}^2} \left[h_{ij}^{(0)} + \sum_{n=1}^{2} \sum_{m_1=1}^{27} \sum_{m_2=1}^{27} h_{m_n,ij}^{(n)} \prod_{k=1}^{n} \widetilde{v}_{m_k} \right] \tag{10}$$

where $\mathscr{L}$ and $\mathscr{T}$ are here calculated using quantities at Δ_{LES} and the discrete spatial locations indexed by x_i in $\widetilde{v}$ have been rescaled based on the ratio $\Delta_1/\Delta_{LES} = 2$.

The ALES closure does an excellent job of capturing the structure, location, and intensity of the SGS stresses at Δ_1 where the coefficients are optimized. However, the true test of the ALES closure and the scale invariance of the coefficients is performance at Δ_{LES}, shown in Figure 1. The true SGS stress structures are smaller, sharper, and more intermittent than at the test filter scale, but the ALES closure is able to capture nearly all of these features while the Dynamic Smagorinsky model does not. This agreement is remarkable considering the severe truncation applied in Eq. (10) and noting that for each SGS stress component every location in the 3D field uses the same set of ALES coefficients.

The accuracy of the ALES closure can be quantitatively assessed by considering maps of the SGS stress errors shown in Figure 2. The error is defined as $\varepsilon_{ij}(\mathbf{x}) = \tau_{ij}^{\Delta_{LES},True} - \tau_{ij}^{\Delta_{LES},ALES}$. The ALES errors are largely featureless and relatively small, demonstrating that ALES is indeed capturing the SGS stress correctly. The Dynamic Smagorinsky model, by contrast, has errors of the same

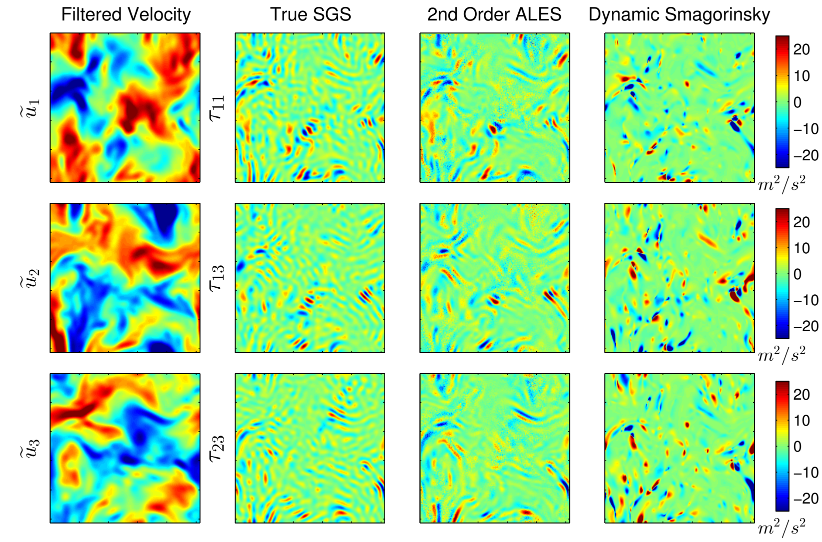

Figure 1. HIT velocity and SGS stress fields at the LES scale from DNS, ALES, and the Dynamic Smagorinsky model show that ALES captures the stresses remarkably well.

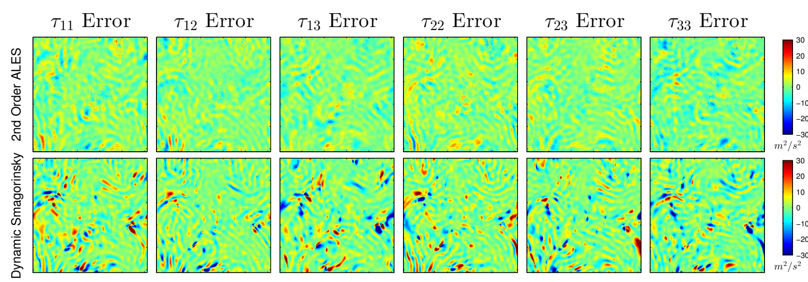

Figure 2. LES scale errors for 2nd order ALES (top row) and the Dynamic Smagorinsky model (bottom row). These error fields confirm that ALES is substantially more accurate than the Dynamic Smagorinsky model.

size, intensity, and structural complexity as the true SGS field itself, showing that it poorly represents the actual local stresses. ALES also appears to be approximately Galilean invariant in initial tests where $u_1(\mathbf{x},t)$ was increased by a large constant but $\mathbf{h}$ was unchanged, revealing no new spatial patterns or bias in the ALES error field.

HST and Truncated SVD Results

We also test ALES on HST data and apply a TSVD regularization. The *a priori* analysis of HST uses the same ALES truncations as in Eqs. (9) and (10) and also the same stencil, sampling, and QR decomposition as in the HIT analysis. The solution is regularized by keeping approximately $1/7^{\text{th}}$ of the original 3403 nonzero singular values based on the discrete Picard condition. One set of ALES coefficients is found for the entire volume, whereas the Dynamic Smagorinsky model requires averaging across homogeneous directions, producing an optimization for each horizontal plane. This suggests ALES may be an advantageous approach in complex or inhomogeneous flows. The TSVD approach allows us to calculate the truncated pseduoinverse $\mathbf{G}^{\dagger} = \mathbf{V}_{p'}\mathbf{\Sigma}_{p'}^{-1}\mathbf{U}_{p'}^{T}$ once, and then quickly find the TSVD model solution for each component of the SGS stresses with a simple matrix-vector multiplication $\mathbf{h}_{\dagger} = \mathbf{G}^{\dagger}\mathbf{d}$. The ALES estimate of the SGS stresses is then given by the TSVD model solution and the full $\mathbf{G}$ matrix as $\boldsymbol{\tau}_{ij}^{\Delta_{LES}} = \mathbf{G}\mathbf{h}_{\dagger}$.

Figure 3 shows the HST ALES SGS field at Δ_{LES} and the error maps are shown in Figure 4. The ALES closure is again substantially more accurate than the Dynamic Smagorinsky model. The ℓ^2 norm of the error at Δ_{LES} decreases by 14.4% with HST when using the TSVD approach and $p' = 500$. Conversely, with HIT we only find a 3.6% decrease in the ℓ^2 norm of the error, suggesting that the ALES process is more prone to overfitting the flow realization for HST than HIT.

SUMMARY AND DISCUSSION

We have presented a fundamentally new and highly promising *autonomic* approach, termed ALES, to estimating the SGS stresses needed for closure in LES of turbulent flows. The approach is based on the most general nonlinear nonparametric functional form relating the local subgrid-stress tensor to all resolved-scale variables at all points and times. This closure is fully adaptive and self-optimizing, allowing the relation between the subgrid stresses and the resolved-scale fields to change freely as the local turbulence state changes. Lack of comparable adaptivity in conventional SGS models, which are based on predefined constitutive equations for the subgrid stresses in terms of the resolved strain rate or other resolved-scale quantities, may be a key reason why such models have failed to give accurate results for the subgrid stresses.

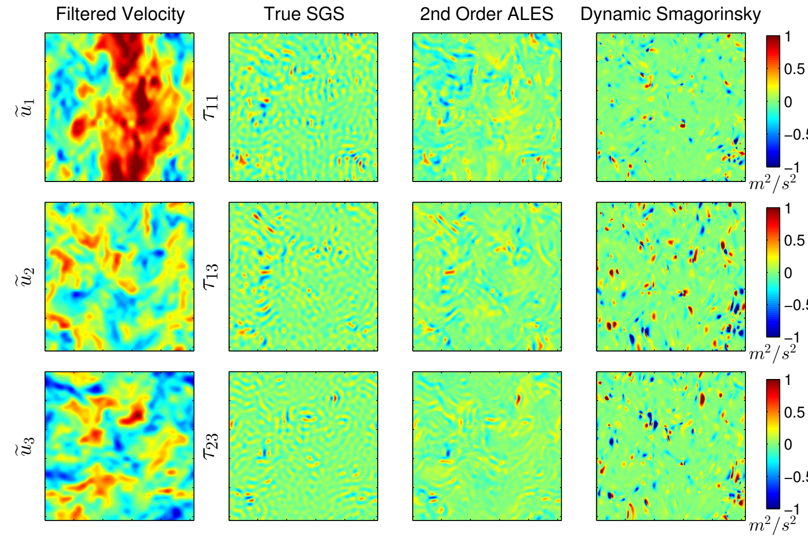

Figure 3. HST velocity and SGS stress fields at the LES scale from DNS, ALES, and the Dynamic Smagorinsky model show that the TSVD regularization helps ALES capture the SGS stresses in challenging sheared flows.

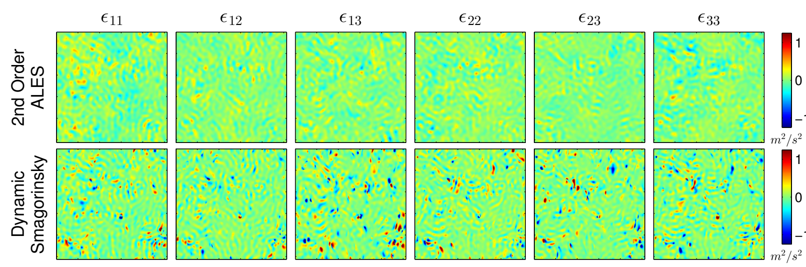

Figure 4. The LES scale errors confirm that the TSVD regularized ALES approach provides more accurate results than the Dynamic Smagorinsky model.

Results presented here from *a priori* tests of ALES in homogeneous isotropic and sheared turbulence show that the new approach provides highly accurate estimates for the subgrid stress fields $\tau_{ij}(\mathbf{x},t)$ using only the resolved-scale fields available in large eddy simulations. This is true even for a stringent truncation to 2$^{\text{nd}}$ order velocity terms, no memory, and a small $(3\times3\times3)$ stencil, which can only accommodate second-order spatial central differences. The accuracy of these test results, even for this small stencil, suggests that the autonomic closure can be implemented in a computationally efficient manner in practical LES. Moreover, the stencil size and memory can be increased if higher-order gradients or time derivatives of resolved-scale quantities are needed to accurately capture states of turbulence that may occur under strong nonequilibrium or other extreme conditions.

Future work will focus on integrating the ALES closure into a forward model simulation and performing *a posteriori* tests. Additional work will characterize the tradeoffs between truncation, regularization, and computational cost. Implementing the general Volterra series expansion and ALES optimization will require additional attention when considering filters with broad spectral support. Finally, it may be possible to extend this autonomic closure approach to steady and unsteady Reynolds averaged Navier-Stokes simulations and find a comparable model-free autonomic closure for the Reynolds stresses.

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