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Verified predictions of shape sensitivities in wall-bounded turbulent flows by an adaptive finite-element method

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ABSTRACT

A Continuous Sensitivity Equation (CSE) method is presented for shape parameters in turbulent wall-bounded flows modeled with the standard k–ϵ turbulence model with wall functions. Differentiation of boundary conditions and their complex dependencies on shape parameters, including the two-velocity scale wall functions, is presented in details along with the appropriate methodology required for the CSE method. To ensure accuracy, grid convergence and to reduce computational time, an adaptive finite-element method driven by asymptotically exact error estimations is used. The adaptive process is controlled by error estimates on both flow and sensitivity solutions. Firstly, the proposed approach is applied on a problem with a closed-form solution, derived using the Method of the Manufactured Solution to perform Code Verification. Results from adaptive grid refinement studies show Verification of flow and sensitivity solvers, error estimators and the adaptive strategy. Secondly, we consider turbulent flows around a square cross-section cylinder in proximity of a solid wall. We examine the quality of the numerical solutions by performing Solution Verification and Validation. Then, Sensitivity Analysis of these turbulent flows is performed to investigate the ability of the method to deal with non-trivial geometrical changes. Sensitivity information is used to estimate uncertainties in the flow solution caused by uncertainties in the shape parameter and to perform fast evaluation of flows on nearby configurations.

1. Introduction

Sensitivity Analysis (SA) has been the topic of active research for many years because of its numerous industrial applications. In design optimization, it refers to the gradient of the cost functions with respect to design variables which can be efficiently obtained through adjoint methods. In a more general framework, sensitivities are the derivatives of the dependent variables with respect to any (physical or numerical) parameter. They are more general in the sense that the derivatives of cost functions can be deduced from the sensitivities of dependent variables; the reciprocal being false. We refer to them as *flow sensitivities*. The body of work on SA has shown that it provides improved insights into the physic of complex problems and allows for a better understanding of them.

Irrespective of the approach employed, computing sensitivities is more involved for parameters that influence the problem through the modification of its geometry. They are referred to as *shape parameters* as opposed to *value parameters*. Indeed, a number of difficulties arises when considering shape parameters both from the theoretical and the practical side that will be discussed in what follows.

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There are several approaches for computing sensitivities: (1) Finite Differences (FD); (2) Complex Variable Method (CVM); and (3) Sensitivity Equation Methods (SEM). The first option requires only evaluations of dependent variables and computes their derivatives by finite differences. This simple approach requires minimal additional development. However, it is costly because the problem at hand must be solved at least as many times as there are parameters. Furthermore, numerical evaluations of sensitivities of pointwise quantities is often difficult because of technical problems arising from non-matching meshes. However, the main disadvantage of this approach is that the calculation of derivatives may suffer from subtractive cancellation errors leading to large errors in the evaluations if the parameter perturbations are too small. This approach is often used as a verification tool for the other methodologies (see e.g. [1–3]).

The CVM is similar to the FD idea with the exception that a complex perturbation is taken. The key improvement is that computed derivatives are not affected by round-off errors [4]. However, the CVM does not offer a saving of resources when compared to using FD [5] since the problem must be solved at a perturbed state for each parameter. Furthermore, the required memory for the solver essentially doubles due to the use of complex declarations of floating point variables (the CPU time of the original solver is also increased by a significant factor).

The last option is provided by the SEM which corresponds to numerically solving a set of equations for the sensitivities. These equations are obtained by differentiation of the (discrete or continuous) equations for the dependent variables. Since they are always linear, the SEM always compute a sensitivity for a fraction of the cost of computing the flow making these methodologies very attractive. In the Continuous Sensitivity Equation (CSE) approach, the governing equations are first differentiated and then discretized, whereas in the Discrete Sensitivity Equation (DSE) approach, discretization is performed prior to differentiation. The advantages of each methodology and their differences have been extensively discussed in the literature (see e.g. [6,7]). One of the main advantages of the DSE approach is that it can be handled through Automatic Differentiation (AD). It is a powerful approach because the code for calculating sensitivities is almost automatically generated from the code for computing dependent variables. Yet, in many cases, implementation requires user interventions to ensure efficiency of the resulting sensitivity code both in terms of accuracy and CPU time. See [8–10] for more details on AD and on the most common softwares. One of the main advantage of the CSE method is that it avoids the differentiation of non-differentiable terms arising from discretization schemes such as limiters, blending functions or stabilization terms (since differentiation is performed on the continuous flow equations). Furthermore, the continuous approach offers more flexibility at the discretization stage. Here, we present a CSE approach.

When a shape parameter a is considered, independent variables (say $\mathbf{x}$) depend on a. Dependent variables (say $\mathbf{u}$) always depend both on $\mathbf{x}$ and $a : \mathbf{u}(\mathbf{x}, a)$. Hence, for a shape parameter, one can consider either the *Eulerian* sensitivity $\partial\mathbf{u}/\partial a$ (partial derivative of $\mathbf{u}$ with respect to a) or the *Lagrangian* sensitivity $D\mathbf{u}/Da$ (total derivative of $\mathbf{u}$ with respect to a). The major difficulty in using Lagrangian sensitivities is the requirement to define and manage the domain deformation induced by the boundary displacement when the parameter changes (the definition being non-unique). Eulerian sensitivities avoid this delicate issue but special attention must be paid when deriving and evaluating boundary conditions. It is worth noting that the DSE methods presented in the literature all use Lagrangian sensitivities which lead to the need for evaluating mesh sensitivities. This requires the delicate issue of differentiating the mesh generation code or mesh deformation procedure which is both involved and computationally demanding. To circumvent these difficulties, we propose the use of the Eulerian sensitivities and present a suitable methodology for handling boundary conditions for the corresponding Sensitivity Equations in turbulent flow problems. Moreover, this approach simplifies the use of adaptive grid methods which have proved to be extremely powerful for achieving mesh independent solutions of complex problems [11,12].

In Computational Fluid Mechanics (CFD), there is a wealth of publication on SEM for laminar flows (see e.g. Refs. [13,6,14–18,3]). However, the situation is quite different for the case of turbulent flows for which there is a paucity of literature. The additional equations for turbulence modeling greatly increase the level of complexity of the system of PDE and its discretization. The DSE approach has been applied to turbulent flows and value parameters using AD in Refs. [19,20] and to shape parameters using hand-differentiation in Refs. [21,22]. The CSE method for turbulent flows and value parameters is presented in Refs. [23–25]. To the authors' knowledge, this work is the first attempt to derive a CSE method for turbulent flows and shape parameters.

To this end, wall-bounded turbulent flows are modeled with the RANS equations and the standard k–ϵ turbulence model with wall functions using two velocity scales. The CSE are obtained by direct differentiation of this set of PDE and their associated boundary conditions. There are two major challenges when treating shape parameters. The first difficulty arises from the differentiation of wall functions which is not straightforward due to their complex shape parameter dependencies. For example, the boundary condition for the flow in the tangential direction is prescribed as a function of the tangential velocity (mixed or Robin boundary condition). Secondly, it leads to a difficult requirement: the accurate evaluation of the first and second-order derivatives of the velocity at the boundary. Duvigneau and Pelletier [26] have recently proposed a constrained Taylor-series least-squares procedure to achieve accurate boundary gradients for laminar flows. For this work, we extend the constrained Taylor-series least-squares procedure to wall-bounded turbulent flows (see Section 5.4).

The accurate evaluation of flow and shape sensitivity solutions of wall bounded turbulent problems is a tedious task. Indeed, the flow exhibits features whose strength and location are difficult to capture. They are also hard to predict *a priori* so that a good mesh is difficult to design *ab initio*. This difficulty is compounded when sensitivity variables are added because their features are less intuitive than that of the flow variables. Furthermore, the transpiration terms in their boundary conditions result in very thin regions where sensitivity variables exhibit sharp variations. And, when considering several design parameters, each sensitivity has its own region of rapid variations. Hence, their successful computation requires appropriate