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On the proper treatment of grid sensitivities in continuous adjoint methods for shape optimization

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A B S T R A C T

The continuous adjoint method for shape optimization problems, in flows governed by the Navier–Stokes equations, can be formulated in two different ways, each of which leads to a different expression for the sensitivity derivatives of the objective function with respect to the control variables. The first formulation leads to an expression including only boundary integrals; it, thus, has low computational cost but, when used with coarse grids, its accuracy becomes questionable. The second formulation comprises a sum of boundary and field integrals; due to the field integrals, it has noticeably higher computational cost, obtaining though higher accuracy. In this paper, the equivalence of the two formulations is revisited from the mathematical and, particularly, the numerical point of view. Internal and external aerodynamics cases, in which the objective function is either the total pressure losses or the force exerted on a solid body, are examined and differences in the computed gradients are discussed. After identifying the reason behind these discrepancies, the adjoint formulation is enhanced by the adjoint to a (hypothetical) grid displacement model and the new approach is proved to reproduce the accuracy of the second adjoint formulation while maintaining the low cost of the first one.

1. Introduction – state of purpose

Based on the literature, the continuous adjoint method can be formulated following two different approaches. Both result to the same adjoint field equations and boundary conditions, with, however, two distinct expressions for the sensitivity derivatives (SD) of the objective function J with respect to (w.r.t.) the design variables $\vec{b}$. The first published formulation, [1], led to SD expressions including field integrals (*FI*) of the variations in the coordinates $\vec{x}$ w.r.t. $\vec{b}$, the so-called grid, or mesh, sensitivities. These formulations, to be referred to as *FI*, are costly due to integrating over the entire domain and the need of computing $\delta\vec{x}/\delta\vec{b}$; computing them using finite differences (FD), leads to computational cost that scales linearly with the number of design variables, needing two grid displacement PDEs solutions per design variable. The cost of solving the, usually elliptic, grid displacement PDEs so many times dominates the time needed for the computation of the sensitivity derivatives, after solving the primal and adjoint equations.

Later, following a paper by Anderson, [2], for incompressible flows and another one by Jameson, [3], for compressible ones, the so-called "reduced gradient" formulations, which led to SD expressions including only surface integrals (*SI*), be-

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came very popular. As an extension to the aforementioned work by Jameson, which was restricted to structured grids, it was proved in [4] that the same formulation is also valid for any grid type, so it can be used on unstructured grids as well. In the present paper, any formulation of the continuous adjoint method that excludes field integrals from the SD expression will be referred to as *SI*.

For a given shape parameterization with a moderate number of design variables, the cost of *FI* is higher than that of *SI*, but it might still be affordable. If the adjoint method is used to compute sensitivity maps (such as the derivatives of J w.r.t. the normal displacements of hundreds of thousands of grid points on the body surface), the cost of the *FI* approach becomes definitely prohibitive. The problem becomes much more pronounced in unsteady adjoint solvers, [5,6], in which, for a time-averaged objective function, the SD computation must be repeated for each and every time-step. In the same problem, the cost of *SI* is still negligible.

Despite the perfect mathematical equivalence of the *SI* and *FI* formulations, see Sections 2 and 3, according to the authors' experience, if the grid used is not sufficiently fine, inaccuracies in the *SI* computed SD may appear. This may happen even in cases in which the grid is adequately fine to solve the flow equations with acceptable accuracy. Representative cases in which these inaccuracies appear are presented and discussed in Section 3. This issue has already been reported in some papers, [2,7,8].

In view of the above, this paper proposes a new continuous adjoint formulation which leads to SD expressions depending only on surface integrals (it, thus, shares the advantages of the *SI* formulation) while alleviating the accuracy issue. In other words, the proposed enhanced *SI* (E-*SI*) formulation is as fast as the standard *SI* and as accurate as the *FI* one.

In Section 2, the general formulation of the continuous adjoint method is presented. Both the *SI* and *FI* formulations are discussed and proved to be mathematically equivalent. Then, in Section 3, using some selected test problems, SD computed with both formulations are compared and it is observed that discrepancies occasionally appear. To identify the reason of the aforementioned discrepancies, a term-by-term comparison of the different SD expressions follows; the mathematical analysis is confirmed by numerical tests. Though the mathematical analysis is presented for laminar flows only, numerical results include both laminar and turbulent flows. For the latter, the adjoint to the turbulence model PDEs are additionally solved. Two different turbulence models are used, so as to convince the reader that the problem is not related to any specific turbulence model. From the results presented in Section 3, it becomes clear that a term derived from the use of the Leibniz theorem for integral variations is responsible for the contributing effect of grid sensitivities when the *SI* formulation is used. Usually this Leibniz term is ignored; the reason for this omission along with its implications are explained in detail in Section 3. Because the Leibniz term is difficult to compute with accuracy, an alternative expression, based on field integrals of the coordinate variations, is identified. To avoid computing such a numerically costly term, an enhanced continuous adjoint formulation is presented in Section 4, where hypothetical grid displacement PDEs[1] are included in the augmented objective function. This formulation leads to the adjoint grid displacement PDEs, whose solution cost is negligible, and yields an SD expression including only surface integrals. In other words, the proposed E-*SI* formulation leads to accurate objective function gradients, computed using only surface integrals and has the same cost as the standard *SI* formulation.

The novelties of the present paper are briefly summarized below:

- The continuous adjoint method for shape optimization problems including a generic grid displacement PDE model is absolutely new in the literature.
- The major source of inaccuracies in the continuous adjoint method is identified and an adjoint formulation yielding gradients free of field integrals of the grid sensitivities is presented, thoroughly discussed and demonstrated on test problems. To the authors knowledge, there is no other paper on continuous adjoint for turbulent flows dealing with this problem. Only a couple of them mention the problem, [2,7], in laminar and inviscid flows, and discuss this issue without providing a solution based on a purely continuous adjoint approach. It is worth mentioning that in [2], a hybrid discrete–continuous adjoint method has been proposed to take the grid sensitivities into account; this alleviates the accuracy issue but the cost of computing them scales with the number of design variables. In this context, the solution is considered to be capable of computing accurate sensitivities with a computing cost that doesn't scale with the number of design variables.

2. Continuous adjoint formulations – an overview

2.1. General continuous adjoint formulations

Assume an optimization problem, expressed by the objective function J to be minimized, controlled by the design variables b_n $(n = 1, \dots, N)$ and constrained by the state equations $R_i = 0$ $(i = 1, \dots, E$, where E is the number of equations). The formulation of the continuous adjoint method starts by defining the augmented objective function or Lagrangian

$$L = J + \int_{\Omega} \Psi_i R_i d\Omega \tag{1}$$

[1] During the development of continuous adjoint, referring to "grid" might be improper. However, the "grid displacement" terminology was adopted, since this is widely used in discrete adjoint literature.