Advances in LES-based Turbulence Modeling

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Abstract

Recent research progress in turbulence modeling are discussed with focus on two topics: optimal LES and optimal theory based performance estimation. Optimal LES is an approach in which the subgrid model is formulated as minimum mean square error estimate. It has the advantage of being perfectly general, but requires information about the statistics of the small-scale turbulence. New advances in representing the multi-point correlations in both isotropic and wall-bounded flows are discussed, as is the performance of LES simulations based on these models. In the second part, some recent progress in analyzing the performance of models used to described turbulent combustion are discussed. Based on the concept of optimal error estimation, conventional models for the sub-filter variance of mixture-fraction are analyzed. A new dynamic procedure that provides improved performance is also discussed. Finally, the interaction of numerical errors with sub-filter models is studied in an effort to identify the more suitable formulations for LES-based combustion simulations.

Keywords: large eddy simulation, optimal estimation, dynamic modeling procedure.

Large eddy simulation (LES) is now considered an attractive tool for studying turbulent flows. While many applications of LES have shown very good prediction of the flow field, many lingering questions regarding sub-filter modeling and the interaction of numerical and modeling errors still remain. One approach to describing these errors in the optimal LES procedure.

Optimal LES is is based on the observation that the large scale fields being simulated do not provide sufficient information to reconstruct the small, scales, or even the evolution of the large scales [?]. The unknown small scales and therefore the LES evolution thus need to be treated statistically. Optimal LES models are formulated by postulating a model dependency and then minimizing the mean square error in representing the exact model term. Such models

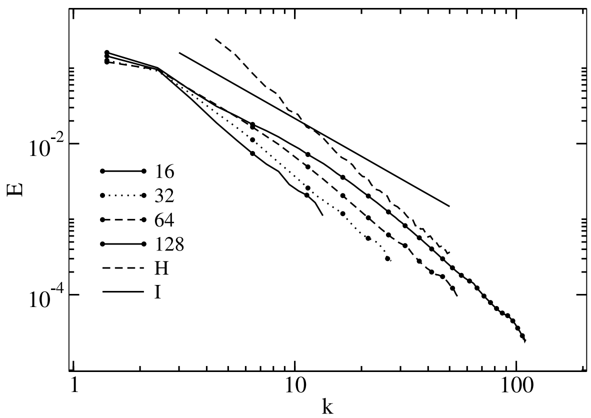

Figure 1: Three-dimensional energy spectra from finite-volume optimal LES of infinite Reynolds number isotropic turbulence using a range of resolutions from 16^3 to 128^3. Also shown is the $k^{-5/3}$ slope and the result of filtering a $k^{-5/3}$ spectrum.

can be formulated in terms of small-separation multi-point velocity correlations. The problem of LES modeling is thus explicitly reduced to the problem of modeling these correlations. Given this information, optimal models can be constructed that account for the errors of the numerical scheme used to solve the equations[**?**], and that are valid even in the presence of strong anisotropy and inhomogeneity[**?**]. Optimal LES is thus one approach which can address the shortcomings of current LES models.

The required multi-point correlations include the 2-point second order, 3-point third order and 4-point fourth order correlations. For high Reynolds number isotropic turbulence, where a Kolmogorov inertial range exists, models for these correlations are available or have recently been developed[**?**]. They have been used to construct optimal LES models, which yield remarkably good results. For example, an isotropic LES based on a finite-volume discretization (filter) and the correlation models produces spectra that are consistent with the finite volume filtering of a Kolmogorov $k^{-5/3}$ spectrum (figure 1). In a wall bounded flow, however, modeling the correlations is more difficult. A new formulation for the anisotropy and inhomogeneity of the two-point second correlation based on the structure tensors of Kassinos *et al* [**?**] has been developed. A comparison of thse model correlations with those determined from a DNS is shown in figure 2.

Details of the optimal LES and multi-point correlation modeling approaches will be discussed, as will their appliaction in LES simulation.

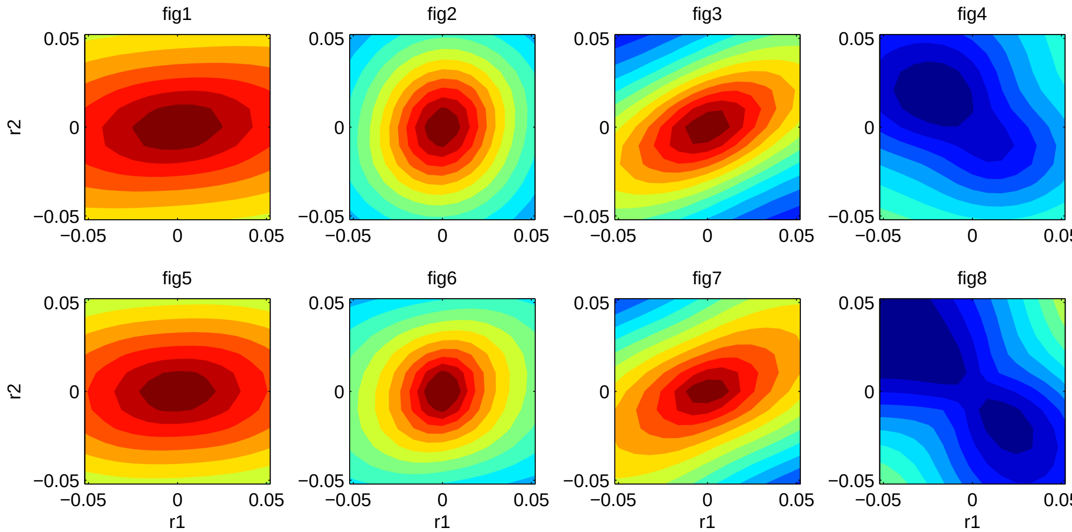

Figure 2: Comparison of the two-point correlation tensor components from the model and DNS in the x-y plane with no separation in z. The correlations are centered at $y^+ = 100$ in a turbulent channel flow, with $Re_\tau = 940$

In the second part of the lecture, we discuss the performance of models used to describe turbulent combustion. Most combustion models use a passive scalar, termed mixture fraction, to describe the thermochemical state of the gas-phase. In LES, the filtered gas-phase properties can be obtained if the sub-filter variance of mixture fraction is known. This measure of sub-filter scalar energy has to be modeled and several models are available in literature. Recently, the optimal error estimation procedure was used to evaluate sub-filter models [**?**, **?**]. It was found that the dynamic models, not surprisingly, provided the least error for a range of filter-widths. However, simple Taylor's series based analysis of the dynamic procedure found that certain key terms are being neglected in the model formulation [**?**]. When included, the new procedure was found to provide lower errors compared to the conventional procedure.

To understand the impact of numerics on model performance, *apriori* tests were conducted using different discretization schemes. It was found that the numerical error is of the same order as modeling error. Further, numerical errors have a "benign" effect on certain models leading to reduced overall error. These interesting findings also indicate that mathematical structure of the model is very important for reducing the inaccuracies due to numerical discretization [**?**, **?**].

References

[1] J. Langford and R. Moser, "Optimal LES formulations for isotropic turbulence," *Journal of Fluid Mechanics* **398**, 321 (1999).

[2] P. S. Zandonade, J. A. Langford, and R. D. Moser, "Finite volume optimal large-eddy simulation of isotropic turbulence," *Physics of Fluids* **16**, 2255 (2004).

[3] S. Volker, P. Venugopal, and R. D. Moser, "Optimal large eddy simulation of turbulent channel flow based on direct numerical simulation statistical data," *Physics of Fluids* **14**, 3675 (2002).

[4] H. Chang and R. D. Moser, "An intertial range model for the three-point third-order velocity correlation," *Physics of Fluids* **19**, 105111 (2007).

[5] S. Kassinos, W. Reynolds, and M. Rogers, "One-point turbulence structure tensors," Journal of Fluid Mechanics **428**, 213 (2001).

[6] A. Moreau, O. Teytaud, and J. P. Bertoglio. Optimal estimation for large-eddy simulation of turbulence and application to the analysis of subgrid models. *Phys. Fluids*, **18**, 1-10, 2006

[7] G. Balarac, H. Pitsch and V. Raman, "Modeling of sub-filter scalar variance using the concept of optimal estimator", *Physics of Fluids*, **20** 035114, 2008

[8] G. Balarac, H. Pitsch and V. Raman, "Modeling of the sub-filter scalar dissipation rate using the concept of optimal estimators", *Submitted to Physics of Fluids*, 2008

[9] V. Raman, G. Balarac, and H. Pitsch, "Minimizing numerical errors in the computational sub-filter scalar variance", *To be Submitted to Physics of Fluids*, 2008