Turbulent Backward-Facing Step Flow: Reliability Assessment of Large-Eddy Simulation Using ILSA

Bernard J. Geurts, Amirreza Rouhi, and Ugo Piomelli

Abstract Reliability assessment of large-eddy simulation (LES) of turbulent flows requires consideration of errors due to shortcomings in the modeling of sub-filter scale dynamics and due to discretization of the governing filtered Navier-Stokes equations. The Integral Length-Scale Approximation (ILSA) model is a pioneering sub-filter parameterization that incorporates both these contributions to the total simulation error, and provides user control over the desired accuracy of a simulation. The performance of ILSA, implemented as eddy-viscosity models, for separated turbulent flow over a backward-facing step is investigated here. We show excellent agreement with experimental data and with predictions based on other, well-established sub-filter models. The computational overhead is found to be close to that of a basic Smagorinsky sub-filter model.

Keywords Turbulence · Large-eddy simulation · ILSA modelling · Reliability

1 Introduction

Large-eddy simulation (LES) of turbulent flow has a long and rich history. During the 1960s first parameterizations, such as Smagorinsky's eddy-viscosity model [1]

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were proposed to capture the effects of localized turbulent motions on the large energy-carrying scales. The coarsening length-scale of choice was directly linked to the mesh-size in the computational grid, often chosen as the cube-root of the volume of a grid cell [2]. While coarsening is helpful in reducing the computational effort required for a simulation of a particular flow, it also introduces uncertainty regarding the accuracy of the results [3, 4]. Achieving a clear estimation and control of the level of uncertainty in the coarsened predictions, is a crucial pacing item in LES research. We review the recent ILSA proposal (Integral Length-Scale Approximation) which is a first framework that can address dynamic error control systematically, closely following [5, 6].

The computational grid for LES is often defined independent of the flow. Correspondingly, also the grid-based local coarsening length-scale is decoupled from the actual local flow. However, LES coarsening could in principle differ from location to location and from time to time, in response to local turbulence levels and variations in length- and time scales. Such would allow for lower resolution in regions of rather quiescent flow and higher resolution where required by the locally more detailed flow [7]. Recently, in Piomelli et al. [5] an alternative coarsening length-scale was put forward for LES, based on flow physics rather than on the grid scale. This idea was implemented in the form of an eddy-viscosity model based on the local integral length-scale. The model coefficient is specified with reference to the concept of 'sub-filter activity' as suggested in Geurts and Fröhlich [8]. The eddy-viscosity is such that an *a priori* user-defined measure for the error level can be maintained. Effective model parameters that implement this sub-filter activity level can be inferred computationally from exploratory coarser simulations, following the SIPI (Successive Inverse Polynomial Interpolation) error minimization [9]. Combined, ILSA is a first, complete formulation in which the issue of LES reliability for a particular flow is key.

In this paper we review the ILSA modeling strategy and discuss the development and testing of the new model for flow over a backward-facing step, showing that the new eddy-viscosity model compares closely with experimental data by Vogel and Eaton [10]. ILSA does not require the introduction of any *ad hoc* user-defined parameters, other than the target sub-filter activity, i.e., the desired level for the total simulation error. The ILSA model allows to separate the problem of *representing small-scale turbulent motions* in a coarsened flow model from that of *achieving accurate numerical resolution* of the solution. The formulation supports the notion of grid-independent LES, in which a prespecified reliability measure is used to determine the local coarsening length-scale. This is basic to achieving *a priori* error control.

The organization of this paper is as follows. In Sect. 2 we briefly review reliability issues in LES. Basic ILSA is presented in Sect. 3 in which the original 'global' ILSA and the 'local' ILSA extension are discussed. Section 4 presents results for turbulent backward-facing step flow, closely following [6]. Summarizing remarks are collected in Sect. 5.

2 Reliability Issues in Large-Eddy Simulation

In this section we briefly review the main components that make up the total simulation error in LES and discuss the error-landscape approach to visualize interacting error contributions. A standard formulation for LES assumes a spatial convolution filter with an effective width Δ, coupling the unfiltered Navier-Stokes solution to the filtered solution. In this paper we work with incompressible flows, governed by conservation of mass and momentum respectively,

$$\partial_j \overline{u}_j = 0$$
$$\partial_t \overline{u}_i + \partial_j (\overline{u}_i \overline{u}_j) + \partial_i \overline{p} - \frac{1}{\text{Re}} \partial_{jj} \overline{u}_i = -\partial_j (\overline{u_i u_j} - \overline{u}_i \overline{u}_j)$$

where the overbar denotes the filtered variable. Here, we use Einstein's summation convention and use p for the pressure and $\boldsymbol{u}$ for the velocity field. Time is denoted by t and partial differentiation with respect to the jth coordinate by the subscript j. Relevant length (L) and velocity (U) scales, and the constant density and kinematic viscosity (ν) are used to make the equations dimensionless and define the Reynolds number $Re = UL/\nu$. On the left-hand side we observe the incompressible Navier-Stokes formulation in terms of the filtered variables. On the right hand side the filtered momentum equation has a non-zero contribution expressed in terms of the divergence of the sub-filter stress tensor

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$$

The sub-filter tensor expresses the central 'closure problem' in LES, as it requires both the filtered as well as the unfiltered representation of the solution. Since only the filtered solution is available in LES, the next step in modeling the coarsened turbulent flow is to propose a sub-filter model M in terms of the filtered solution only. Numerous sub-filter models have been proposed for LES, among which eddy-viscosity models [3, 11] regularization models [12] and similarity models [13]. In this paper we restrict ourselves to eddy-viscosity models, in which the anisotropic part of sub-filter stress tensor is given by, where S_{ij} denotes the rate of strain tensor of the filtered velocity field, i.e., the symmetric part of the velocity gradient, and ν_{sfs} is the sub-filter scale eddy viscosity.

A central premise of numerical simulation asserts that the solution to a given PDE problem should be obtained accurately and efficiently, while simultaneously, a close upper-bound for the error should be estimated. In the context of LES this not only implies a study of the effects of numerical discretization errors on the dynamics of the simulated solution, but also includes the role of the model for the sub-filter stress tensor as well as the interaction between these two basic sources of error [14–16]. However, in practice the computational costs of simulating a flow on N^3 grid points, using an explicit time-stepping method, scales $\sim N^4$ with N the number of grid points along a coordinate direction. This cost implies a large role of the numerical

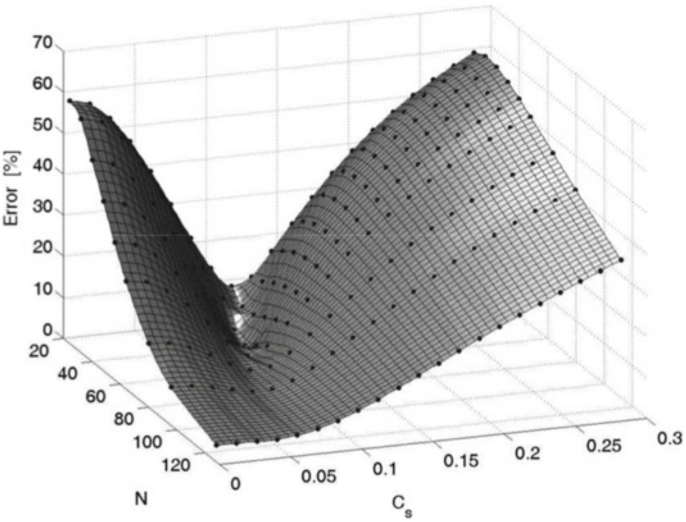

Fig. 1 Error landscape for LES based on the Smagorinsky model applied to decaying homogeneous isotropic turbulence at a Taylor Reynolds number of 100. The error in the resolved enstrophy, relative to the DNS prediction, is shown as function of the spatial resolution *N* and the Smagorinsky coefficient—reproduced with permission from Meyers et al. [18]. Each dot on the error-surface corresponds to a particular LES

method in capturing the actual LES solution [17]. Hence, at practically feasible, likely marginal resolution, both the selected sub-filter model as well as the adopted spatial discretization method can have a significant influence on the simulated dynamics. Together, these influences give rise to the total simulation error.

Since the modeling and discretization error effects can partially counteract each other [19–23] it is not straightforward to assess the overall simulation error in a given flow property. Instead, one can resort to a computational assessment of the simulation error for selected cases [24, 25]. This is known as the error-landscape approach. In Fig. 1 we show such an error-landscape for LES of homogeneous isotropic turbulence, based on the Smagorinsky model. The error is based on the relative deviation of the turbulent kinetic energy between, on the one hand, a particular LES (at given spatial resolution *N* and value of the Smagorinsky coefficient C_S) and, on the other hand, the underlying direct numerical simulation. Each dot on the error-landscape surface denotes the error in a particular LES. At zero Smagorinsky coefficient, e.g., the LES corresponds to a 'no-model' or under-resolved simulation. We observe that the error decreases rapidly and smoothly with increasing spatial resolution, indicating convergence toward DNS predictions at high enough spatial resolution. Moreover, we notice that at fixed, coarse, spatial resolution *N* and sufficiently large values of the Smagorinsky coefficients, also rather large errors arise. In between the 'no model' case and a very large C_S there appears a minimum in which possible partial cancellation of modeling and discretization error effects is achieved optimally at that value of grid resolution *N*. This would yield the lowest total simulation error at the corresponding computational cost. The optimal refinement strategy can be inferred by determining these minima as function of N. Knowledge about such error behavior can be used to classify errors due to numerical dissipation and sub-filter contributions [26]. Strictly speaking, the optimal refinement strategy can be inferred only after a database of LESs is collected—the optimal Smagorinsky coefficient at given spatial resolution is a quantity that currently cannot be predicted in advance theoretically [27].

A computational estimate of the optimal Smagorinsky coefficient at given spatial resolution can be obtained at modest additional cost using the SIPI method (Successive Inverse Polynomial Interpolation) [9]. At given N this method takes error levels at three prior simulations using different C_S values, and, via quadratic interpolation, progresses to converge C_S to achieve the error minimum. Since the dependence of the optimal Smagorinsky coefficient on the spatial resolution is quite modest, one may proceed in two steps. First, at coarse resolution the optimal Smagorinsky coefficient is determined. Subsequently, at finer resolution, production simulations can be executed with this optimal coarse grid value. This approach is also basic to the original ILSA model to which we turn next.

3 ILSA—Integral Length-Scale Approximation

We review the length-scale definition for LES based on the resolved turbulent kinetic energy (TKE) and its dissipation. Rather than working with a grid-based length-scale, as in traditional LES, referring to sub-*grid* scales, we propose a flow-specific length-scale distribution defining the filter-width and hence refer to the LES approach as modelling the sub-*filter* scales.

The global ILSA model is an eddy-viscosity model in which the anisotropic part of the sub-filter stress tensor is given by $\tau_{ij}^a = -2\nu_{sfs} S_{ij}$ with turbulent eddy-viscosity defined as

$$\nu_{sfs} = (C_m \Delta)^2 \left|\overline{S}\right| \equiv (C_m C_\Delta L)^2 \left|\overline{S}\right| \equiv (C_k L)^2 \left|\overline{S}\right|$$

where $C_k = C_m C_\Delta$ is referred to as the 'effective model coefficient', and the filter-width Δ is expressed as a fraction of the local integral length-scale, $\Delta = C_\Delta L$, inferred from

$$L = \frac{\langle K_{res} \rangle}{\langle \varepsilon_{tot} \rangle}$$

where the resolved turbulent kinetic energy (TKE) and total dissipation rate are given by

$$K_{res} = \frac{1}{2}\overline{u}_i'\overline{u}_i'; \quad \varepsilon_{tot} = 2(\nu + \nu_{sfs})\overline{S}_{ij}'\overline{S}_{ij}'$$

in terms of resolved velocity fluctuations and the corresponding rate-of-strain tensor. Using the resolved TKE rather than the total one does not affect the estimated length-scale significantly [5, 28]. The choice to use the integral length scale L implies that the local LES resolution adapts itself dynamically to the turbulence characteristics of the flow. The local grid resolution h should at least resolve the integral length scale L, i.e., $L/h >> 1$. By selecting h appropriately, an approximately grid-independent LES prediction may be obtained. Moreover, variations in L automatically can be used to generate (adaptive) non-uniform grids on which to simulate the turbulent flow at hand [7].

Aside from the local integral length-scale L, a key ingredient toward the ILSA model is that adaptations in the effective model coefficient are made consistent with a measure toward explicit error control. This way, the effective model coefficient C_k should be obtained in response to the local flow characteristics. For this purpose the concept of sub-filter activity [8] is used. This approach is conceptually related to the famous 'Pope 80% rule' [3] in which it is put forward that accurate LES requires the local filter-width to be such that the resolved turbulent kinetic energy is at least 80% of the total turbulent kinetic energy. Likewise, requiring a bounded sub-filter activity, we inherit a dynamic model response compliant with a desired level of error control.

The local ILSA model uses invariants of the sub-filter stresses directly. Following Rouhi et al. [6] we introduce

$$s_\tau = \left(\frac{\left\langle \tau_{ij}^a \tau_{ij}^a \right\rangle}{\left\langle \left(\tau_{ij}^a + R_{ij}^a\right)\left(\tau_{ij}^a + R_{ij}^a\right)\right\rangle}\right)^{1/2}$$

where the anisotropic part of the sub-filter tensor is denoted by τ_{ij}^a and the anisotropic part of the resolved stress tensor by $R_{ij}^a = \overline{u}_i'\overline{u}_j' - \overline{u}_k'\overline{u}_k'\delta_{ij}/3$. In case of an eddy-viscosity model the anisotropic sub-filter tensor $\tau_{ij}^a = -2\nu_{sfs}\overline{S}_{ij}$ with $\nu_{sfs} = (C_k L^2)|\overline{S}|$. This model implies

$$\left\langle \tau_{ij}^a \tau_{ij}^a \right\rangle = 4\left\langle \nu_{sfs} S_{ij} S_{ij} \right\rangle = \left\langle 2L^4 |S|^4 \right\rangle C_k^4 \equiv \chi_1 C_k^4$$
$$\left\langle \tau_{ij}^a R_{ij}^a \right\rangle = \left\langle -2\nu_{sfs} S_{ij} R_{ij}^a \right\rangle = -\left\langle 2L^2 |S| S_{ij} R_{ij}^a \right\rangle C_k^2 \equiv \chi_2 C_k^4$$

If we denote in addition $\left\langle R_{ij}^a R_{ij}^a \right\rangle \equiv \chi_3$ then we infer a fourth order polynomial equation governing the effective model coefficient as

$$\chi_1\left(1 - \frac{1}{s_\tau^2}\right)C_k^4 + 2\chi_2 C_k^2 + \chi_3 = 0$$

from which the unknown coefficient C_k can be obtained once the desired sub-filter activity is set to an appropriate value.

4 Local ILSA for Flow Over a Backward-Facing Step

In this section we illustrate the performance of the local ILSA model for turbulent flow over a backward-facing step at $Re_c = U_c h_s/\nu = 28{,}000$ based on the centerline velocity U_c at the inlet ($x = 0$) and step height h_s. We compare results with the Lagrangian dynamic model [29], and show close agreement of local ILSA with experimental reference data by Vogel and Eaton [10]. We analyze the induced eddy-viscosity model on the computational grid and argue better numerical behavior in the ILSA model, contributing to the overall model performance. Figure 2: Structured grid for the backward-facing step flow on a coarse grid of $256 \times 100 \times 64$ grid points, clustered at characteristic locations in the domain, i.e., near the boundaries and shear layers inside the domain. All scales are normalized by the step height.

In Fig. 2 we show the computational grid used for the backward-facing step simulations. The height of the inflow channel is 4 step heights and the spanwise width is 3 step heights. The inflow length of the channel is 32 step heights and the velocity field at $x = -5h_s$ is recycled to the inflow located at $x = -32h_s$ to generate a well-developed turbulent inflow. At the outflow at $20h_s$ a convective boundary condition was adopted.

In Fig. 3 the mean flow statistics are shown at three spatial resolutions, comparing local ILSA with the Lagrangian dynamic model, with ‘no model’ and with experimental data. The LES results agree closely with each other and with the experimental data—only on the coarsest grid there is a slight difference between the local ILSA and Lagrangian dynamic model. This difference is most notable in the recovery region after the reattachment. The ‘no model’ option shows that the inclusion of a sub-filter model is beneficial for the accuracy of predictions.

The central model parameters of the local ILSA model are illustrated in Fig. 4. We compare the standard definition of the filter width (Fig. 4a) with the estimated integral scale L (Fig. 4b). The local integral length-scale decreases considerably where the

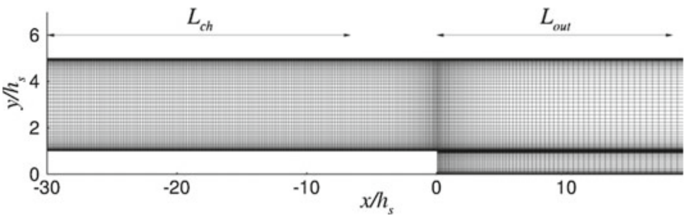

Fig. 2 Structured grid for the backward-facing step flow on a coarse grid of $256 \times 100 \times 64$ grid points, clustered at characteristic locations in the domain, i.e., near the boundaries and intense shear layers inside the domain. All scales are normalized by the h_s step height

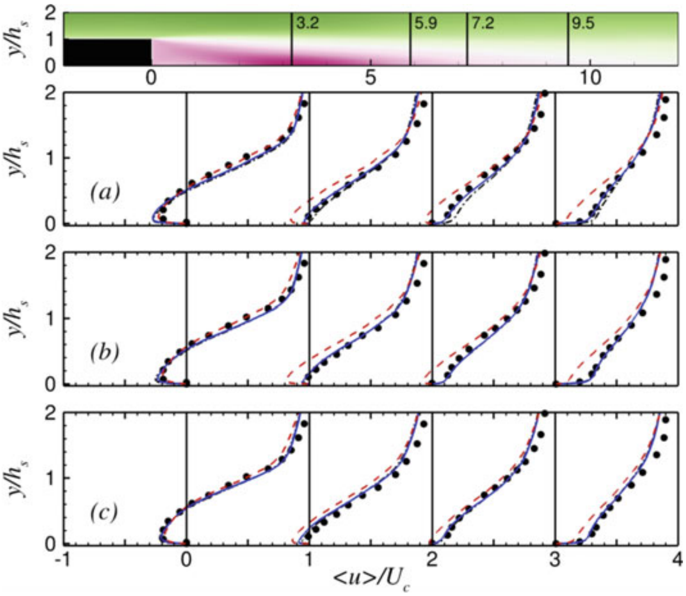

Fig. 3 Mean velocity normalized by the centerline velocity at the inlet, determined at a number of locations downstream of the step on different grids: **a** 256 × 100 × 64 points, **b** 384 × 150 × 96 points, **c** 512 × 200 × 128 points. Experimental data [10] shown with full circles, Lagrangian dynamic model in dash-dot, no-model in dashed line and local ILSA in solid line (reproduced with permission from Rouhi et al. [6])

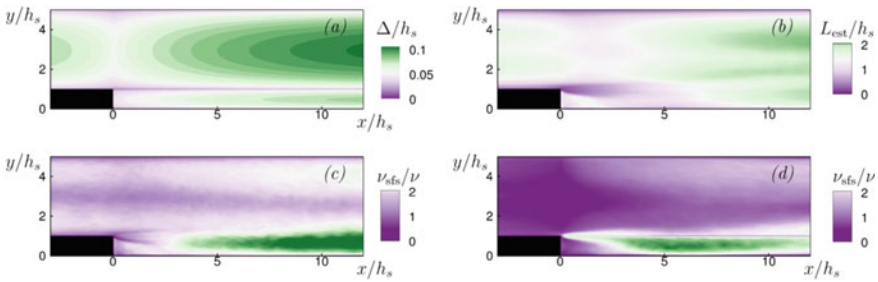

Fig. 4 SFS quantities for the backward-facing step flow. **a** Filter size; **b** integral scale; **c** eddy viscosity, local ILSA model; **d** eddy viscosity, dynamic Lagrangian model. Intermediate grid, 384 × 150 × 96 points

flow has small scale features, i.e., in the boundary layers and near the shear layers. Away from these locations, L increases as the typical scales that need resolving become larger. The structured character of the grid implies that a refined mesh is used in regions where the turbulent eddies are not small, for instance downstream of the step, $x/h_s \simeq 5$–10 and $y/h_s \simeq 1$. As a consequence, the Lagrangian eddy viscosity has an unphysical sharpness along the region where the grid is refined (Fig. 4d), which is not observed when the local ILSA model is used (Fig. 4c). Such large variations in the local filter-width are linked to commutator errors [30, 31]. By allowing a smooth variation of the eddy-viscosity/filter-width, these commutator errors can largely be removed [32, 33].

5 Concluding Remarks

We discussed recent progress in the assessment of the reliability of LES predictions. The basic limitation in LES quality stems from an interplay between on the one hand effects of discretization errors and on the other hand modeling error. This can be clarified comprehensively in terms of a computed error-landscape in which the total simulation error is computed as function of spatial resolution and model coefficient. A key concept in dynamic error control for LES is 'sub-filter activity'. Adhering to a description that keeps the measure for the sub-filter activity near a pre-specified target value, allows some level of control over the dominant LES errors.

The ILSA model requires little extra computational overhead and yields close agreement with DNS and experimental reference material for backward-facing step flow. The main model innovation, implies using the local integral length scale to represent changes in the local flow physics. Much of the non-uniform variations in the turbulence properties is already reflected in changes in the integral length scale—the rest of the eddy-viscosity definition is less sensitive to flow details and was found to yield a natural adaptation of the sub-filter model to the flow.

The local ILSA model holds promise to be effective in LES also for wider classes of turbulent flow. Further studies to underpin this should include stronger variations in flow properties, including re-laminarization. Moreover, investigating the role of the target value for the sub-filter activity level on the reliability of the LES predictions and the convergence with spatial resolution are items of ongoing research toward a genuine error-bar for CFD.

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