Gradient Calculus for a Class of Optimal Design Problems in Engineering

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Abstract This chapter reviews some recent works in which the analysis and control of partial differential equations are applied to optimal design in some problems appearing in aerodynamics and elasticity. From a mathematical point of view, the idea is to apply a descent algorithm to a cost functional defined on a part of the boundary. More specifically, we focus here on problems where the cost functional is defined on the part of the boundary to be optimized. This is the case, for instance, when the goal is to improve the lift or the drag in aerodynamic problems or to uniformize the tangential stresses along the boundary of a elastic material.

1 Introduction

This work contains a series of applications of control problems to aerodynamics and elasticity problems with the aim of improving the industrial software in simulation. We focus mainly on aerodynamic applications since they have been more extensively studied in the last years. However the methodology considered here is general and can be easily adapted to structural optimization, as we show in Sect. 6.

In the last years, advanced software for automatic aerodynamic design optimization has been extensively used by engineers to avoid expensive experimental proofs in wind tunnels (see the early works by A. Jameson [15] and O. Pironneau [22] or the more recent book [20] and the references therein). This optimization software is based on gradient methods to minimize a suitable cost or objective function

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(drag coefficient, deviation from a prescribed surface pressure distribution, etc.) with respect to a set of design variables (defining, for example, an airfoil profile). This is a complex problem where several difficulties arise: parametrization of complex geometries, suitable choice of the correct systems of equations to model the fluid according to the underlying physics (Euler equations, Navier–Stokes, RANS, turbulence models, etc.), numerical methods to solve the differential equations, mesh generation, mesh adaptivity to small changes in the geometry, cost function approximation, gradient approximation, etc. These and other industrial constraints make any practical application of such a technology a very complex task. Mathematical analysis can be useful to improve some of the factors involved in this process. Here we focus on the computation of the gradient of cost functionals associated to optimal design.

To fix the problem we consider a fluid domain Ω bounded by a typically disconnected boundary $\partial\Omega$ which is divided into a far-field component Γ_∞ and a wall boundary S (Fig. 1). Aeronautic optimization problems seek the minimization of a certain cost function, such as the deviation of the pressure on S from a prescribed pressure distribution in the so-called inverse design problems, or integrated force coefficients (drag or lift) in force optimization problems. In these examples the cost function J can be defined as an integral over the wall boundary S of a suitable function $f(U,S)$ of the flow variables, referred to as a vector U, and the geometry S

$$J(S) = \int_S f(U,S)\,ds. \tag{1}$$

The flow variables U satisfy a suitable flow model (Euler, Navier–Stokes, RANS, etc.), that we write as

$$R(U) = 0, \qquad x \in \Omega, \tag{2}$$

including initial and boundary conditions.

Note that the cost functional depends on a part S of the boundary of the domain, which will be referred to as the control variable. The set of admissible controls is therefore a set of different geometries for S that we refer as S_{ad}. We are interested in the following problem: Find $S_{min} \in S_{ad}$ such that,

$$J(S_{min}) = \min_{S \in S_{min}} J(S). \tag{3}$$

To prove the existence of solution for the above minimization problem is, in general, a difficult problem which strongly depends on the flow equations, the restrictions included in S_{ad}, and the functional itself.

However, since these aerodynamical problems are very sensitive to perturbations of the domain, rather than looking for an optimal S, in the applications one tries to improve a given “natural” design by performing small perturbations. Therefore,

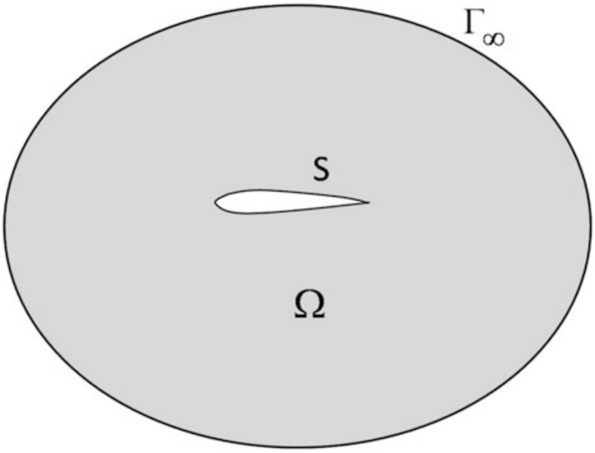

Fig. 1 Exterior domain with boundary S

the main interest is to make a sensitivity analysis of J with respect to small perturbations of the boundary S. Once this is done, the deformation for which the functional decreases with highest rate is chosen: the best descent direction. In other words, the main objective is to compute the shape derivative of J.

Another important point is that, in the engineering practice, instead of computing the exact continuous objective function, one computes a discrete approximation in which the time and physical domain are discretized. The objective function is evaluated by means of a discrete integration rule and the variables U are estimated by means of a numerical approximation scheme for solving the flow equations. Therefore our real optimization problem is in fact a discrete version of (1)–(3), and the sensitivity analysis should be done for such discrete version. This is usually referred to as a *discrete approach* to obtain sensitivity (see for example [19, 20]). Note that this sensitivity analysis will depend on the discretization aspects, such as the numerical scheme used to approximate the flow variables, the mesh, the numerical approximation of the cost functional, and even on the implementation issues such as multigrid techniques and, possibly, parallel computation.

In contrast with this *discrete approach* there is the alternative *continuous approach* where the sensitivity analysis is obtained for the continuous system and then discretized to obtain the optimal descent direction for the discrete model (see [14]). The validity of this *continuous approach* to obtain an accurate sensitivity analysis of the discrete model is not obvious. It is usually based on strong convergence results of the chosen discretization for (1)–(3) and the smoothness of solutions. On the other hand, the continuous approach makes easier the analysis and reduce the dependence on the numerical scheme chosen to obtain the flow variables. We refer to [21] for a comparison between both approaches, the discrete and continuous.

In this work we focus on the continuous approach of the sensitivity analysis, that we will briefly describe.

In order to define the shape deformation of the control boundary S we introduce a suitable parametrization of S given by $\mathbf{x} : [0, 1] \to \mathbb{R}^2$. A generic deformation of the boundary can be described as a vector field $\delta \mathbf{x}(s)$ such that the new geometry S' is parametrized by $\mathbf{x}'(s) = \mathbf{x}(s) + \delta \mathbf{x}(s)$. For sufficiently small perturbations, $\delta \mathbf{x}(s)$ can be described by normal displacements as follows:

$$\delta \mathbf{x}(s) = \alpha(s)\mathbf{n}, \quad \mathbf{n} \text{ normal vector to } S, \tag{4}$$

since tangent deformations are equivalent to reparameterizations of the boundary. The function α represents a perturbation profile which describes the amount of displacement, in the normal direction, at each point of S. This α is usually taken in a finite dimensional subspace generated by some basis functions (polynomial, trigonometric, etc.)

$$\tilde{U}_{ad} = span(\alpha_1, \alpha_2, \ldots, \alpha_n).$$

The sensitivity analysis for the continuous model consists in finding the shape derivative of J, i.e. the derivative of J with respect to any deformation profile $\alpha \in \tilde{U}_{ad}$, and then the best decreasing rate is chosen. This will constitute the descent direction for J. There are two main approaches that have been tried in industrial applications: *finite differences* and *adjoint methodology*.

In the finite difference approach, shape derivatives are calculated by computing the finite difference

$$\frac{J(S_{\alpha_k,\varepsilon}) - J(S)}{\epsilon}, \quad \varepsilon << 1,$$

where $S_{\alpha_k,\varepsilon}$ is the new geometry obtained from S with the parametrization $\mathbf{x}(s) + \varepsilon \alpha_k \mathbf{n}(s)$. This is done for each $k = 1, .., n$. The parameter ε should be chosen small enough to recover the linear behavior but not too small to avoid round errors. In this way, partial derivatives with respect to each α_k are computed. The one with the highest decreasing rate is chosen as the descent direction for computing the new geometry. The main drawback of this approach is that it is computationally too expensive. Note that each finite difference of J requires an evaluation of the cost functional and therefore a new solution of the flow equations. On the other hand, the choice of the value of ε is difficult and an adequate strategy to estimate it has to be used.

A more efficient way to compute a descent direction for J is the adjoint method, in which one seeks for the following representation of the Gateaux derivative of J with respect to α,

$$\delta J = \int_S G(s)\alpha(s)\, ds,$$

for some function $G(s)$, usually known as gradient of J. Once this is known, an optimal descent direction is chosen by projecting $-G(s)$ in the subspace of admissible deformations $\tilde{U}_{ad}$.

The computation of G involves shape derivatives, in the sense given by Hadamard (see [12]), and classical control theory which reduces the computation of the gradient to the resolution of a suitable adjoint system. In contrast with the finite difference approach, only one system has to be solved to obtain the descent direction. However, this adjoint system does not issue from a physical fluid problem but from an algebraic calculation. Therefore the usual numerical methods for fluids are not well-adapted to solve it, in general, and a particular numerical analysis is needed to find efficient methods.

The adjoint method is in fact a particular application of the classical control theory for partial differential equations. This theory was significantly developed due, in particular, to the works of J.-L. Lions [18]. Later on O. Pironneau investigated the application of the control theory to the optimal shape design for elliptic equations [22]. In the late eighties A. Jameson [15] was the first to apply these techniques to the Euler and Navier–Stokes equations in the field of aeronautical applications. From these pioneering works a lot of new results and applications have made of this topic an essential tool in optimal design.

In this work we review the continuous adjoint, when considering different models to approximate the flow variables, namely the Euler equation (Sect. 3), Navier–Stokes equations (Sect. 4), and Euler equations in presence of shock waves (Sect. 5). The analysis has been validated with two-dimensional and three-dimensional examples. At this moment, the Navier–Stokes sensitivity analysis is implemented in experimental versions of high performance codes as SU2 (Standford University) and TAU (developed in Germany by DLR). It is worth mentioning that the extension of the continuous approach to the sensitivity analysis of RANS equations with Spalart–Allmaras model for turbulence has been studied in [6], where gradient formulas are derived. In Sect. 6 we show an application of this technique in the context of elasticity problems.

2 Gradient Computation

In this section we describe the methodology to obtain gradient formulas for the cost functional in a systematic way. It is worth mentioning that this calculus is formal since it assumes that solutions of the underlying differential equations are smooth. This is not true in general. As it is well known, Euler equations may produce discontinuities even for a smooth initial data. For simplicity, we focus on dimension $n = 2$ but the case $n = 3$ can be treated similarly.

Let us consider $U_{ad} \subset L^2(0, 1)$ and the functional $J : U_{ad} \to \mathbb{R}$

$$J(\alpha) = \int_S j(U)\, ds \tag{5}$$

where S is described as a normal perturbation of a reference geometry S_0 in such a way that $S = S_0 + \alpha(s)\mathbf{n}$ and $\alpha \in \tilde{U}_{ad} \subset L^2(0,1)$. The vector function U is the solution of system (2). All the functionals considered below can be written in this form.

Classical shape derivatives allow us to write the Gateaux derivative of J, δJ, in the generic direction α (see [23]), as follows:

$$\delta J = \int_S \left(\frac{\partial j}{\partial U} \delta U + (\partial_n j + \kappa j)\alpha \right) ds \tag{6}$$

where κ represents the curvature of S (in 3-d the boundary S will be a surface and κ should be replaced by $2H$ with H the mean curvature of S). The vector function δU represents the Gateaux derivative of U in the direction given by α and it is obtained by linearization of system (2),

$$\frac{\partial R}{\partial U} \delta U = 0, \qquad x \in \Omega. \tag{7}$$

Now we introduce an adjoint state Ψ for which

$$\int_S \frac{\partial j}{\partial U} \delta U \, ds = \int_S \mathscr{B} \Psi \delta\alpha \, ds, \tag{8}$$

where $\mathscr{B}$ is a certain operator and Ψ satisfies the so-called adjoint system

$$\mathscr{A} \Psi = 0, \qquad x \in \Omega. \tag{9}$$

The operators $\mathscr{A}$ and $\mathscr{B}$ strongly depend on the flow equations and boundary conditions included in $R(U)$, and they must be computed specifically for each problem. We show an example in the appendix below.

Once obtained the adjoint state we can replace (8) into (6),

$$\delta J = \int_S (\mathscr{B}\Psi + \partial_n j + \kappa j) \, \delta\alpha \, ds, \tag{10}$$

and therefore

$$G(s) = \mathscr{B}\Psi(s) + \partial_n (j(U(s))) + \kappa j(U(s)).$$

Remark 1. In general, the operator $\mathscr{A}$ is closely related to the linearized system (7) and its numerical approximation should take into account this fact. There are several ways to deduce numerical schemes for (7) but the more stable ones are usually obtained by a suitable adjoint of the linearization of the numerical methods for $R(U)$. This can be done at several levels, from a specific code based on the linearized numerical scheme to automatic differentiation tools that provides a linearization of the whole numerical code used to solve $R(U)$, including parallelization, multigrid, preconditioners, etc.

3 Continuous Adjoint Formulation for Euler System

We first consider the case of steady inviscid two dimensional flows. We present a brief description of the continuous adjoint formulas. We refer to [1,7] for a complete analysis and full formulation.

The governing equations in this case are

$$\nabla \cdot F = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} = 0, \quad \text{in } \Omega, \quad U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}, \tag{11}$$

$$F_x = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ \rho u H \end{pmatrix}, \qquad F_y = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + P \\ \rho v H \end{pmatrix}. \tag{12}$$

Here, ρ is the density, u and v are the Cartesian velocity components, E is the total energy, and P and H are the pressure and enthalpy, given by the following relations:

$$P = (\gamma - 1)\rho\left[E - \frac{1}{2}(u^2 + v^2)\right], \quad H = E + \frac{P}{\rho}, \tag{13}$$

where γ is the ratio of specific heats. The above system must be completed with suitable boundary conditions. We consider characteristic-type boundary conditions [16] on the far-field boundary Γ_∞, and non-penetrating boundary conditions on solid wall boundaries,

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \mathbf{v} = (u, v) \quad \mathbf{n} = (n_x, n_y), \quad \text{normal vector on } S. \tag{14}$$

$$\text{Far field boundary conditions on } \Gamma_\infty. \tag{15}$$

The operator $R(U)$ in this case contains the whole system of equations and boundary conditions (11)–(15).

Concerning the cost function, there are several possibilities according to different interests. Conventional cost functions include specified pressure distributions (inverse design), force (drag or lift) or moment coefficients, efficiency (i.e., lift over drag), etc. All these cost functionals can be written in the general form:

$$J(S) = \int_S g(P, \mathbf{n})\, ds \tag{16}$$

for some function $g(P, \mathbf{n})$. For example, in the particular case of lift-drag coefficients, the cost functional take the form

$$J(S) = \int_S C_p(\mathbf{n} \cdot \mathbf{d})\, ds, \qquad \mathbf{d} = \begin{cases} (\cos\beta, \sin\beta), & (drag), \\ (\sin\beta, \cos\beta), & (lift), \end{cases} \tag{17}$$

where β is a constant parameter (angle of attack), $C_p = (P - P_\infty)/C_\infty$, $C_\infty = \gamma M_\infty^2 P_\infty/2$, and P_∞ and M_∞ are freestream pressure and Mach number respectively.

Following the general framework in Sect. 2 above $j(U) = g(P(U), \mathbf{n})$.

The final expression for G in the case of (16) is given by

$$G = \frac{\partial g}{\partial P}\partial_n P + \mathbf{t}\cdot\partial_{tg}\frac{\partial g}{\partial \mathbf{n}} - \kappa\left(g - \frac{\partial g}{\partial \mathbf{n}}\cdot\mathbf{n}\right)$$
$$-\nabla\cdot\mathbf{v}(\rho\psi_1 + \rho\mathbf{v}\cdot\boldsymbol{\varphi} + \rho H\psi_4) + \mathbf{t}\cdot\mathbf{v}\partial_{tg}(\rho\psi_1 + \rho\mathbf{v}\cdot\boldsymbol{\varphi} + \rho H\psi_4)$$

where κ is the curvature of S (for 3D flows the mean curvature appears), $\mathbf{t}$ is the unitary tangent vector to S, ∂_n the normal derivative and ∂_{tg} the tangential derivative. The adjoint variables

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \qquad \boldsymbol{\varphi} = (\psi_2, \psi_3),$$

satisfy the adjoint system

$$A^T\nabla\Psi = 0, \qquad A = \left(\frac{\partial F_x}{\partial U}, \frac{\partial F_y}{\partial U}\right),$$

and the boundary conditions

$$\varphi\cdot\mathbf{n} = \frac{\partial g}{\partial P}, \qquad \text{on } S,$$
$$\text{adjoint far field conditions on } \Gamma_\infty.$$

We refer to [13] for details on how this adjoint boundary conditions are obtained and implemented numerically.

4 Continuous Adjoint Formulation for Navier–Stokes System

In this section we consider the Navier–Stokes system. We refer to [7] for the full expression of the adjoint system, the derivation of the gradient formula, and some numerical experiments. The gradient formula for 3D flows is also given in [7].

The governing equations, for steady viscous laminar flows in two dimensions, are

$$\nabla \cdot F - \nabla \cdot F^v = 0, \quad \text{in } \Omega, \tag{18}$$

where $F = (F_x, F_y)$ has been defined in (12) and

$$F_x^v = \begin{pmatrix} 0 \\ \sigma_{xx} \\ \sigma_{xy} \\ u\sigma_{xx} + v\sigma_{xy} + k\frac{\partial T}{\partial x} \end{pmatrix}, \qquad F_y^v = \begin{pmatrix} 0 \\ \sigma_{xy} \\ \sigma_{yy} \\ u\sigma_{yx} + v\sigma_{yy} + k\frac{\partial T}{\partial y} \end{pmatrix}. \tag{19}$$

The viscous stresses may be written as

$$\sigma_{xx} = \frac{2}{3}\mu\left(2u_x - v_y\right), \qquad \sigma_{yx} = \sigma_{xy} = \mu\left(u_y + v_x\right),$$
$$\sigma_{yy} = \frac{2}{3}\mu\left(2v_y - u_x\right),$$

where μ is the laminar viscosity coefficient. The coefficient of thermal conductivity and the temperature are computed as follows:

$$k = \frac{c_p}{Pr}\mu, \qquad T = \frac{P}{R\rho},$$

where c_p is the specific heat at constant pressure, Pr is the Prandtl number, and R is the gas constant.

Equation (18) is complemented with characteristic-type boundary conditions on the far field, and nonslip conditions on solid walls

$$u = v = 0, \quad \text{on } S.$$

An additional boundary condition has to be imposed to the temperature on the solid walls, which can be either adiabatic or isothermal (constant temperature)

$$\partial_n T = 0, \quad \text{adiabatic},$$
$$T = T_0, \quad \text{constant temperature}.$$

In the adiabatic case, the expression for G is given by

$$G = \frac{\partial g}{\partial P}\partial_n P + \mathbf{t}\cdot\partial_{tg}\frac{\partial g}{\partial \mathbf{n}} - \kappa\left(g - \frac{\partial g}{\partial \mathbf{n}}\cdot\mathbf{n}\right)$$
$$-(\mathbf{n}\cdot\partial_n\mathbf{v})(\rho\psi_1 + \rho H\psi_4) + \mathbf{n}\cdot\Sigma\cdot\partial_n\mathbf{v} - \psi_4(\mathbf{n}\cdot\sigma\cdot\partial_n\mathbf{v})$$
$$+\psi_4(\sigma : \nabla\mathbf{v}) - k(\partial_{tg}\psi_4)(\partial_{tg}T),$$

where ' :' denotes the double dot contraction of second order tensor fields. The adjoint variables satisfy the adjoint system

$$(A + A^v)^T \nabla \Psi = 0, \qquad A^v = \left(\frac{\partial F_x^v}{\partial U}, \frac{\partial F_y^v}{\partial U} \right),$$

with boundary conditions

$$\varphi = \frac{\partial g}{\partial P} \mathbf{n}, \qquad \text{on } S$$

and adjoint farfield boundary conditions on Γ_∞.

The second order tensor Σ is defined as follows

$$\Sigma = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}, \qquad \Sigma_{xx} = \frac{2}{3}\mu(2\partial_x \psi_2 - \partial_y \psi_3),$$

$$\Sigma_{xy} = \Sigma_{yx} = \mu(\partial_y \psi_2 + \partial_x \psi_3), \qquad \Sigma_{yy} = \frac{2}{3}\mu(2\partial_y \psi_3 - \partial_x \psi_2).$$

5 Continuous Adjoint Formulation for Euler System in the Presence of Shock Waves

So far, we have considered smooth solutions of flow equations. In this case, the perturbation of the flow field variables with respect to shape changes can be approximated by linearizing the governing equations. However, inviscid flows described by the Euler equations can develop discontinuities (shocks or contact discontinuities) due to the intersection of characteristics. In this case, the smooth analysis in Sect. 3 is no longer valid. We refer to [2] for the complete formulation and analysis of this section.

In this section we restrict ourselves to the particular case where there is a single discontinuity located on a smooth curve Σ (Fig. 2). When this occurs, Euler system (11) must be completed with the Rankine–Hugoniot conditions that relate the flow variables on both sides of the discontinuity. Thus, we replace (11) by

$$\begin{cases} \nabla \cdot F = 0, & \text{in } \Omega \backslash \Sigma, \\ [F \cdot \mathbf{n}]_\Sigma = 0, & \text{on } \Sigma, \end{cases} \tag{20}$$

where $[A]_\Sigma$ represents the jump of A across the discontinuity curve Σ, i.e. $[A]_\Sigma = A^+ - A^-$.

The sensitivity analysis in this case is much more complex since a perturbation of the boundary S may affect to the position of the discontinuity Σ. Thus, the

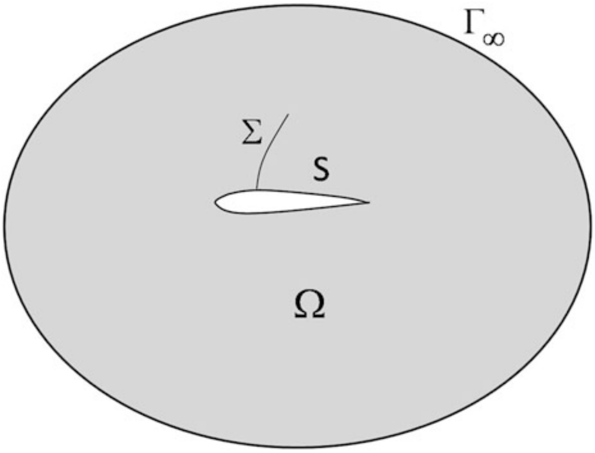

Fig. 2 Exterior domain with boundary S and shockwave

variational calculus must be modified to take into account the position of the discontinuity as a new variable. This analysis has been done in simpler models by different authors (see for instance [3, 4, 10, 11]). Moreover, in [8, 17] the position of the discontinuity is used to improve gradient algorithms in the case of the inviscid Burgers equation in 1-d.

A formal calculus based on this approach allows us to obtain a formula for G in this particular case.

We must distinguish two different situations: either the shock wave Σ meets the boundary S at a point $x_b \in S$, or it does not. We focus on the first case since the second one is simpler. We have the following

$$G = \frac{\partial g}{\partial P}\partial_n P + \mathbf{t}\cdot\partial_{tg}\frac{\partial g}{\partial \mathbf{n}} - \kappa\left(g - \frac{\partial g}{\partial \mathbf{n}}\cdot\mathbf{n}\right)$$
$$-\nabla\cdot\mathbf{v}(\rho\psi_1 + \rho\mathbf{v}\cdot\boldsymbol{\varphi} + \rho H\psi_4) + \mathbf{t}\cdot\mathbf{v}\partial_{tg}(\rho\psi_1 + \rho\mathbf{v}\cdot\boldsymbol{\varphi} + \rho H\psi_4),$$

for $x \in S$ but $x \neq x_b$. Note that this formula is analogous to the gradient formula for smooth solutions. The only difference is that we do not have to compute it at the discontinuity point x_b where the flow variables may have discontinuities and their derivatives may produce singularities. The adjoint system is given by

$$\begin{cases} A^T\nabla\Psi = 0, & \text{in } \Omega\backslash\Sigma \\ \mathbf{t}\cdot\partial_{tg}\boldsymbol{\varphi} = 0, & \text{on } \Sigma, \\ [\Psi]_\Sigma = 0, & \end{cases} \tag{21}$$

together with the adjoint boundary conditions for the far field and

$$\varphi \cdot \mathbf{n} = \frac{\partial g}{\partial P}, \qquad \text{on } S.$$

The second and third equations in (21) are transmission conditions that comes from the Rankine–Hugoniot conditions by duality. They are usually referred as adjoint Rankine–Hugoniot conditions. They establish, in particular, that the adjoint vector variables Ψ must be continuous at Σ.

It is worth mentioning that well-posedness of the adjoint system (21) is a difficult task due to the discontinuity of the matrix coefficients A at Σ. This is a challenging problem even for simpler scalar conservation laws in one dimension [5].

6 An Example in Elasticity

In this section we apply the same strategy in the context of elasticity problems. In particular, we consider optimal design problems whose cost functions depend on the stresses at the boundary to be optimized. An example described in [9] considers the shape optimization of the cross-sectional vault of a tunnel in order to have uniform stresses along the profile (see also [24]). In this way, we avoid regions with larger compression stresses at the boundary that could produce more fatigue. For this specific problem, a two-dimensional elastic problem is solved for the cross-section of the tunnel with the following objective function

$$J(\alpha) = \frac{1}{2} \int_S (\sigma_t - \sigma_{tm})^2 \, ds, \tag{22}$$

where σ_t represents the tangential stresses along S ($\sigma_t = \mathbf{t} \cdot \sigma \cdot \mathbf{t}$ where σ is the stress tensor and $\mathbf{t}$ the tangent vector to S) and σ_{tm} a reference value that can be either a given constant or the average of the tangential stresses along S,

$$\sigma_{tm} = \frac{\int_S \sigma_t \, ds}{\int_S ds}.$$

Of course, other functionals are also possible according to the interest of the application.

Let us state the problem: consider the elasticity system defined on a domain $\Omega \subset \mathbb{R}^2$ with boundary $\partial\Omega = \Gamma \cup S$ and $\Gamma \bigcap S = \emptyset$, (Fig. 3) and the objective function

$$J(\alpha) = \int_S j(\mathbf{t} \cdot \sigma \cdot \mathbf{t}) \, ds, \tag{23}$$

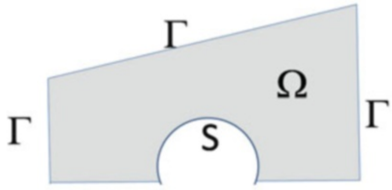

Fig. 3 Cross section of a tunnel vault

for some function j, where $\sigma = \sigma_{\alpha\beta}$ is the second order stress tensor and $\mathbf{t}$ the tangent vector to S that we obtain rotating $\pi/2$ the outward normal clockwise. The stress tensor is obtained by solving the elasticity system

$$\sigma_{\alpha\beta,\beta} + f_\alpha = 0, \quad \mathbf{x} \in \Omega, \quad \alpha, \beta = 1, 2, \tag{24}$$

$$\sigma_{33} = \nu(\sigma_{11} + \sigma_{22}), \quad \mathbf{x} \in \Omega, \tag{25}$$

$$\varepsilon_{\alpha\beta} = \frac{1+\nu}{E}\sigma_{\alpha\beta} - \frac{\nu}{E}\sigma_{kk}\delta_{\alpha\beta}, \tag{26}$$

$$\varepsilon_{13} = \varepsilon_{23} = \varepsilon_{33} = 0, \tag{27}$$

where $\mathbf{x} = (x_1, x_2) \in \Omega$ is a generic point of the elastic body, (f_1, f_2) the components of the external forces, $\delta_{\alpha\beta}$ the Kronecker delta and $\varepsilon_{\alpha\beta}$ are the components of the strain tensors respectively. The elastic constants of the isotropic material are the Young modulus E and Poisson ratio ν. Partial derivative is denoted by a comma (,). The expression of the strain tensor components are given as a function of the displacements as follows:

$$\varepsilon_{\alpha\beta} = \frac{1}{2}\left(u_{\alpha,\beta} + u_{\beta,\alpha}\right). \tag{28}$$

To fix ideas, the following boundary conditions are assumed

$$u_\alpha = \bar{u}_\alpha, \quad \mathbf{x} \in \Gamma, \quad \alpha = 1, 2 \tag{29}$$

$$\sigma_{\alpha\beta} n_\beta = 0, \quad \mathbf{x} \in S, \quad \alpha, \beta = 1, 2 \tag{30}$$

where $\bar{u}_\alpha$ are specified displacement, $\mathbf{n} = (n_1, n_2)$ is the outward normal unit vector to the boundary Γ. Other boundary conditions are also possible.

The gradient in this case is given by

$$G = -\partial_{tg}(j'(\sigma_t)(\mathbf{n}\cdot\sigma\cdot\mathbf{t} + \mathbf{t}\cdot\sigma\cdot\mathbf{n})) - \Psi\cdot\partial_n\sigma\cdot\mathbf{n} + \partial_{tg}(\Psi\cdot\sigma\cdot\mathbf{t})$$
$$-\frac{\nu}{1-\nu}j'(\sigma_t)\mathbf{n}\cdot\partial_n(\sigma)\cdot\mathbf{n} + [\kappa j(\sigma_t) + \partial_n\left(j(\sigma_t)\right)]$$

where ∂_{tg} and ∂_n represent the tangential and normal derivatives respectively, and $\Psi = (\psi_1, \psi_2)$ satisfies the adjoint problem,

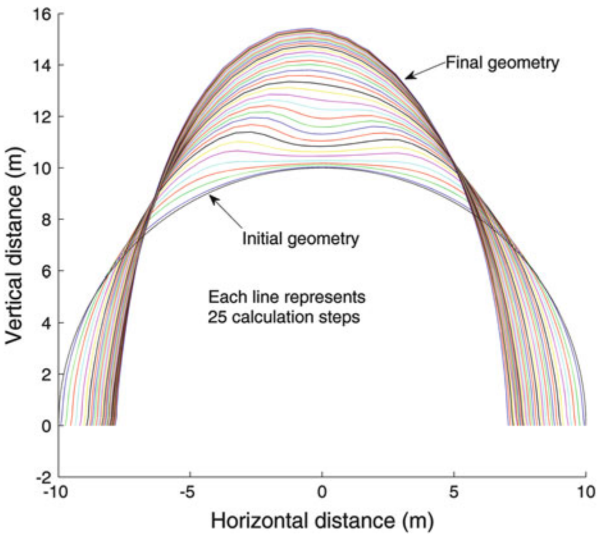

Fig. 4 Cross-sectional designs obtained with a gradient type method

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\begin{aligned}
\frac{\partial \sigma^*_{\alpha\beta}}{\partial \beta} &= 0, \quad x \in \Omega, \quad \alpha, \beta = 1, 2, \\
\sigma^*_{33} &= \nu(\sigma^*_{11} + \sigma^*_{22}), \quad x \in \Omega, \\
\epsilon^*_{\alpha\beta} &= \frac{1+\nu}{E}\sigma^*_{\alpha\beta} - \frac{\nu}{E}\sigma^*_{kk}\delta_{\alpha\beta}, \\
\epsilon^*_{\alpha\beta} &= \frac{1}{2}\left(\frac{\partial \psi_\beta}{\partial \alpha} + \frac{\partial \psi_\alpha}{\partial \beta}\right), \\
\epsilon^*_{13} &= \epsilon^*_{23} = \epsilon^*_{33} = 0,
\end{aligned}
$$

with the following boundary conditions:

$$
\begin{aligned}
\psi_\alpha &= 0, \quad x \in \Gamma, \quad \alpha = 1, 2, \\
\sigma^*_{\alpha\beta} n_\beta &= \frac{-E}{1-\nu^2}\partial_{tg}\left(j'(\sigma_t)\right) t_\alpha, \quad x \in S, \quad \alpha = 1, 2.
\end{aligned}
$$

The practical implementation of these formulas and some numerical experiments are given in [9]. As an example Figs. 4 and 5 show the different profiles obtained by a gradient-type algorithm applied to the functional (22). In this example, the initial geometry is a semicircle that is transformed into a parabolic profile after the optimization procedure.

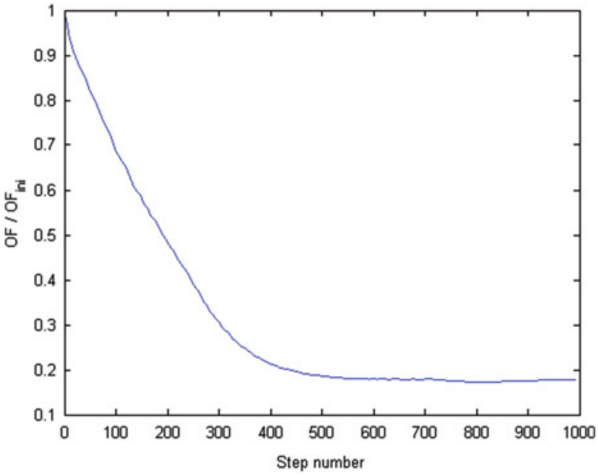

Fig. 5 Evolution of the cost functional

Appendix

In this section we show how to compute the adjoint operators $\mathscr{A}$ and $\mathscr{B}$ in (8)–(9) for one of the examples above. As it has been said, this computation strongly depends on the specific problem, but nevertheless the methodology is straightforward as it will be shown here.

We focus on the 2D elasticity problem described in Sect. 6. The objective function is given by (23) so that, according to (8) we look for $\mathscr{B}$, $\mathscr{A}$ and an adjoint state Ψ such that

$$\int_S \delta(j(\mathbf{t}\cdot\sigma\cdot\mathbf{t}))\,ds = \int_S \mathscr{B}\Psi\delta\alpha\,ds, \tag{31}$$

with Ψ satisfying $\mathscr{A}\Psi = 0$.

First of all, observe that, as $\delta\mathbf{t} = \delta\alpha'\mathbf{n}$, we have

$$\begin{aligned}\delta(j(\mathbf{t}\cdot\sigma\cdot\mathbf{t})) &= j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})(\mathbf{n}\cdot\sigma\cdot\mathbf{t}+\mathbf{t}\cdot\sigma\cdot\mathbf{n})\delta\alpha' \\ &\quad + j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})\mathbf{t}\cdot\delta\sigma\cdot\mathbf{t},\end{aligned} \tag{32}$$

where the tensor $\delta\sigma$ is the solution of the linearized elasticity system

$$\delta\sigma_{\alpha\beta,\beta} = 0, \quad \mathbf{x}\in\Omega, \quad \alpha,\beta = 1,2, \tag{33}$$

$$\delta\sigma_{33} = \nu(\delta\sigma_{11}+\delta\sigma_{22}), \quad \mathbf{x}\in\Omega, \tag{34}$$

$$\delta\varepsilon_{\alpha\beta} = \frac{1+\nu}{E}\delta\sigma_{\alpha\beta} - \frac{\nu}{E}\delta\sigma_{kk}\delta_{\alpha\beta}, \quad \mathbf{x}\in\Omega, \tag{35}$$

$$\delta\varepsilon_{\alpha\beta} = \frac{1}{2}\left(\delta u_{\alpha,\beta} + \delta u_{\beta,\alpha}\right), \quad \mathbf{x} \in \Omega, \tag{36}$$

$$\delta\varepsilon_{13} = \delta\varepsilon_{23} = \delta\varepsilon_{33} = 0, \quad \mathbf{x} \in \Omega, \tag{37}$$

and the linearized boundary conditions

$$\delta\mathbf{u} = 0, \quad \mathbf{x} \in \Gamma, \tag{38}$$

$$\delta\sigma \cdot \mathbf{n} + \partial_n(\sigma) \cdot \mathbf{n}\delta\alpha - \sigma \cdot \mathbf{t}\alpha'(s) = 0, \quad \mathbf{x} \in S. \tag{39}$$

The only term that requires further analysis in (32) is the last one, i.e.

$$\int_S j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\mathbf{t} \cdot \delta\sigma \cdot \mathbf{t}\, ds. \tag{40}$$

To simplify it we write the linearized stress-strain tensor given in (34)–(35) with respect to the local system of coordinates associated to S, $\{\mathbf{t}, \mathbf{n}\}$. The following expression for $\delta\sigma_{\alpha\beta}$ is obtained:

$$\begin{aligned} \mathbf{t} \cdot \delta\sigma \cdot \mathbf{t} &= \frac{E}{1-\nu^2}\mathbf{t} \cdot \delta\varepsilon \cdot \mathbf{t} + \frac{\nu}{1-\nu}\mathbf{n} \cdot \delta\sigma \cdot \mathbf{n} \\ &= \frac{E}{1-\nu^2}\partial_{tg}(\delta\mathbf{u} \cdot \mathbf{t}) - \frac{\nu}{1-\nu}\mathbf{n} \cdot \partial_n(\sigma) \cdot \mathbf{n}\delta\alpha. \end{aligned} \tag{41}$$

In the last equality, we have used

$$\mathbf{t} \cdot \delta\varepsilon \cdot \mathbf{t} = \partial_{tg}(\delta\mathbf{u} \cdot \mathbf{t}),$$

and the boundary conditions to be satisfied for $\delta\mathbf{u}$ and $\mathbf{u}$ on S.

Therefore (40) can be written as

$$\begin{aligned} \int_S j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\mathbf{t} \cdot \delta\sigma \cdot \mathbf{t}\, ds &= \frac{E}{1-\nu^2}\int_S j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\partial_{tg}(\delta\mathbf{u} \cdot \mathbf{t})\, ds \\ &\quad - \frac{\nu}{1-\nu}\int_S j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\mathbf{n} \cdot \partial_n(\sigma_{\alpha\beta}) \cdot \mathbf{n}\delta\alpha\, ds \\ &= -\frac{E}{1-\nu^2}\int_S \partial_{tg} j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})(\delta\mathbf{u} \cdot t)\, ds \\ &\quad - \frac{\nu}{1-\nu}\int_S j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\mathbf{n} \cdot \partial_n(\sigma_{\alpha\beta}) \cdot \mathbf{n}\delta\alpha\, ds. \end{aligned} \tag{42}$$

In order to eliminate the term $\delta\mathbf{u}$ the adjoint problem to the linearized system is introduced

$$\frac{\partial \sigma^*_{\alpha\beta}}{\partial \beta} = 0, \quad x \in \Omega, \quad \alpha, \beta = 1, 2, \tag{43}$$

$$\sigma^*_{33} = \nu(\sigma^*_{11} + \sigma^*_{22}), \quad x \in \Omega, \tag{44}$$

$$\epsilon^*_{\alpha\beta} = \frac{1+\nu}{E}\sigma^*_{\alpha\beta} - \frac{\nu}{E}\sigma^*_{kk}\delta_{\alpha\beta}, \tag{45}$$

$$\epsilon^*_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial \psi_\beta}{\partial \alpha} + \frac{\partial \psi_\alpha}{\partial \beta}\right) \tag{46}$$

$$\delta\epsilon^*_{13} = \delta\epsilon^*_{23} = \delta\epsilon^*_{33} = 0, \tag{47}$$

with the following boundary conditions

$$\psi_\alpha = 0, \quad x \in \Gamma, \quad \alpha = 1, 2, \tag{48}$$

$$\sigma^* \cdot \mathbf{n} = \frac{-E}{1-\nu^2}\partial_{tg} j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\mathbf{t}, \quad x \in S. \tag{49}$$

Multiplying the equations of the linearized system by $\Psi = (\psi_1, \psi_2)$ and integrating by parts it is easily obtained

$$0 = -\int_\Omega \delta\sigma : \epsilon^* \, dx - \int_S \Psi \cdot \left(\partial_n \sigma \cdot \mathbf{n}\delta\alpha - \sigma \cdot \mathbf{t}\delta\alpha'\right) \, ds, \tag{50}$$

where : represents the double dot product of second order tensors.

A straightforward computation allows us to write the first term in this formula as follows,

$$\int_\Omega \delta\sigma : \epsilon^* \, dx = \int_\Omega \sigma^* : \delta\epsilon \, dx. \tag{51}$$

Now we integrate by parts in the right hand side of (51), taking into account the boundary conditions for $\mathbf{u}$ and Ψ,

$$\begin{aligned} \int_\Omega \sigma^* : \delta\epsilon \, dx &= -\int_\Omega \delta u_\alpha \frac{\partial \sigma^*_{\alpha\beta}}{\partial \beta} dx + \int_S \delta\mathbf{u} \cdot \sigma^* \cdot \mathbf{n} \, ds \\ &= -\frac{E}{1-\nu^2}\int_S \partial_{tg} j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\delta\mathbf{u} \cdot \mathbf{t} \, ds. \end{aligned} \tag{52}$$

Therefore, combining (50)–(52) the following equation is obtained

$$\frac{E}{1-\nu^2}\int_S \partial_{tg} j'(\mathbf{t} \cdot \sigma \cdot \mathbf{t})\delta\mathbf{u} \cdot \mathbf{t} \, ds = \int_S \Psi \cdot \left(\partial_n \sigma \cdot \mathbf{n}\delta\alpha - \sigma \cdot \mathbf{t}\delta\alpha'\right) \, ds. \tag{53}$$

Substituting (53) into (42) we obtain the final expression for (40),

$$\int_S j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})\mathbf{t}\cdot\delta\sigma\cdot\mathbf{t}\,ds = -\int_S \Psi\cdot\left(\partial_n\sigma\cdot\mathbf{n}\delta\alpha - \sigma\cdot\mathbf{t}\delta\alpha'\right)\,ds$$
$$-\frac{\nu}{1-\nu}\int_S j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})\mathbf{n}\cdot\partial_n(\sigma_{\alpha\beta})\cdot\mathbf{n}\delta\alpha\,ds. \tag{54}$$

From this formula together with (32) we obtain in the left hand side of (31) an expression where all the terms contain a factor with $\delta\alpha$ or its derivative. Integrating by parts on S and assuming that either S has no boundary or $\delta\alpha = 0$ at the boundary of S we easily obtain the expression for $\mathscr{B}$ in (31),

$$\mathscr{B} = -\partial_{tg}(j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})(\mathbf{n}\cdot\sigma\cdot\mathbf{t}+\mathbf{t}\cdot\sigma\cdot\mathbf{n}))$$
$$-\Psi\cdot\partial_n\sigma\cdot\mathbf{n} + \partial_{tg}(\Psi\cdot\sigma\cdot\mathbf{t}) - \frac{\nu}{1-\nu}j'(\mathbf{t}\cdot\sigma\cdot\mathbf{t})\mathbf{n}\cdot\partial_n(\sigma)\cdot\mathbf{n}.$$

The operator $\mathscr{A}\Psi = 0$ contain all the adjoint equations and boundary conditions (43)–(49).

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