Journal of Computational and Applied Mathematics 296 (2016) 334–351

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Shape derivatives for the compressible Navier–Stokes equations in variational form

Matthias Sonntag[a,*], Stephan Schmidt[b], Nicolas R. Gauger[a]

[a] Chair for Scientific Computing, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

[b] University of Würzburg, Emil-Fischer-Str. 30, 97074 Würzburg, Germany

ARTICLE INFO

Article history:
Received 6 February 2015
Received in revised form 30 July 2015

MSC:
49Q10
49Q12
65K10
76Nxx
76M30

Keywords:
Shape derivative
Variational form
Compressible Navier–Stokes equations

ABSTRACT

Shape optimization based on surface gradients and the Hadamard-form is considered for a compressible viscous fluid. Special attention is given to the difference between the "function composition" approach involving local shape derivatives and an alternate methodology based on the weak form of the state equation. The resulting gradient expressions are found to be equal only if the existence of a strong form solution is assumed. Surface shape derivatives based on both formulations are implemented within a Discontinuous Galerkin flow solver of variable order. The gradient expression stemming from the variational approach is found to give superior accuracy when compared to finite differences.

0. Introduction

Shape optimization is a research field that has received much attention in the past. In general, any problem where the boundary of the domain is part of the unknown can be considered a shape optimization problem. In most applications, the physics are modeled by partial differential equations, making shape optimization a special sub-class within the field of PDE-constrained optimization. Usually, the derivation of the sensitivities and adjoint equations follows a function composition approach, i.e. some set of design variables defines the geometry and within this geometry the PDE is solved, thereby generating the state variables that enter the objective function [1–3]. Therefore, the necessity to consider sensitivities or derivative information with respect to the geometry adds additional complexity to the shape optimization problem when compared to general PDE-constrained optimization. Because it is often not immediately clear how to compute these "mesh sensitivities", that is the variation of the PDE with respect to a change in the geometry, there is often a strong desire for a very smooth parameterization of the domain with as few design parameters as possible. Although there have been successful attempts to incorporate problem structure exploitations in order to efficiently compute these partial derivatives for very large problems, such as differentiating the entire design chain at once or by considering the adjoint process of the mesh deformation [4,5], very often one is still forced into finite differencing, which means the PDE residual at steady state has to be evaluated on meshes that have been perturbed by a variation in each design parameter of the shape, a process that makes large scale optimization usually prohibitive. This negates some of the advantages of the adjoint approach, such as

* Corresponding author.
E-mail addresses: matthias.sonntag@rhrk.uni-kl.de (M. Sonntag), stephan.schmidt@mathematik.uni-wuerzburg.de (S. Schmidt), nicolas.gauger@rhrk.uni-kl.de (N.R. Gauger).

http://dx.doi.org/10.1016/j.cam.2015.09.010
0377-0427/

the independence of the number of design parameters. More severely, it also makes fast optimization strategies such as the one-shot approach [6–8] somewhat unattractive in terms of wall-clock-time.

A more recent trend to overcome the cumbersome computation of these geometric sensitivities is the use of shape calculus. Shape calculus summarizes the mathematical framework used when considering problems where the shape is the unknown in the continuous setting. Manipulations in the tangent space of the unknown object can be used to circumvent any necessity of knowing discrete geometric sensitivities, because these can be directly included in a surface gradient expression on the continuous level. More details on this theoretical framework can be found in [9,10]. Traditionally, this methodology was primarily used to address the very difficult question of existence and uniqueness of optimal shapes [11], but more recently this methodology has also been used in very large scale aerodynamic design and computational optimization [12–14]. In [15], for example, the complete optimization of a blended wing–body aircraft in a compressible inviscid fluid is considered. Because this approach solely relies on the problem formulation in the continuous setting and only afterwards discretizes the continuous boundary integral expressions for the shape derivative, great care must be taken when making the initial assumptions and when implementing the respective continuous expressions, especially at singular points in the geometry, such as the trailing edge of an airfoil [16]. Because this approach is indeed truly independent of the number of design parameters, it enables the most detailed possible parameterization, that is using all surface mesh nodes as design unknowns. This is sometimes called "free node parameterization". However, these highly detailed shape parameterizations usually lack any kind of inherent regularity preservation and as such, one usually finds this approach paired with some sort of smoothing procedure that projects or embeds the respective optimization iterations into a desired regularity class, which can nicely be paired with an SQP or Newton-type optimization scheme, which is sometimes also called a "Sobolev Method" [17,18].

As part of this work, we study how to further increase the accuracy of shape derivatives when used within viscous compressible aerodynamic design optimization. Within applied aerodynamic shape optimization, it is customary to exploit the above mentioned function composition approach in order to derive and implement the adjoint equation and gradient expression. This has been used with great success, both within the context of continuous and discrete adjoint based aerodynamic shape optimization [19,20,13,21] and general shape optimization [22]. However, common to these approaches is the assumption that the state equation has a strong form solution and each of the steps within the shape differentiation process of the function composition exists, which usually means the existence of so-called local shape derivatives. For elliptic problems, this existence can usually be shown, making the above mentioned approach somewhat of an established procedure, see for example Chapter 3.3 in [10]. However, for the hyperbolic equations governing some compressible fluids, the existence of a strong form solution is not clear. Rather, in the presence of shock waves and discontinuities in the flow, one can usually only expect the variational form of the equation to hold, a property which is very often not taken into account when studying the derivative. Shape differentiation of problems governed by PDEs in weak or variational forms are not very often considered in the literature, except in [23] and especially in [24], where the incompressible Navier–Stokes equations are considered for this purpose from a rigorous theoretical standpoint. Thus, we revisit the shape optimization problem previously considered in [25], but the gradient is derived using elements of the variational approach as shown in [24]. Furthermore, we simultaneously follow the function composition approach, outlining the exact differences comparing these two approaches. One can nicely see how both methodologies reduce to the same gradient expression when assuming the existence of a strong from solution of the state equation. We conclude with a numerical error analysis based on comparing finite differencing with either implementation, demonstrating the higher accuracy of the gradient formulation based on the variational form of the compressible Navier–Stokes equations.

The structure of the paper is as follows. In Section 1, we begin by recapitulating the compressible Navier–Stokes equations in both strong and variational form. Next, Section 2 serves as an introduction and quick overview of shape calculus, including shape derivatives and the Hadamard or Hadamard–Zolésio Structure Theorem, which leads to a preliminary form of the shape derivative of the aerodynamic cost functions. The next section, Section 3, is used to work out the differences between the shape derivative of the compressible Navier–Stokes equations stemming from either the function composition or the variational approach. In Section 4, we then summarize the idea of adjoint calculus. This is used to differentiate the Navier–Stokes equations, thereby discussing the Hadamard form of the respective objective functions both for the strong as well as the variational form of the state constraint. Finally, in the last section, numerical results achieved with both methods are compared to shape derivatives computed by finite differences, showing a considerable gain in accuracy when using shape derivatives based on the variational form.

1. Fluid mechanics

1.1. Flow domain and boundary conditions

In the following ρ, $v = (v_1, v_2)^\top$, p, E and T denote the density, velocity, pressure, total energy and temperature. The domain of the fluid is denoted by Ω, with wall and far-field boundaries Γ_W and Γ_∞. At the wall Γ_W, the no-slip boundary condition $v = 0$ is imposed for the velocity. With respect to temperature, either the isothermal boundary condition $T = T_W$ or the adiabatic boundary condition $\nabla T \cdot n = 0$ holds. The isothermal and adiabatic parts of the wall are named Γ_{iso} and Γ_{adia} and we assume $\Gamma_W = \Gamma_{iso} \cup \Gamma_{adia}$ disjoint.