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Optimal Closures in a Simple Model for Turbulent Flows

Turbulent flows at high Reynolds numbers continue to challenge both scientists studying their fundamental properties and engineers interested in diverse technical applications involving fluid mechanics. In particular, accurate and efficient numerical simulation of turbulent flows will remain an open problem in computational science for the foreseeable future. As a result, one must rely on solving various simplifications and obtain approximate solutions of the flow problem. One such approach which has gained widespread popularity in engineering practice relies on the so-called Large-Eddy Simulation (LES). In this talk, I will introduce a computational framework for determining optimal closures of the eddy-viscosity type for LES of a broad class of PDE models, such as the Navier-Stokes equation. The proposed framework is thoroughly tested on a model problem involving the LES of the 1D Kuramoto-Sivashinsky equation, where the optimal closure relations are obtained as generalizations of the standard Smagorinsky model. Since this leads to a PDE optimization problem with a nonstandard structure, the solution is obtained computationally with a flexible and efficient gradient approach relying on a combination of modified adjoint-based analysis and Sobolev gradients, which will be discussed along with some results.