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Reliability of large-eddy simulation

Bernard J. Geurts b.j.geurts@utwente.nl

University of Twente, MMS, Applied Mathematics Faculty EEMCS, 7500AE Enschede, NL
Eindhoven University of Technology, AT, Fluid Dynamics Lab, Applied Physics, 5600MB Eindhoven, NL

Turbulence readily arises in numerous flows in nature and technology. The large number of degrees of freedom of turbulence poses serious challenges to numerical approaches aimed at understanding and controlling such flows. While the Navier-Stokes equations are commonly accepted to precisely describe fluid flow, including turbulence, alternative coarsened descriptions need to be developed. These coarsened descriptions aim at capturing the primary features of a flow, at considerably reduced computational effort. Such coarsening introduces a `closure problem' that requires additional phenomenological modeling. Careful analysis and fundamental understanding of turbulence and numerical methods are needed to achieve successful closure and accurate computational strategies.

Large-eddy simulation (LES) forms an emerging computational tool for the prediction of turbulent flows. The methodology combines an accurate representation of turbulent flow phenomena with a computationally affordable representation of the flow dynamics. To this end, the Navier-Stokes equations, which govern the flow physics, are low-pass filtered, and the effects of small-scale turbulent motions, which would require very fine grid representations in direct numerical simulations (DNS), are instead incorporated using a subgrid-scale closure.

An overview of the large-eddy simulation (LES) approach is sketched in which we present the phenomenology of coarsened turbulence, linking RANS and LES and discussing the central closure problem. Sub-filter modeling is reviewed and several models proposed in literature are discussed, including eddy-viscosity models, dynamic models, regularization models, variational multiscale approach and approximate inverse modeling. Testing of LES computational strategies is discussed and illustrated for (i) homogeneous, isotropic, decaying turbulence, (ii) turbulent combustion. Error-assessment for large-eddy simulation is given attention; predictions of LES are principally flawed due to shortcomings in the closure modeling and errors in the numerical treatment. A systematic framework for estimating these errors is presented, error-decomposition is illustrated and the error-landscape concept is introduced and adopted for optimization of numerical and model parameters. Finally, an illustration of the error-landscape approach to turbulent combustion is provided.

At the coarse resolutions that are commonly adopted in present-day large-eddy simulations, an important problem is the intricate interaction between errors due to the subgrid-scale model and errors introduced by the discrete representation of the resolved-scale flow dynamics. The realization is growing that a proper understanding of the complex error dynamics, involving numerical errors and subgrid-scale modeling errors, is paramount for the credibility of LES as a valid prediction tool for turbulent flows. Various contributions have been presented recently, aiming at the identification of modeling and numerical errors, or the formulation of reliability guidelines.

A central issue in the assessment of LES is the methodology, which is used to identify the quality of results. Various effects can play a role, which complicates the interpretation of the reliability of a simulation. Numerical discretization, specific properties of the subgrid-scale closure, the flow conditions of the selected reference case, the use of explicit filtering or de-filtering during the simulation or during postprocessing, etc., can all contribute strongly to the accumulated total simulation error. One recently proposed approach to assess LES consists of the systematic variation of simulation parameters. Such a database-analysis allows to obtain a general overview of the error behavior in the form of so-called "error landscapes."

Based on the systematic variation of the Smagorinsky model-parameter, the spatial resolution and the Reynolds number in LES of decaying homogeneous isotropic turbulence, it was demonstrated that errors resulting from such a well-known "Smagorinsky-fluid" might strongly interact with discretization errors. Moreover, "optimal refinement trajectories" were obtained, which provide the optimal model parameter, resulting in the lowest simulation error at given resolution. Later, these optimal refinement trajectories were compared with the predicted model-coefficient that results from the dynamic eddy-viscosity model. This showed that the error-landscape approach can also be very instructional in the interpretation of the quality other eddy-viscosity subgrid models. We recall that the error-landscape for a "Smagorinsky fluid" provides a detailed overview of a selected simulation error as function of the spatial resolution *N* and the Smagorinsky parameter *C*. Each point in the *C*-*N* plane corresponds to a particular large-eddy simulation, which displays its own specific deviation from the exact direct numerical simulation results. An “error landscape” is created by considering the total simulation-error for a systematically varied set of *C*-*N* points, leading to an extensive database approach. In this error landscape the line *C*(N)*, for which the total simulation-error is minimal at given resolution *N*, represents the “optimal refinement strategy.” An illustration is given in FIG. 1, showing error-landscapes for the energy and enstrophy in homogeneous, isotropic turbulence at Taylor *Re*=100.

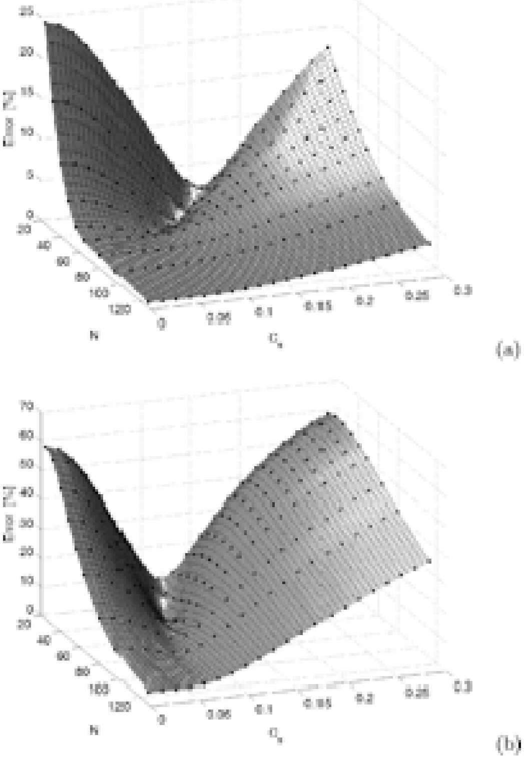

FIG. 1. Error surfaces of LES employing the Smagorinsky model for the *Re*_=100 case. Errors are related to the resolved kinetic energy (a) and to the resolved enstrophy (b). The locations indicated by the dots correspond to the different simulations that were included in the database. A fourth order accurate spatial discretization was adopted.

In order to obtain *(C, N)* combinations that are ‘near optimal’ for a set of physical quantities simultaneously, we show the optimal refinement and a band of parameters such that the error is within 20% of the optimum in FIG. 2. We observe that accurate prediction of a combination of several quantities simultaneously, leads to more strict requirements on the main parameters *(C, N)*. At low resolution there can be even no parameter choices that comply with acceptably accurate predictions of both quantities. These observations can be extended to turbulent non-premixed combustion, as will be included in the presentation.

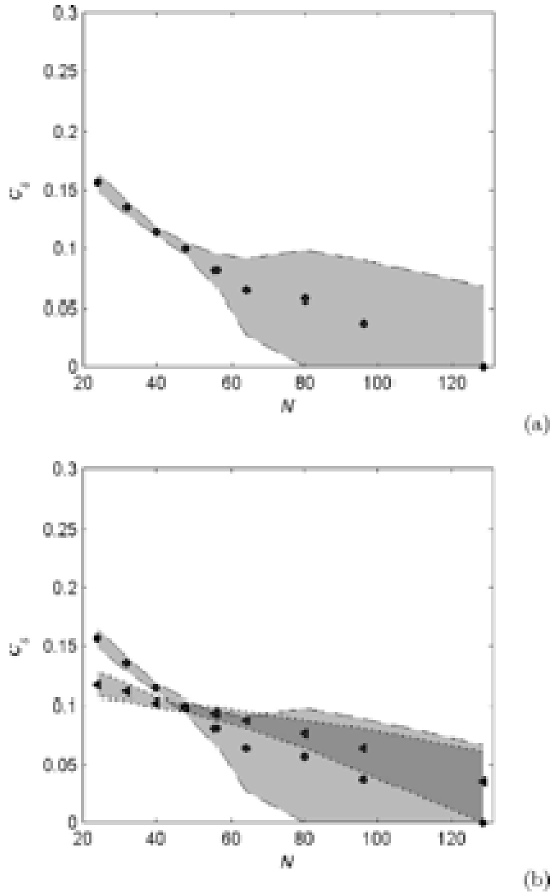

FIG. 2. “Near optimal” regions related to different error definitions for the standard Smagorinsky model at *Re*=100 for energy (a) and for energy and enstrophy (b).The “near optimal” regions are shaded gray and semitransparent, such that parameters in which both overlap appear with darker shades of gray. Symbols correspond to the optimal refinement strategy for the different error definitions.