Autonomic Subgrid-Scale Closure for Large Eddy Simulations

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Exascale computing creates opportunities for entirely new approaches for simulating turbulent flows. A prime example of this is "autonomic closure" for large eddy simulations (LES). Autonomic subgrid-scale closure is a highly innovative approach that leverages high-performance computing to completely eliminate the need for specifying a predefined turbulence model for the subgrid-scale stresses in LES. Instead it applies advances in optimization and machine learning to provide "on-the-fly" autonomic identification of the best local relation between subgrid stresses and resolved-scale variables at every point and time in a simulation. This new closure is "autonomic" in the sense that it is self-optimizing without user inputs or training data, and is essentially unlimited in its ability to represent widely varying turbulence states in essentially any flow. While the approach can be generalized to other subgrid-scale processes, our work has focused on its use for subgrid stress closure in LES. Results to date have been remarkable and suggest that autonomic closure is practical way of achieving dramatically higher-fidelity large eddy simulations of turbulent flows.

Autonomic subgrid-scale closure shows enormous promise as a conceptually revolutionary, fundamentally better, and potentially transformative way – enabled by the increasing availability of high-performance computing resources – to achieve essentially model-free simulations of nonlinear, nonlocal, and nonequilibrium effects in large eddy simulations.

Summarizing the key ideas, we are developing a fundamentally new autonomic approach to subgrid-scale stress (SGS) closure that, instead of using a predefined turbulence model, solves a nonlinear nonparametric system identification problem to adaptively find the best local SGS closure at each point and time. This autonomic approach to LES closure (abbreviated as "ALES" and summarized in Figure 1) 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 [1], and nonequilibrium [2, 3] 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 SGS stresses at a test filter scale. The optimized coefficients are then projected to the LES scale by invoking scale similarity. The optimization process is self-

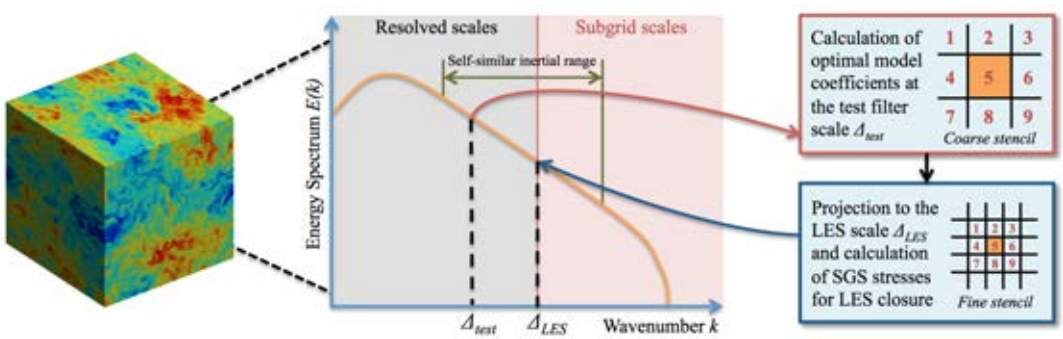

Figure 1: Conceptual schematic of the autonomic closure approach, showing the LES filter scale Δ_{LES} and test filter scale Δ_{test}. Coefficients in the Volterra series relating SGS stresses to resolved-scale variables are determined autonomically via optimization at Δ_{test}. The optimal coefficients are then applied at Δ_{LES} after appropriate renormalization, allowing SGS stresses at the LES filter scale to be obtained from the resolved-scale variables.

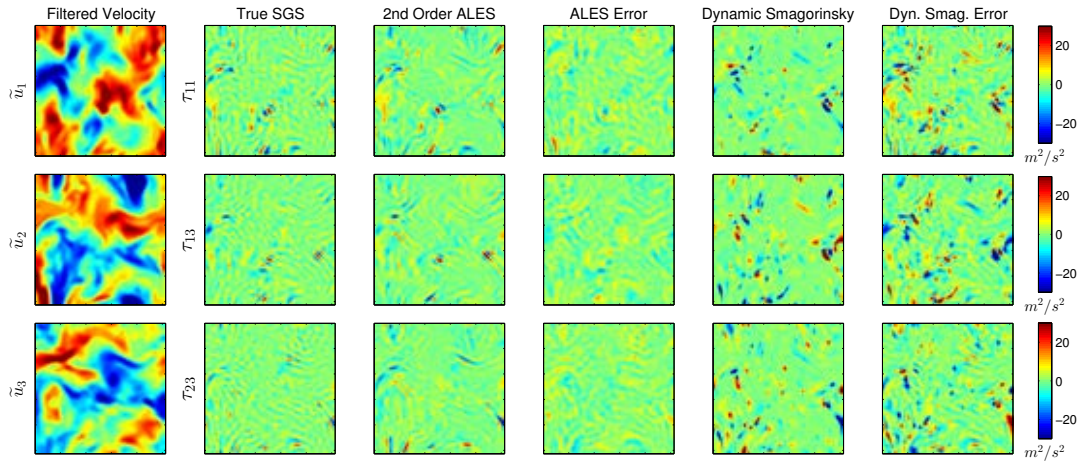

Figure 2: Homogeneous isotropic turbulence velocity and SGS stress fields at the LES scale from direct numerical simulations, ALES, and the dynamic Smagorinsky model show that ALES captures the stresses remarkably well.

contained and complete in that it does not require external training data, nor a predefined model structure, nor tuning coefficients that must be specified ahead of time. The ALES approach thus avoids the need to explicitly specify a turbulent constitutive model and instead identifies an optimal model "on the fly."

This highly innovative and potentially transformative new *autonomic* approach to LES closure has become computationally feasible due to recent advances in constrained optimization and machine learning techniques, as well as to the increasing availability of co-processor acceleration on modern supercomputers. In particular, the ALES approach can be coupled with a suitable co-processor accelerated optimization method in order to implement the closure in an LES code. Preliminary results from *a priori* tests of the autonomic closure in homogeneous isotropic and sheared turbulence have shown that even a truncated version of the fully general autonomic closure gives substantial improvements over the dynamic Smagorinsky model (e.g., Figure 2 and Refs. [5, 6]).

Details of this autonomic approach to LES closure are given in Refs. [5, 6]. The approach can be generalized to account for other subgrid processes, such as mixing, in which scale-similarity in the inertial range allows the optimized coefficients in the Volterra series to be projected from a test filter scale to the LES scale. As such, it provides a new and dramatically improved method – made possible by the availability of high-performance computing resources – to achieve essentially model-free closure in large eddy simulations of turbulent flows that inherently adapts to the degree of nonlinear, nonlocal, and nonequilibrium effects in the local turbulence state at every point and time in a simulation.

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