ACCURACY CONTROL FOR LARGE-EDDY SIMULATION OF TURBULENT MIXING - INTEGRAL LENGTH-SCALE APPROACH

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ABSTRACT

Turbulent flow at high Reynolds numbers is currently not accessible on the basis of direct numerical simulation (DNS) of the Navier-Stokes equations - the computational complexity is too high to allow DNS in most realistic flow conditions. Instead, Large-Eddy Simulation (LES) offers an alternative in which the focus is on capturing the larger dynamic scales of a problem. However, the fundamental closure problem in LES induced by spatial filtering of non-linear terms, and the role of discretization errors in the numerical treatment of the LES equations, induce a principal uncertainty in any LES prediction. This uncertainty requires quantification and control. We investigate error control capabilities of the Integral Length-Scale Approximation (ILSA) and apply this modeling to transitional and turbulent mixing, focussing on the achieved reliability of LES as function of the grid resolution and 'sub-filter activity'.

INTRODUCTION

Rigorous and rational methods for the computational modeling of turbulent flow at high Reynolds numbers include direct numerical simulation (DNS) and Large-Eddy Simulation (LES). These approaches have different strengths and limitations and can find successful application in a number of flow problems. LES arises from spatial filtering of the Navier- Stokes equations. In this approach, an externally specified length-scale, the so-called 'filterwidth' Δ, is introduced, giving some control over the range of dynamical features that are included in the computational model. The spatial filtering potentially simplifies the dynamics, but it also gives rise to a fundamental closure problem in LES, forcing the introduction of a particular sub-filter scale model to represent the effects of the motions on scales smaller than Δ. In addition, the numerical treatment of the LES equations, to which a specific sub-filter model is added, introduces discretization errors that may influence the behavior of the resolved scales. Together, the sub-filter modeling and the discretization induce a principal uncertainty in LES that requires quantification and control. We consider the Integral Length-Scale Approximation (ILSA) (Piomelli *et al.* (2015); Rouhi *et al.* (2016)). Previously, ILSA was applied successfully to homogeneous isotropic turbulence, turbulent channel flow, flow over a backward-facing step, in a separating boundary layer (Wu & Piomelli (2018)), a sphere, and the Ahmed body (Lehmkuhl *et al.* (2019)). In this contribution we include transitional as well fully developed turbulent flow and focus on turbulent mixing in a temporal mixing layer model (Vreman *et al.* (1997)). Modeling and discretization errors can to some extent be controlled in the ILSA framework - we illustrate this here.

Large-eddy simulation (LES) of turbulent flow has a long and rich history in which already during the 1960s first parameterizations, such as Smagorinsky's eddy-viscosity model Smagorinsky (1963) were proposed to capture the effects of localized turbulent motions on the large scales. The coarsening length-scale of choice was the mesh-size, often chosen as the cube-root of the volume of a grid cell Schumann (1975). However, the grid is often defined prior to any flow simulation and a direct, quantitative link between the grid-based length-scale and the actual local flow is not made. Moreover, while coarsening is helpful in reducing the computational effort, it also introduces uncertainty regarding the accuracy of the achieved results (Pope (2000); Geurts (2003)). We adopt the recent ILSA (Integral Length-Scale Approximation) proposal which is a first framework that can address LES error control systematically (Piomelli *et al.* (2015); Rouhi *et al.* (2016); Geurts *et al.* (2019)).

In this contribution we systematically look into the level of total error control achievable in turbulent mixing. The basic limitation in LES quality stems from an interplay between effects of discretization and modeling errors. A key concept in error control for LES is 'sub-filter activity' (Geurts & Fröhlich (2002)). The error behavior in LES has two simplifying limits. First, at low sub-filter activity the LES model contribution is small and fine grid resolution (proper for DNS) is required to remove the discretization error. The cost of such an academic limit may be unrealistic. Second, at high sub-filter activity (significant coarsening of the turbulent flow), one gains control over the computational cost, but looses direct influence on the achievable accuracy. In fact, a systematic error associated with the adopted sub-filter model is inherent in this limit. In practice, one seeks an intermediate value for the sub-filter activity that yields the optimal accuracy at fixed computational costs. We quantify the accuracy against filtered DNS and study the relation between 'achieved accuracy' and 'target value for sub-filter activity'. Keeping the sub-filter activity near a pre-specified target value, allows some control over the LES errors , and knowing what this target value implies for the total simulation error defines a deterministic 'uncertainty quantification' for LES. Investigating the relation between this target value and the reliability of the LES predictions is an items of ongoing research toward a genuine error bar for CFD.

In the context of LES, a study of the total simulation error implies consideration of effects (i) of numerical discretization errors, (ii) of the role of the sub-filter modeling error due to the sub-filter model and (iii) of the interaction between these two basic sources of error (Geurts (1999); Van der Bos *et al.* (2007)). Since the modeling and discretization errors can partially counteract each other it is not straightforward to assess the overall simulation error. Instead, one may resort to a computational assessment, known as the error-landscape approach (Meyers *et al.* (2003)). In a study of homogeneous isotropic turbulence using Smagorinsky's eddy-viscosity model, the error-landscape displays a clear minimal total error as function of spatial resolution N and model parameter, marking an 'optimal refinement strategy'. A computational estimate of the optimal Smagorinsky coefficient at given spatial resolution can be obtained at modest cost using the Successive Inverse Polynomial Interpolation (SIPI) method, (Geurts & Meyers (2006)). Since the dependence of the optimal coefficient on the spatial resolution is quite modest, one may proceed in two steps. First, at coarse resolution the optimal coefficient is determined. Subsequently, at finer resolution, production simulations can be executed with this optimal coarse grid value.

In the ILSA formulation (Piomelli *et al.* (2015)), the filter width Δ is a fraction of the local integral length-scale based on the resolved turbulent kinetic energy K_{res} and the total dissipation rate ε_{tot}. Another key ingredient in ILSA model is the model parameter C_k. In ILSA's original formulation (Piomelli *et al.* (2015)), C_k was adjusted using SIPI. In its local formulation, C_k is adjusted dynamically, consistent with a measure for explicit error control. For such a measure for the error several options can be considered - we focus on an invariant of the sub-filter stress tensor. An approach based on the concept of sub-filter activity (Geurts & Fröhlich (2002)) the appropriate model coefficient can be determined. In this contribution we sketch the details of the method next. Afterwards, we introduce the problem of turbulent mixing in a transitional and turbulent temporal mixing layer. Subsequently, we consider predictions of the evolution of the momentum thickness and compare ILSA predictions with filtered DNS results and findings based on other, well-known, sub-filter models. Concluding remarks are collected afterwards.

THE INTEGRAL LENGTH SCALE APPROACH

In this Section we briefly review the main components that make up the total simulation error in LES and discuss the possible error-cancellation implying that the total simulation error may not simply be the sum of the absolute values of modeling and discretization errors (Geurts, 1999; Geurts 2002). 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. We consider incompressible flows, governed by conservation of mass and momentum respectively,

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

where the overbar denotes the filtered variable. Here, we adopt Einstein's summation convention and use p for the pressure and u for the velocity field. Time is denoted by t and partial differentiation with respect to the j-th coordinate by the subscript j. Relevant length- (λ) and velocity (U) scales, and constant kinematic viscosity (ν) are used to non-dimensionalize the equations and define the Reynolds number $Re = U\lambda/\nu$. 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. In this paper we restrict ourselves to eddy-viscosity models, in which the anisotropic part of sub-filter stress tensor is given by $\tau^a_{ij} = -2\nu_{sfs}\overline{S}_{ij}$, where $\overline{S}_{ij}$ 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.

To define an eddy-viscosity ν_{sfs} we follow the standard proposition that $\nu_{sfs} \sim \ell^2|\overline{S}|$ in which $|\overline{S}|$ is the sized of the filtered strain-rate tensor and ℓ a suitable length-scale. We review the length-scale definition ℓ for LES based on the resolved turbulent kinetic energy (TKE) and the dissipation rate of total TKE. 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 modeling the sub-filter scales. An important benefit of this distinction is the fact that by resolving the new length-scale on the computational grid, a smoothly varying filter width is generated that is consistent with the local flow state, independent of the grid topology (Rouhi *et al.* (2016); Lehmkuhl *et al.* (2019)). Additionally, with this grid-independent filter width, grid convergence study is feasible, allowing to discriminate between discretization and sub-filter modeling contributions to the overall error.

The global ILSA model is an eddy-viscosity model in which the anisotropic part of the sub-filter stress tensor is given by with turbulent eddy-viscosity defined as

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

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

$$L = \frac{\langle K_{res} \rangle^{3/2}}{\langle \varepsilon_{tot} \rangle}$$

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

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

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 (Piomelli *et al.* (2015)), as long as more than 80% of TKE is resolved (Pope (2000)) Pope (2000). 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., $L/h \gg 1$. 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 (Boersma et al., 1997).

Aside from the local integral length-scale L, a key ingredient of the ILSA model is that adaptations in the effective model coefficient are made consistent with a measure toward explicit LES resolution control. This way, the effective model coefficient C_k should be obtained in response to the flow characteristics. For this purpose the concept of sub-filter activity (Geurts & Frhlich, 2002) is used. We exploit the local formulation of ILSA in which the spatially and temporally non-uniform C_k can be found based on invariants of the sub-filter stresses directly. We introduce

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

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 for the anisotropic sub-filter tensor $\tau_{ij}^a = -2\nu_{sfs}S_{ij}$ with $\nu_{sfs} = (C_k L)^2|\overline{S}|$. The key innovation of ILSA is in the fact that the user may specify the level of LES resolution in terms of the sub-filter activity s_τ. Extensive studies have been conducted into turbulent channel flow and turbulent flow over a backward-facing step (Rouhi *et al.* (2016)). Recently, the model has also been applied to more complex flows, including separating boundary layers ((Wu & Piomelli (2018)), a sphere, and the Ahmed body (Lehmkuhl *et al.* (2019)). Most of these studies involve fully developed turbulence; a notable exception is the simulation of the flow over the sphere, in which the boundary layer is laminar, and the flow transitions to turbulence in the separated shear layer. In this case the model was shown to have the correct behavior: the eddy viscosity vanished where the flow was laminar, and only developed once turbulence was established. In the laminar-flow region the integral length scale of turbulence was zero, as expected, so that the ratio L/h was not larger than unity, as the model requires. However, at appropriate resolution, the laminar flow can be well captured at zero eddy viscosity. To understand better the behavior of the ILSA model during laminar-to-turbulent transition, here we consider a time-evolving flow in a temporal mixing layer that starts from a laminar initial state and develops into turbulence in the course of time. This flow problem is discussed next.

TURBULENT MIXING - TRANSITIONAL AND TURBULENT FLOW

To assess the quality of ILSA for turbulent mixing we consider the classical model of a temporal mixing (Vreman *et al.* (1997)). In a rectangular domain of $L_x \times L_y \times L_z$ a tanh-profile is adopted for the streamwise velocity u as function of y and zero velocity in the y and z directions. Periodic conditions are assumed in the x and z directions, while a free-slip condition is applied at the boundaries in the y direction. Apart from the initial mean velocity, also a combination of linear stability eigenfunctions is added to trigger a fast transition to a developed turbulent flow.

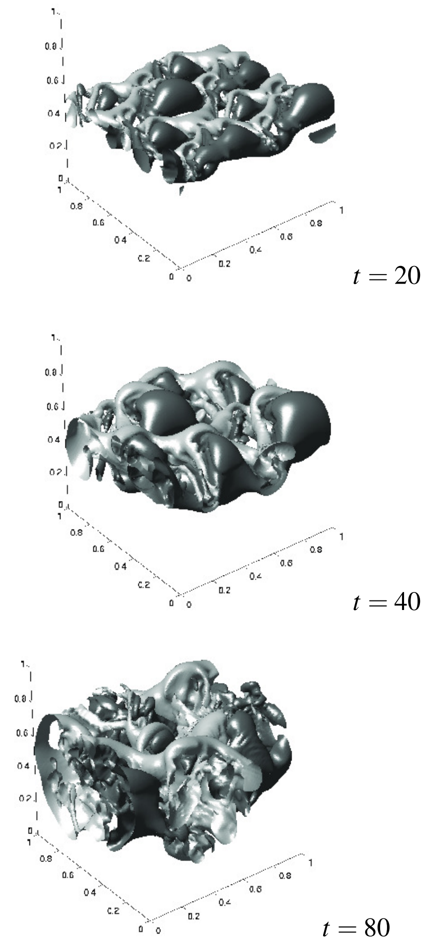

Figure 1. Snapshots of the vertical velocity in a 'temporal' mixing layer at a Reynolds number of 50. The light (dark)contours correspond with upward (downward) flow.

Adopting a Reynolds number of 50, based on the initial momentum thickness, the flow can be simulated in full detail using a grid of 256^3 cells and a central second order, conservative finite volume spatial discretization. Three snapshots of the vertical velocity at $t = 20,\ 40$ and 80 are shown in Figure 1. Initially, the roll-up of spanwise roller structures dominates the flow, showing somewhat parallel structures. These spanwise rollers grow and by $t = 40$ show have well saturated and give rise to a subsequent self-similar development of the mixing layer in which, e.g., the momentum thickness of the mixing layer increases linearly in time.

ASSESSMENT OF ILSA FOR TURBULENT MIXING

Mixing processes play an important role in a multitude of technologies. A characteristic model for a 'mixing layer' can be obtained experimentally by bringing together two parallel streams of fluid, each with its own velocity. As a consequence of the velocity differences on the upper and lower side of the so-called splitter-plate, shear stresses emerge where the two flows join. Fluid from the lower layer is transported to the upper layer and vise versa, giving rise to an effective turbulent mixing near the center of the mixing layer. This flow is often modeled in a simpler temporal setting (Vreman *et al.* (1997)). The temporal flow captures the main physics of the mixing as is illustrated in figure 1. The configuration is a box with periodic boundary condition in the streamwise and spanwise directions and free-slip condition at the top and bottom boundaries.

A key quantity of interest is the momentum thickness. Extensive simulations have been conducted to compare different LES predictions with filtered DNS findings. For the LES 32^3 grid points were used. In Figure 2 we show a comparison of filtered DNS data against a range of well-known sub-filter models. This flow configuration offers full assessment of dynamic error control in ILSA as will be presented in the full paper.

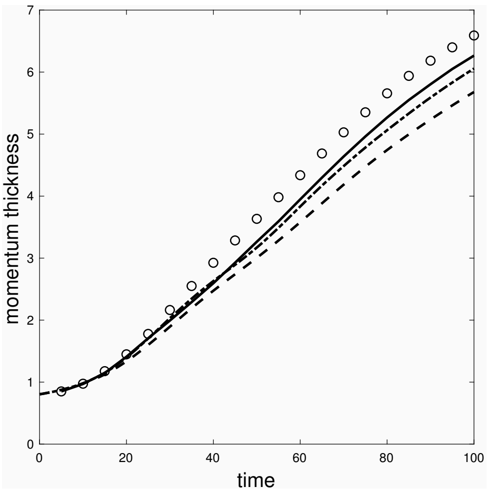

Figure 2. Momentum thickness predicted by: filtered DNS (marker o), ILSA (solid), dynamic eddy-viscosity (dashed), Leray (dash-dotted).

CONCLUDING REMARKS

We investigated the reliability of LES predictions for transitional and turbulent mixing in a temporal mixing layer. The basic limitation in LES quality stems from an interplay between effects of discretization errors and modeling error. A key concept used for dynamic error control for LES in this paper is the 'sub-filter activity'. This measures the dynamic relevance of scales that were removed from the dynamics through spatial filtering. Depending on whether 'a lot' of small scales were removed during coarsening or not, the main source of total simulation error may vary from that of being dominated by sub-filter modeling error to that of being dominated by spatial discretization error. 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 these dominant LES errors.

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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