Quality and Reliability of Large-Eddy Simulations

ERCOFTAC SERIES

VOLUME 12

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ISBN: 978-1-4020-8577-2 e-ISBN: 978-1-4020-8578-9

Library of Congress Control Number: 2008927470

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Printed on acid-free paper

9 8 7 6 5 4 3 2 1

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Preface

Computational resources have developed to the level that, for the first time, it is becoming possible to apply large-eddy simulation (LES) to turbulent flow problems of realistic complexity. Many examples can be found in technology and in a variety of natural flows. This puts issues related to assessing, assuring, and predicting the quality of LES into the spotlight. Several LES studies have been published in the past, demonstrating a high level of accuracy with which turbulent flow predictions can be attained, without having to resort to the excessive requirements on computational resources imposed by direct numerical simulations (see, e.g., [1]). This is also corroborated in the current volume, which contains the proceedings of the first QLES meeting on Quality and Reliability of Large-Eddy Simulation, held October 22–24, 2007 in Leuven (QLES07).

The setup and use of turbulent flow simulations requires a profound knowledge of fluid mechanics, numerical techniques, and the application under consideration. The susceptibility of large-eddy simulations to errors in modelling, in numerics, and in the treatment of boundary conditions, can be quite large due to nonlinear accumulation of different contributions over time, leading to an intricate and unpredictable situation. A full understanding of the interacting error dynamics in large-eddy simulations is still lacking. To ensure the reliability of large-eddy simulations for a wide range of industrial users, the development of clear standards for the evaluation, prediction, and control of simulation errors in LES is summoned. The workshop on Quality and Reliability of Large-Eddy Simulations (QLES2007) provided one of the first platforms specifically addressing these aspects of LES. Its main objective was to address fundamental aspects of the LES-quality issue by bringing together mathematicians, physicists, and engineers, thereby confronting entirely different approaches to the subject, doing justice to the complexity of this field. The problem of treating one flow problem correctly is easily an order of magnitude more challenging than the feasibility problem of doing one simulation at all. The latter illustrates the state-of-the-art in LES of a decade ago, while the former represents a more timely challenge.

One of the main difficulties arising in the evaluation of errors in large-eddy simulation, is the nonlinear accumulation of different error sources. Most notorious is the possible interaction between subgrid-scale modelling errors and numerical errors [9, 33]. A problem which is not so well recognized, is the fact that there is no consensus on the definition of errors among researchers. Moreover, differing views exist on the role of the subgrid-scale model relative to that of the numerics in LES. Obviously, such differences handicap the exchange of ideas on accuracy and reliability of LES. These elements will be addressed in some more detail next, to provide an introduction to the current volume.

In early large-eddy simulations, subgrid-scale models were nothing more than a numerical stabilization mechanism [29], regularizing the coarse-mesh solution of the Navier–Stokes equations. Later (see, e.g. [18, 17]) a physical interpretation was linked to the subgrid-scale model, based on the formal application of a low-pass filter to the Navier–Stokes equations. In particular, attention was given to an analysis of the exchange of energy between so-called resolved and unresolved scales, corresponding roughly to scales larger or smaller than the width of the presumed spatial filter, respectively. In modern-day LES, both approaches still exist, i.e., numerical stabilization of the Navier–Stokes equations versus a physics-based subgrid-scale model.

Many examples exist of physics-based models, such as the Lilly–Smagorinsky model [18], backscatter models [22], VMS-Smagorinsky models [12], and several of their variants [28, 32, 25, 31, 13, 26]. Mathematically, these models are used to close the low-pass filtered Navier–Stokes equations. Hence, a natural point of reference for the definition of errors are the low-pass filtered results from either direct numerical simulations or experiments [34]. In such a framework, it was realized early on that, apart from subgrid modelling issues, also numerical discretization was central for the quality of LES [20]. In Mansour's approach [20], a spectral cut-off filter is considered, and spectral discretization is used as a point of reference for the quality of a numerical discretization scheme. In this context, Ghosal [9] pointed out that discretization and modelling errors are of the same order of magnitude, and further work along these lines was presented in [4, 3]. In a different approach to numerical errors Mason [21] proposed to increase the ratio of the filter scale to the grid size Δ/h. At high values of Δ/h, any consistent numerical discretization will converge to a grid-independent solution. Using this framework to define discretization and modelling error, Vreman, Geurts & Kuerten [33] showed a strong interaction between both error sources when $\Delta = h$. In this context, it was also shown that $\Delta/h > 1$ does not necessarily guarantee a reduction in total errors [33, 7, 23]. From a computational-cost point of view, both $\Delta/h > 1$ and higher order numerics are expensive, and avoided in most large-scale computations of realistic applications. In addition, recent research seems to suggest that low-order schemes and $\Delta/h = 1$ may be beneficial to the global simulation error at coarse resolutions [24].

In an alternative approach to LES one may introduce a direct regularization of the Navier–Stokes equations. In this case a change is made to the dynamical properties of the equations, such that they can be accurately solved at a much coarser mesh than DNS. Such an alteration can be performed on the level of the continuous equations, e.g., addressing the convective nonlinearity, as is done in Leray regularization [8, 16], in the NS-α model [5], or in the ADM approach [30, 15]. Alternatively, it has been suggested that this 'regularization' may be absorbed into the discretization scheme; examples are the spectral vanishing viscosity method [14], MILES [6], and several others [11, 10]. In contrast to the classical subgrid-scale model approach described above, in a numerical stabilization approach, no explicit distinction is made between numerical errors and modelling errors. This is a cause of deep methodological disagreements among different LES practitioners – an element that re-appears in several of the contributions.

We believe that the main challenge for LES today is not lying anymore in the development of new modelling or regularization approaches. Aside from the important, unresolved problem of LES and high-Re boundary layers, most of these techniques produce very satisfactory results when used appropriately. Rather, a main challenge is in the development of a transparent standard which helps practitioners in the correct use of LES. A fully consistent theory on errors in LES still requires a huge amount of work. While empirical qualitative comparisons with reference data have been used for decades to conclude on possible improvements in the numerics and physical closures, a mathematically grounded quantitative error measure, like the one proposed by Hoffman, is certainly needed. The definition of such an error measure is a tricky issue, since it appears that in some flows the error can evolve in an counter-intuitive way [33, 27]. A related issue is LES sensitivity: how sensitive is a given LES result to computational setup parameters? A reliable simulation must be stable, in the sense that a small variation of the setup parameters should not yield a dramatic change in the quality of the results. Here again, only very few results are available, and advanced mathematical tools are required (e.g. [19]).

For Reynolds-averaged Navier–Stokes simulations, which are nowadays commonly used in industry, advice on best practise is well known, e.g., ERCOFTAC's Best practice guidelines [2]. Certainly, such an exercise would also be extremely useful for LES. This motivated a concerted effort to arrive at 'Best practice for LES' as identified as a central target of the COST Action 'LESAID', that started in 2006. However, for LES more should be possible: not only guidelines for good quality, but also a 'first-principles' framework may be feasible, in which the quality of LES is guaranteed. It was this context which motivated the organization of a dedicated workshop on quality and reliability of LES. Different contributions were grouped into four sessions. This is also reflected in the current book, which is divided into four parts, i.e., (1) Numerical and mathematical analysis of subgrid-scale-model and discretization errors,

(2) Computational error-assessment, (3) Modelling and error-assessment of near-wall flows, (4) Error assessment in complex applications.

For the organization we relied considerably on the members of the scientific committee: N. A. Adams (Technische Universität München, Germany), M. Baelmans (Katholieke Universiteit Leuven, Belgium), A. Boguslawski (Politechnika Czestochowska, Poland), D. Carati (Université Libre de Bruxelles, Belgium), E. Dick (Universiteit Gent, Belgium), D. Drikakis (Cranfield University, United Kingdom), A. G. Hutton (QinetiQ, United Kingdom), J. Jiménez (Universidad Politecnica Madrid, Spain), M. V. Salvetti (Università di Pisa, Italy), and G. S. Winckelmans (Université Catholique de Louvain, Belgium). We gratefully acknowledge their help.

The workshop on quality and reliability of large-eddy simulations was supported financially by a number of institutions. On a European scale, support was provided by COST Action P20 'LESAID' (LES – Advanced Industrial Design) and ERCOFTAC (European Research Community on Flow, Turbulence and Combustion). At the Belgian level, financial support was provided by the Research Foundation – Flanders (FWO – Vlaanderen), and by the research council of the K.U.Leuven. This support was crucial to the organization of this workshop and is gratefully acknowledged.

Leuven,
January 2008

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