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Variational sensitivity analysis and design optimization

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ABSTRACT

Variational method (VM) is employed to derive the co-state equations, boundary (transversality) conditions, and functional sensitivity derivatives. The converged solutions of the state equations together with the steady state solution of the co-state equations are integrated along the domain boundary to uniquely determine the functional sensitivity derivatives with respect to the design function. The application of the variational method to aerodynamic shape optimization problems is demonstrated on internal flow problems at supersonic Mach number range of 1.5. Optimization results for flows with and without shock phenomena are presented. The study shows that while maintaining the accuracy of aerodynamical objective function and constraint within the reasonable range for engineering prediction purposes, variational method provides a substantial gain in computational efficiency, i.e., computer time and memory, when compared with the finite difference computations.

1. Introduction

1.1. Variational sensitivity analysis

The new emerging sensitivity analysis technique for gradient-based optimization method is the continuous or variational sensitivity analysis. From a modified functional, variational method derives a set of partial differential equations, i.e., the co-state equations with their boundary conditions and the sensitivity derivatives. In computing the sensitivity derivatives with respect to the control points or design variables, this methodology utilizes the converged solutions of the state and co-state equations.

In recent years, variational sensitivity analysis has significantly contributed to the progress of aerodynamic design optimization. Pironneau [1] showed the usefulness of variational approach in fluid mechanical problems by illustrating how to compute the minimum drag profile in two-dimensional viscous and laminar flows. Chen and Seinfeld [2] developed a methodology to compute the performance sensitivity derivatives using optimal control theory. Koda et al. [3] used this procedure to solve atmospheric diffusion problems. Koda [4–6] further developed this approach and outlined a numerical algorithm for the computation of functional derivatives. Meric [7,8] treated optimal control problems governed by parabolic and elliptic partial differential equations and solved them numerically using variational method. In their effort to compare the gradients obtained by "implicit" and "variational" approaches, Shubin and Frank [9] implemented VM to optimize the shape of a nozzle of a variable cross-sectional area for steady one-dimensional Euler equations. Jameson [10] regarded the boundary of the flow domain as a control parameter and then designed airfoils using the potential as well as the two- and three-dimensional compressible inviscid flows. Cabuk and Modi [11] implemented a perturbation method to compute the optimum profile of a diffuser for a maximum static pressure in a two-dimensional steady viscous incompressible flow. Ta'asan et al. [12] have successfully implemented variational method and optimized an airfoil in the potential flow field. Ibrahim and Baysal [13] demonstrated the versatility of the variational method to solve aerodynamical design problems for internal flows in different Mach number regimes including shock flows. Following the same approach as Jameson [10], Reuther and Jameson [14] optimized airfoils in potential flows. Iollo and Salas [15] used variational method to solve a two-dimensional internal flow optimization problem with embedded shock to match a pressure distribution. References [17,28–30,33,34] applied variants of discrete sensitivity approaches to optimize engineering problems. Epstein and Peigin [26] used Genetic Algorithm to optimize three-dimensional lifting surfaces for wing-body aircraft configuration. In all these classes of optimization, the functional sensitivity derivatives are directly coupled to the solution of a set of linear partial differential equations, i.e., the co-state equations and their boundary conditions that result from the variation of the augmented Lagrangian function [27,31,32]. The success of any optimization by this approach is, therefore, destined to a stable and converged solution of the state and co-state equations.

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1.2. Generality of the variational approach

Since the co-state equations are derived from the continuous PDE of the state equations, any robust solution method can be adopted to furnish the converged solution of these equations. Further more, any convenient discretization method different from the type of discretization one uses for the state equations can be selected for the co-state equations. The requirement that the co-state equations be discretized exactly the same way as the state equations is shown not to be necessary, at least for quasi one-dimensional Euler equations [16]. In addition to that, any time integration method different from the time integration method used for the state equations can be selected to advance the co-state equations to steady state. The last point to mention is that the shape of the domain is considered as the design parameter, and its contribution to the functional and gradient sensitivity derivatives is directly incorporated.

The distinction of variational method from the discrete approach is that it first integrates and then differentiates the modified functional, i.e., weak formulations for many non-linear problems such as shock phenomena. The most important aspect of variational method is that the constraint sensitivity equation with the sensitivity equation of the objective function are used to determine the magnitude and sign of the search vector which in turn keeps the design variables in the design space until the optimum shape is reached.

2. Aerodynamic design optimization and sensitivity analysis

2.1. Constrained optimization methodology

A constrained optimization method in general encompasses three elements of optimization, i.e., design variables, constraints, and objective function. These are here briefly discussed.

2.1.1. Design variables in variational sense

In most aerodynamic optimization problems, the design variables are generally of a combination of flow field related or geometric nature, such as the coefficients of some geometric functions, surface grid points [17], aero-functions [18], or polynomial functions such as Bezier–Bernstein functions [19,20] and Spline functions [21].

In this study, variational method treats the boundary of the domain in a continuous fashion, and therefore, the boundary is considered as part of the solution to the design problem. With the assumption that the domain Ω is sufficiently regular, the location of points on the boundary $\vec{X}_\Gamma$ can be considered as a continuous design variable. Mathematically, the coordinates of the varying boundary in the continuous sense can be expressed as

$$\vec{X}_\Gamma = \vec{f}(\vec{X}_D) \tag{1}$$

where $\vec{X}_D$ are the design variables. In aerodynamic optimization problems, the vector of design variables is provided for very limited and simplified geometries, for instance, four digit NACA airfoils and some nozzles. However, for general-purpose geometries, these control points must be determined through iterative methods from certain functional relationships such as the Bezier–Bernstein polynomials [19]. Because these polynomial functions are known to generate smooth curves and surfaces for a minimal number of control points, the function $\vec{f}$ which describes the curve for the two-dimensional problem, is given by [20]

$$\vec{f}(\vec{X}_D) = \sum_{i=0}^{n} \vec{X}_{d,i} B_{i,n}(\bar{u}) \quad \text{for} \quad \bar{u} \in [0,1], \tag{2}$$

where

$$B_{i,n}(\bar{u}) = C(n,i)\bar{u}^i(1-\bar{u})^{n-i}, \tag{3}$$

and

$$C(n,i) = \frac{n!}{i(n-i)!}. \tag{4}$$

In (2)–(4), $B_{i,n}(\bar{u})$ are the blending functions, $C(n,i)$ are the binomial coefficients, $\bar{u}$ is the normalized arc length, $\vec{X}_{di}$ are the control points associated with $\bar{u}$ and n is the order of the Bezier–Bernsten polynomials.

2.1.2. Constraints

Constraints are the integral parts of the optimization procedure that influence the final outcome of the functional. They can be geometrical, flow-type, equality or inequality constraints, or a combination of all or some that depend on the particular optimization problem one wants to address.

In variational formulation of design optimization problems, the flow-type constraints are expressed in the integral forms. The geometrical and side constraints, on the other hand, can be formulated either in the integral or discrete forms. For the general variational approach, generic flow-type constraints are expressed as

$$G_j(\vec{Q},\vec{n}) = \int_{\bar{\Gamma}} g_j(\vec{Q},\vec{n})d\bar{\Gamma} \le 0 \quad \text{for} \quad j = 1,2,\ldots,\text{nconf}, \tag{5}$$

where $\bar{\Gamma}$ is the deformed boundary, $\vec{Q}$ is the vector of conserved flow field variables, $\vec{n}$ is the normal vector and nconf is the number of generic fluid-type constraints. The generic geometric-type and the side constraints can also be given as

$$G_j(\vec{X}_D) \le 0 \quad \text{for} \quad j = \text{nconf}+1, \text{nconf}+2,\ldots,\text{ncon}, \tag{6}$$

and

$$X_{iD}^{\text{lower}} \le X_{iD} \le X_{iD}^{\text{upper}} \quad \text{for} \quad i = 1,2\ldots,\text{ndv}, \tag{7}$$

where ncon is the total number of constraints, and ndv is the number of design variables, respectively.

2.1.3. Objective functional

In the variational method approach, the objective functional is defined in the form of a definite integral involving an unknown state function $\vec{Q}$, which can be dependent on some normal vectors $\vec{n}$ and other problem parameters. Then, the objective functional is extremized at the converged state solution over the curve of the surface described by the vector of design variables. Mathematically, a generic functional on the boundary $J_{\bar{\Gamma}}$, is defined as

$$J_{\bar{\Gamma}}(\vec{Q},\vec{n}) = \int_{\bar{\Gamma}} D(\vec{Q},\vec{n})d\bar{\Gamma}, \tag{8}$$

where D is the objective function specified on the curve or boundary. The selection of the objective function is mostly dictated by the flow physics.

2.2. Variational formulation of aerodynamic optimization problem

When constraints are involved in the optimization problem, the partial derivatives of the functional and the constraints cannot be zero at the same time since they are functionally related to each other through the optimality criteria [22,23]. To start the derivation of the optimality criteria, the residual, $\bar{R}(\vec{Q})$ is written as

$$\bar{R}(\vec{Q}) = \bar{E}_x + \bar{F}_y = \vec{0}, \tag{9}$$

where $\bar{E}_x$ and $\bar{F}_y$ are the conservative fluxes in the x and y directions. The generic boundary constraints are expressed also given as

$$\bar{H}(\vec{Q},\vec{n}) = \vec{0}. \tag{10}$$

Without changing its value, the objective functional $J_{\bar{\Gamma}}$ can now be modified as