Development of regularization modeling and error-control in large-eddy simulation

Bernard J. Geurts

1Multiscale Modeling and Simulation, J.M. Burgers Center, Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands
2Anisotropic Turbulence, Fluid Dynamics Laboratory, Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

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Abstract: Numerical simulation is developing into a viable research-tool to help understand dispersion and structure in turbulence. In order to make progress toward simulating flows under realistic flow-conditions and in complex flow-domains, large-eddy simulation appears an essential stepping-stone. This requires a combination of accurate numerical treatment and proper (subgrid) modeling of the dynamic effects of small-scale turbulence. It will be shown that accurate subgrid models may be systematically derived from mathematical regularization principles. This will be illustrated for the Leray and NS-$\alpha$ models. Moreover, a database analysis of interacting modeling and simulation errors in large-eddy simulation will be discussed in terms of error-landscapes. The optimality of the dynamic procedure will be quantified and a new inverse polynomial interpolation method will be proposed with which model parameters can be optimized to approximate the ‘optimal refinement strategy’.

Mathematical regularization of the nonlinear terms in the Navier-Stokes equations is found to provide a systematic approach to deriving subgrid closures for numerical simulations of turbulent flow (Geurts and Holm, 2003). By construction, these subgrid closures imply existence and uniqueness of strong solutions to the corresponding modeled system of equations. We will consider the large eddy interpretation of two such mathematical regularization principles, i.e., Leray and NS-$\alpha$ regularization. The Leray principle introduces a smoothed transport velocity as part of the regularized convective nonlinearity. The NS-$\alpha$ principle extends the Leray formulation in a natural way in which a filtered Kelvin circulation theorem, incorporating the smoothed transport velocity, is explicitly satisfied. These regularization principles give rise to implied subgrid closures which are implemented in large eddy simulation.

Comparison with filtered direct numerical simulation data and with predictions obtained from popular dynamic eddy-viscosity modeling shows that these mathematical regularization models provide considerably more accuracy at a lower computational cost than the dynamic approaches (Geurts and Holm, 2006). In particular, the regularization models perform especially well in capturing the flow features characteristic of the smaller resolved scales. Variations in spatial resolution and Reynolds number establish that the Leray model is more robust but also slightly less accurate than the NS-$\alpha$ model. The NS-$\alpha$ model retains more of the small-scale variability in the resolved solution. However, this requires a corresponding increase in the required spatial resolution. When using second order finite volume discretization, the potential accuracy of the implied NS-$\alpha$ model is found to be realized by using a grid spacing that is not larger than the length scale $\alpha$ that appears in the definition of this model.

Next to the quality of the subgrid modeling, the accuracy of large-eddy simulations is limited by the numerical contamination of the smaller retained flow-structures. We analyze the effects of discretization and modeling errors in a database-approach and assess the total simulation error and its numerical and modeling contributions (Meyers et al., 2003). The interaction between the different sources of error is shown to lead to their partial cancellation. From this analysis one may identify an ‘optimal refinement strategy’ for given subgrid model, discretization method and flow conditions, leading to minimal total simulation error at given computational cost. We provide full detail for homogeneous decaying turbulence in a ‘Smagorinsky fluid’.

The optimal refinement strategy is compared with the error-reduction that arises from grid-refinement of the dynamic eddy-viscosity model (Meyers et al., 2005). The main trends of the
optimal refinement strategy as function of resolution and Reynolds number are found to be adequately followed by the dynamic model. This yields significant error reduction upon grid refinement, although at coarse resolutions significant error-levels remain. To address this deficiency, a successive inverse polynomial interpolation procedure is adopted with which the optimal Smagorinsky constant may be efficiently approximated at given resolution. The computational overhead of this procedure is shown to be well justified in view of the achieved reduction of the error-level relative to the 'no-model' and dynamic model predictions. This approach is sketched next.

Central to an optimization procedure for large-eddy modeling is the definition of a 'cost-function' that measures the error-level at given parameters. We compare LES predictions for the resolved kinetic energy with filtered DNS data. For the Smagorinsky model the relative error is expressed by $\delta E(\xi_S)$ where $\xi_S = (C_S \Delta)/h$ is the resolution of the Smagorinsky length $\xi_S$ in terms of the Smagorinsky constant $C_S$, the filter-width $\Delta$ and the grid-spacing $h$. Only minimization algorithms that do not rely on the explicit use of derivatives of $\delta E$ will be considered. Locally around its minimum we assume that the cost-function may be approximated by a parabola. This motivates the use of successive inverse parabolic interpolation (SIPI) to obtain a next estimate for $\xi_S$.

Referring to figure 1(a), we start by constructing an interpolating parabola through the original bracketing triplet, $(a, \delta E(a))$, $(b, \delta E(b))$ and $(c, \delta E(c))$. The location of the minimum of this parabola may be determined, which indicates a new value for $\xi_S$ to be used in the next simulation. Subsequently, the total simulation error is evaluated at $\xi_S = d$. From this information a new bracketing triplet may be identified which defines a new interpolating polynomial, and the process may be continued.

Successive inverse parabolic interpolation and evaluation of $\delta E$ leads to a sequence of bracketing triplets which quite rapidly converges to the optimum. If $\delta E$ has a continuous second derivative which is positive at the minimum, then convergence is super-linear. The application of this method to the Smagorinsky fluid at $R_\lambda = 100$ and a spatial resolution of $N = 32^3$ or $N = 48^3$ is illustrated in figure 1(b). In these cases the combination of a 'no-model simulation', a 'dynamic eddy-viscosity simulation' at $\xi_S = \xi_d$ and a Smagorinsky simulation with $\xi_S = \xi_d/2$ already yields about a factor of 4 reduction of the error relative to the no-model case. Application of SIPI yields rapid convergence; after about 2-3 iterations the optimum is quite well approximated and a relative error of about 1-2 % remains.

Figure 1: (a): Illustration of successive inverse parabolic interpolation (SIPI) to approximate the optimal resolution of the Smagorinsky length-scale $\xi_S = (C_S \Delta)/h$. The initial triplet $(a, b, c)$ defines an interpolating polynomial (dashed), whose minimum yields a next approximation $d$ at which a new large-eddy simulation should be performed. (b) Application of SIPI to the total simulation error at $R_\lambda = 100$ and $N = 32$ (solid) and $N = 48$ (dashed). The initial triplet is indicated with $\circ$, the first iterand with $\ast$, the second with a 'diamond' and the third with a 'square'.


