Introduction to Shape Design and Control

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1 Introduction

In this lecture which is the first in a series of four lectures we will lay down the foundation for the ideas presented later. We are concerned with mathematical tools that will enable us the analysis and the construction of efficient algorithms for the solution of shape optimization problems governed by fluid dynamics models, ranging from the full potential equation to the full compressible Navier-Stokes equations. We restrict all our discussions to gradient based methods. We begin this lecture with a short review of basic ideas in optimization where we start with algebraic problems and constraints. We derive the optimality conditions for such cases as an introduction to our problems of interest which include optimal control and shape design. We demonstrate the derivation of the optimality conditions for a control problem and discuss the case of finite dimensional control as well as the infinite dimensional control case. Our last topic is the derivation of optimality conditions for shape design problem. We derive the variation of functionals with respect to the domain (shape) of integration. Examples for optimal shape design problems which minimize the deviation of the pressure from a given pressure distribution, are given for the full potential equation and the Euler equation.

2 Review of The Basics: Gradient Based Methods

We begin by a very elementary discussion of minimization problems in a finite number of design variables. We focus first on the unconstrained case and recall a few of the basic observations made in any textbook on the subject. This is given for completeness of the presentation.

2.1 Unconstrained Optimization

Consider the unconstrained minimization problem

$$\min_{\alpha} E(\alpha) \tag{1}$$

where $\alpha = (\alpha_1, \ldots, \alpha_q)$. We refer to α as the design variable and to $E(\alpha)$ as the cost functional. A change in the design variables by $\tilde{\alpha}$ introduces a change in the functional which can be written as

$$\delta E \equiv E(\alpha + \epsilon\tilde{\alpha}) - E(\alpha) = \epsilon\tilde{\alpha}^T \nabla E + \frac{1}{2}\epsilon^2 \tilde{\alpha}^T \mathcal{H} \tilde{\alpha} + O(\epsilon^3). \tag{2}$$

Here $(\nabla E)^T = (\frac{\partial E}{\partial \alpha_1}, \ldots, \frac{\partial E}{\partial \alpha_q})$ and $\mathcal{H}$ stands for the Hessian, i.e., the matrix of second derivatives of E. We assume the Hessian $\mathcal{H}$ is positive definite, i.e., $\alpha^T \mathcal{H} \alpha > 0$ for all $\alpha \neq 0$ to guarantee a unique minimum. For small ϵ we can neglect second order terms and higher in ϵ and see that a choice of $\tilde{\alpha} = -\nabla E$ result in a reduction of the functional, that is,

$$E(\alpha - \epsilon \nabla E) - E(\alpha) = -\epsilon \|\nabla E\|^2 + O(\epsilon^2). \tag{3}$$

This is the basis for the steepest descent method and other gradient based methods. The gradient ∇E of the functional to be minimized can be easily computed for this case, say, by finite differences. At a minimum the following equations hold,

$$\texttt{Optimality Condition:} \qquad \frac{\partial E}{\partial \alpha_j} = 0 \qquad\qquad j = 1, \ldots, q. \tag{4}$$

These equations are called the (first order) necessary conditions for the problem.

2.2 Constrained Optimization

Consider next the problem

$$\begin{array}{c} \min_\alpha E(\alpha, U(\alpha)) \\ L(U(\alpha), \alpha) = 0 \end{array} \tag{5}$$

where $U = (U_1, \ldots, U_n), \alpha = (\alpha_1, \ldots, \alpha_q), L = (L_1, \ldots, L_n)$. We derive now the optimality conditions for this case. Consider changes in α and correspondingly in U as

$$\begin{array}{c} \alpha \to \alpha + \epsilon\tilde{\alpha} \\ U(\alpha) \to U(\alpha + \epsilon\tilde{\alpha}) = U + \epsilon\tilde{U} + O(\epsilon^2), \end{array} \tag{6}$$

where $\tilde{\alpha}$ and $\tilde{U}$ are related through the equation

$$L_U \tilde{U} + L_\alpha \tilde{\alpha} = 0, \tag{7}$$

which is a linearization of the constraint equation in (5). The variation in the functional can be written as

$$\delta E \equiv E(\alpha + \epsilon\tilde{\alpha}, U(\alpha + \epsilon\tilde{\alpha})) - E(\alpha, U(\alpha)) = \epsilon(\tilde{\alpha}^T E_\alpha + \tilde{U}^T E_U) + O(\epsilon^2). \tag{8}$$

For this formulation we see that a descent direction for the functional depends on $\tilde{U}$, which is not known before we have decided about the direction of change (since $\tilde{U}$ depends on $\tilde{\alpha}$). Using $\tilde{U}$ is not a viable approach and we are going to derive a different one. The idea is to eliminate the dependence of the variation in the functional on $\tilde{U}$. We derive it in details since later on we need to do a similar derivation for partial differential equations (PDE) and there things may look less obvious.

From equation (7) for $\tilde{U}$ we have (by taking transpose),

$$\tilde{U}^T L_U^T + \tilde{\alpha}^T L_\alpha^T = 0 \tag{9}$$

and therefore also

$$(\tilde{U}^T L_U^T + \tilde{\alpha}^T L_\alpha^T)\lambda = 0 \tag{10}$$

for an arbitrary vector $\lambda = (\lambda_1, \ldots, \lambda_n)$. The plan is to add this term, which is zero, to our expression for the variation in the cost functional and then by using a proper choice for λ simplifying the variation of the cost functional such that it does not depend on $\tilde{U}$. Clearly,

$$\delta E = \epsilon(\tilde{\alpha}^T E_\alpha + \tilde{U}^T E_U) + \epsilon(\tilde{U}^T L_U^T + \tilde{\alpha}^T L_\alpha^T)\lambda + O(\epsilon^2) \tag{11}$$

and by recombination of terms

$$\delta E = \epsilon\tilde{\alpha}^T(E_\alpha + L_\alpha^T\lambda) + \epsilon\tilde{U}^T(E_U + L_U^T\lambda) + O(\epsilon^2), \tag{12}$$

and this is true for all λ. Now a proper choice for λ that simplifies (12) is given by

$$\texttt{Adjoint Equation:} \quad L_U^T\lambda + E_U = 0, \tag{13}$$

which leads to

$$\delta E = \epsilon\tilde{\alpha}^T(L_\alpha^T\lambda + E_\alpha) + O(\epsilon^2). \tag{14}$$

Equation (13) for λ is called the adjoint (or costate) equation and λ is called the adjoint (costate) variable, or the Lagrange multiplier. Note the last expression for the variation of E given by (14) does not depends on $\tilde{U}$, but it does depends on λ, which satisfies the adjoint equation listed above. It is clear that the choice

$$\tilde{\alpha} = -(L_\alpha^T\lambda + E_\alpha) \tag{15}$$

is a direction of descent for the functional E, since

$$\delta E = -\epsilon\|L_\alpha^T\lambda + E_\alpha\|^2 + O(\epsilon^2). \tag{16}$$

This direction is called the steepest descent direction, and the method based on it is called the steepest descent method.

At a minimum $L_\alpha^T \lambda + E_\alpha = 0$, giving us the optimality condition (necessary condition)

$$\texttt{Optimality Conditions:} \quad \begin{array}{l} L(U(\alpha), \alpha) = 0 \\ L_U^T \lambda + E_U = 0 \\ L_\alpha^T \lambda + E_\alpha = 0. \end{array} \tag{17}$$

The left hand side of the last equation is the gradient of the functional subject to the constraints,

$$\nabla E = L_\alpha^T \lambda + E_\alpha. \tag{18}$$

2.3 Condition Number of the Hessian

The convergence rate for the steepest descent method is connected to the eigenvalues of the Hessian, in particular, to the ratio of the smallest eigenvalue to the largest one. We discuss this in some details in this section. A basic gradient descent method has the form

$$\alpha \leftarrow \alpha - \delta \nabla E \tag{19}$$

where δ is a step size, whose magnitude is determined using a line search. At the a vicinity of a minimum $\alpha = \alpha^*$, since $\nabla E(\alpha^*) = 0$, we have

$$E(\alpha, U(\alpha)) = E(\alpha^*, U(\alpha^*)) + \frac{1}{2}\tilde{\alpha}^T \mathcal{H} \tilde{\alpha} + O(\|\tilde{\alpha}\|^3), \tag{20}$$

where $\tilde{\alpha} = \alpha - \alpha^*$. From this we see that the gradient in the vicinity of the minimum can be expressed as

$$(\nabla E)(\alpha) = \mathcal{H}\tilde{\alpha}. \tag{21}$$

Substituting the last equality into (19) and subtracting α^* from both sides we get,

$$\tilde{\alpha} \leftarrow (I - \delta \mathcal{H})\tilde{\alpha}. \tag{22}$$

This relation expresses the new errors ($\tilde{\alpha}$ on left) as a function of the old errors ($\tilde{\alpha}$ on right). Convergence rate depends on

$$\|I - \delta \mathcal{H}\|. \tag{23}$$

Now we want to relate the difficulty in solving an optimization problem using the steepest descent method to the condition number of the Hessian. The Hessian is a symmetric matrix and it is also positive definite (if indeed we have a minimum). Let its eigenvalues be μ_j with eigenvectors v_j, i.e.,

$$Hv_j = \mu_j v_j \tag{24}$$

and assume that $0 < \mu_1 \leq \mu_2 \leq \ldots \leq \mu_q$. The iteration matrix was shown to be $I - \delta\mathcal{H}$ and its eigenvalues are $1 - \delta\mu_j$. For convergence we need

$$\max_j |1 - \delta\mu_j| < 1 \tag{25}$$

which implies $\delta < \frac{2}{\mu_q}$. Taking $\delta = \frac{c}{\mu_q}$, with $0 < c < 2$ gives

$$\max_j |1 - \delta\mu_j| = |1 - c\frac{\mu_1}{\mu_q}|. \tag{26}$$

Thus, the convergence rate depends on the ratio of the smallest to the largest eigenvalue of the Hessian. When dealing with symmetric positive matrices this is the condition number of the matrix.

The structure of the minimum is essentially determined by $\mathcal{H}$ and its analysis in the context of fluid dynamics equation will be demonstrated later. It plays a major role in the optimization problem and its solution processes.

Several approaches for calculating gradients of E subject to the constraints exist, and we discuss some of them.

2.4 Gradient Calculation: Constrained Optimization

Black Box Methods are the simplest approach to solve constrained optimization problems and consist of calculating the gradient in the following way. Let δE be the change in the cost functional as a result of a change $\tilde{\alpha}$ in the design variables. The following relation holds

$$\delta E = \tilde{\alpha}^T E_\alpha + \tilde{\alpha}^T U_\alpha^T E_U \tag{27}$$

where U_α are the partial derivatives of U with respect to the design variables, also termed as sensitivity derivatives. All quantities in this expression are straightforward to calculate except U_α. The dimensionality of this quantity is the dimension of U times the dimension of α.

The calculation of U_α is done in this approach using finite differences. That is, for each of the design parameters α_j in the representation of α as $\alpha = \sum_{j=1}^{q} \alpha_j e_j$, where e_j are a set of vectors spanning the design space, one perform the following process

`ALGORITHM: Black-Box Gradient Calculation`

- `Solve` $L(U(\alpha+\epsilon e_j), \alpha+\epsilon e_j) = 0$ `given` α, ϵ
- `Set` $\frac{\partial U}{\partial e_j} \approx (U(\alpha+\epsilon e_j) - U(\alpha))/\epsilon$

Once the above process is completed for $j = 1, \ldots, q$, one combines the result into

$$U_\alpha^T = (\frac{\partial U}{\partial e_1}, \ldots, \frac{\partial U}{\partial e_q}) \tag{28}$$

which is used in calculation of the gradient

$$\nabla E = E_\alpha + U_\alpha^T E_U. \tag{29}$$

Since in practical problems the dimension of U may be thousands to millions, the feasibility of calculating gradients using this approach is limited to cases where the number of design variables is very small.

The Adjoint Method is an efficient way for calculating gradients for constrained optimization problems even for very large dimensional design space. The idea is to use the expression for the gradient as appears in (18). Thus, one introduces into the solution process an extra unknown, λ, which satisfies the adjoint equation (13).

A minimization algorithm is then a repeated application of the following three steps.

`ALGORITHM: Adjoint Method`

- `Given` α `solve` $L(\alpha, U) = 0$ `for` U
- `Given` α, U `solve` $L_U^T \lambda + E_U = 0$ `for` λ
- `Update` α `as` $\alpha \leftarrow \alpha - \delta[E_\alpha + L_\alpha^T \lambda]$

2.5 Quasi-Newton Methods

When considering gradient based methods for the solution of optimization problem it is useful to consider the level lines of the cost functional. If the level lines are close to circles, then gradient based algorithms will be fast to converge since the gradient (with a minus sign) points toward the minimum. If on the other hand, when those level curves are thin ellipses the gradient does not point toward the minimum in general, and therefore gradient based methods will be slow to converge. The thin ellipses correspond to bad conditioning (large ratio of largest to smallest eigenvalue) of the Hessian.

It is important to notice the following two cases. The first is when removing just a few eigenvalues, a well conditioned system is obtain. In such cases methods which use an approximate Hessian which is constructed during the iterative process, such as BFGS, lead to very effective solvers. The second case is when the condition number remains high even after removing a large number of eigenvalues. This is typical to problems arising from discretization of partial differential equations where the number of design variables is large. Iterative algorithms of the BFGS type cannot serve as a remedy in this case and different approaches are needed. Such approaches will be described in lectures 3 and 4 following this one.

3 Control Problems Governed by PDE

Shape optimization problems which are one of our main topics, are related to control problems governed by PDE. An understanding of boundary control problems will help us to get the proper insight into shape optimization problems.

We consider the small disturbance equation, for zero Mach number, in two dimensions. The domain Ω is a rectangle whose bottom boundary has a control variable to be optimized. It is required to achieve a certain pressure distribution on that boundary. Denote by Γ the bottom boundary and by Γ_0 the rest of the boundary Ω. The potential ϕ satisfies the equation

$$\texttt{State Equation:}\quad \begin{array}{ll} \Delta\phi = 0 & \Omega \\ \frac{\partial\phi}{\partial n} = \alpha_x & \Gamma \\ \phi = g & \Gamma_0 \end{array} \tag{30}$$

where α is the design variable. This problem is related to a shape design problem in which the bottom boundary is described by the function α, and the boundary condition for ϕ on this boundary is $\frac{\partial\phi}{\partial n} = 0$. We will come to this relation later on.

We consider the cost functional

$$E(\alpha) = \frac{1}{2}\int_\Gamma (p - p^*)^2 dx \tag{31}$$

where $p = \phi_x$, and we would like to construct a formula for the gradient of this functional. We consider a perturbation of the design variable by $\epsilon\tilde{\alpha}$ and the corresponding change in ϕ by $\epsilon\tilde{\phi}$, which satisfies

$$\begin{array}{ll} \Delta\tilde{\phi} = 0 & \Omega \\ \frac{\partial\tilde{\phi}}{\partial n} = \tilde{\alpha}_x & \Gamma \\ \tilde{\phi} = 0 & \Gamma_0. \end{array} \tag{32}$$

The variation in the functional is

$$
\begin{aligned}
\delta E \equiv E(\alpha+\epsilon\alpha)-E(\alpha) &= \tfrac{1}{2}\int_\Gamma [(p+\epsilon\tilde{p}-p^*)^2-(p-p^*)^2]dx \\
&= \epsilon\int_\Gamma(\phi_x-p^*)\tilde{\phi}_x dx + O(\epsilon^2) \\
&= -\epsilon\int_\Gamma(\phi_x-p^*)_x\tilde{\phi}dx + O(\epsilon^2)
\end{aligned}
\tag{33}
$$

where integration by parts have been used in the last equality. As in the abstract constrained optimization problem we discussed in section (2.2), we see that the change in the functional depends on the the sensitivity derivatives $\tilde{\phi}$, and we would like to eliminate this dependence, in order to get an efficient computation of the gradient. We do it by adding a term to δE which is the differential analog of the term $\tilde{U}^T L_U^T\lambda+\tilde{\alpha}^T L_\alpha^T\lambda$ in the algebraic case. Then a proper choice for λ will result in the desired form for the variation in the functional.

Let λ be an arbitrary function defined in the same domain as ϕ. From equation (32) for $\tilde{\phi}$ we have

$$
0=\int_\Omega \lambda\Delta\tilde{\phi}dx=\int_\Omega\tilde{\phi}\Delta\lambda dx+\int_{\partial\Omega}(\lambda\frac{\partial\tilde{\phi}}{\partial n}-\tilde{\phi}\frac{\partial\lambda}{\partial n})ds \tag{34}
$$

where the second equality follows from integration by parts. This is the analog of equation (10) that we have in the algebraic case. Adding the right hand side of (34) (multiplied by ϵ) to δE we get

$$
\delta E=-\epsilon\int_\Gamma(\phi_x-p^*)_x\tilde{\phi}dx+\epsilon\int_\Omega\Delta\lambda\tilde{\phi}dx+\epsilon\int_{\partial\Omega}(\lambda\frac{\partial\tilde{\phi}}{\partial n}-\tilde{\phi}\frac{\partial\lambda}{\partial n})ds+O(\epsilon^2). \tag{35}
$$

Since $\partial\Omega=\Gamma+\Gamma_0$ we can break the integral $\int_{\partial\Omega}$ into $\int_\Gamma+\int_{\Gamma_0}$ and then combine the $\int_\Gamma$ terms, to obtain

$$
\delta E=-\epsilon\int_\Gamma\tilde{\phi}[(\phi_x-p^*)_x+\frac{\partial\lambda}{\partial n}]ds-\epsilon\int_{\Gamma_0}\tilde{\phi}\frac{\partial\lambda}{\partial n}+\epsilon\int_{\partial\Omega}\lambda\frac{\partial\tilde{\phi}}{\partial n}ds+\epsilon\int_\Omega\tilde{\phi}\Delta\lambda dx+O(\epsilon^2) \tag{36}
$$

In order to eliminate the dependence of δE on $\tilde{\phi}$ we make the following choice for λ

$$
\texttt{Adjoint Equation:}\quad
\begin{array}{ll}
\Delta\lambda=0 & \Omega \\
\frac{\partial\lambda}{\partial n}+(\phi_x-p^*)_x=0 & \Gamma \\
\lambda=0 & \Gamma_0.
\end{array}
\tag{37}
$$

Therefore,

$$
\delta E=\epsilon\int_\Gamma\lambda\frac{\partial\tilde{\phi}}{\partial n}dx+O(\epsilon^2)=\epsilon\int_\Gamma\lambda\tilde{\alpha}_x dx+O(\epsilon^2)=-\epsilon\int_\Gamma\lambda_x\tilde{\alpha}+O(\epsilon^2) \tag{38}
$$

where integration by parts was used in the last equality. The expression for the changes in the functional is given as as a function of the changes in the design variable, as well the adjoint variable λ which satisfies the adjoint equation (37), (or costate equation in control terminology). We would like now to pick a direction of change $\tilde{\alpha}$ that will result in reduction of the cost functional. We distinguish two cases.

I. Finite Dimensional Control. In this case we assume that the design variable $\alpha(x)$ has a representation

$$\alpha(x) = \sum_{j=1}^{q} \alpha_j f_j(x) \tag{39}$$

and a similar expression for $\tilde{\alpha}$, where the functions $f_j, j = 1, \ldots, q$ are prescribed. This implies

$$\delta E = -\epsilon \sum_{j=1}^{q} \tilde{\alpha}_j \int_\Gamma \lambda_x f_j dx + O(\epsilon^2), \tag{40}$$

and hence

$$\frac{\partial E}{\partial \alpha_j} = -\int_\Gamma \lambda_x f_j dx \tag{41}$$

and the choice

$$\tilde{\alpha}_j = \int_\Gamma \lambda_x f_j dx \tag{42}$$

will result in a reduction of the cost functional by

$$\delta E = -\epsilon \sum_{j=1}^{q} (\int_\Gamma \lambda_x f_j dx)^2 + O(\epsilon^2). \tag{43}$$

At a minimum the following conditions hold,

$$\frac{\partial E}{\partial \alpha_j} = -\int_\Gamma \lambda_x f_j dx = 0 \qquad j = 1, \ldots, q. \tag{44}$$

Note that the gradient given in (44) is in terms of λ.

II. Infinite Dimensional Control. In this case we regard the variable α as a function defined on the boundary Γ. A proper choice that will result in a reduction of the functional is given in terms of λ,

$$\tilde{\alpha}(x) = \lambda_x(x) \qquad x \in \Gamma \tag{45}$$

and the corresponding reduction in the functional is given this time by

$$\delta E = -\epsilon \int_\Gamma |\lambda_x|^2 dx + O(\epsilon^2). \tag{46}$$

An algorithm for solving this control problem consists of repeated application of the following three steps, until convergence (of the gradient to zero),

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   ALGORITHM
(1) Solve the state equation (30) for φ
(2) Solve the adjoint equation (37) for λ
(3) Update α by α − δα̃    , where δ is found by line search.
    α̃ is given by (42) or (45).
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4 Shape Design Problems

We consider next problems in which the design variable is the shape of the domain in which a PDE is given. We need to derive formulas for the changes of different cost functionals which depend on the shape. Let us take some examples of practical importance.

Example I: The functional depends on the whole domain. Consider the functional

$$J(\Omega, u) = \int_{\Omega} F(u)dx \tag{47}$$

which depends on the domain as well as on a function $u = u(\Omega)$, which depends on that domain too. For the moment we do not specify exactly the dependence of this function on the domain. Later on this function will be a solution of a PDE defined in Ω, and will change as we change the domain Ω.

We need to calculate the variation of this functional with respect to Ω. To do this we assume that the function $u(\Omega)$ is defined in a slightly larger domain that includes Ω. We examine $J(\Omega_\epsilon, u(\Omega^\epsilon)) - J(\Omega, u(\Omega))$ where Ω_ϵ is a small perturbation of Ω, parameterized by a small number ϵ. The perturbation of the shape is done following Pironneau [13]. The boundary of Ω is perturbed in the direction of the outward normal to Ω by $\epsilon\alpha(s)\mathbf{n}$, where s is a parameterization of the boundary, $\mathbf{n}$ is the outward normal and $\alpha(s)$ is an arbitrary function defined on the boundary. We use the short notation, $u^\epsilon = u(\Omega^\epsilon)$ and $u = u(\Omega)$. We have

$$\begin{aligned} J(\Omega_\epsilon, u^\epsilon) - J(\Omega, u) &= \textstyle\int_{\Omega_\epsilon - \Omega} F(u^\epsilon)dx - \int_{\Omega - \Omega_\epsilon} F(u)dx \\ &\quad + \textstyle\int_{\Omega \cap \Omega_\epsilon} F(u^\epsilon)dx - \int_{\Omega \cap \Omega_\epsilon} F(u)dx \end{aligned} \tag{48}$$

For small ϵ these integrals can be approximated as follows

$$\int_{\Omega_\epsilon - \Omega} F(u)dx = \epsilon \int_{\Gamma^+} \alpha(s)F(u)ds + O(\epsilon^2) \tag{49}$$

$$\int_{\Omega-\Omega_\epsilon} F(u)dx = -\epsilon \int_{\Gamma^-} \alpha(s)F(u)ds + O(\epsilon^2) \tag{50}$$

$$\int_{\Omega\cap\Omega_\epsilon} F(u^\epsilon)dx - \int_{\Omega\cap\Omega_\epsilon} F(u)dx = \epsilon \int_\Omega F_u(u)\tilde{u}dx + O(\epsilon^2) \tag{51}$$

where

$$\tilde{u} = \lim_{\epsilon\to 0} \frac{1}{\epsilon}[u^\epsilon - u] \tag{52}$$

and $\Gamma^+ = \{s \in \Gamma | \alpha(s) > 0\}$ and $\Gamma^- = \{s \in \Gamma | \alpha(s) \leq 0\}$. We conclude that,

$$\frac{1}{\epsilon}[J(\Omega_\epsilon) - J(\Omega)] = \int_\Gamma \alpha(s)F(u)ds + \int_\Omega F_u(u)\tilde{u}ds + O(\epsilon). \tag{53}$$

This formula is useful when we have functionals defined on the interior of the domain up to the boundary. Recall that in order to construct the necessary conditions, or to calculate gradients, we need to consider this type of expression.

Example II: Boundary Functionals. Consider next the functional

$$J(\Gamma, u) = \int_\Gamma f(u)ds \tag{54}$$

where $u = u(\Gamma)$, ds is an area element, and Γ is part of the boundary of a domain Ω. The function u depends on the domain in a way which we do not prescribe at the moment. Again we are interested in perturbations of the domain, and as a result of it perturbations of Γ. It is convenient to use the same type of perturbation as before. The new boundary will be denoted by Γ_ϵ and we want to calculate

$$\frac{1}{\epsilon}[J(\Gamma_\epsilon, u^\epsilon) - J(\Gamma, u)] \tag{55}$$

for small ϵ. This case is slightly more complicated since we have to consider the change of the area element ds as well. Consider a line element ds, where the radius of curvature is given by R. Note that this line element can be written as $Rd\theta$ where R is the radius of curvature and $d\theta$ represent an infinitesimal angle. A change in the boundary by $\epsilon\alpha\mathbf{n}$ changes the line element to $(R-\epsilon\alpha)d\theta = (1-\epsilon\frac{\alpha}{R})Rd\theta = (1-\epsilon\frac{\alpha}{R})ds$. Thus, we obtain a formula, for the two dimensional case, for the new line element

$$ds^\epsilon = (1 - \epsilon\frac{\alpha}{R})ds. \tag{56}$$

For problem in three dimension we consider two orthogonal tangential coordinates and in each direction a similar result hold for the line element. The area element being the product of the two line elements has the formula (56) but now with

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \tag{57}$$

where R_1 and R_2 are the radiuses of curvature in two orthogonal directions on the surface. Note that the quantity $\frac{1}{R}$ does not depends on the choice of coordinate system since it is the trace of the matrix of second derivatives of the surface describing the boundary.

In order to obtain a simple expression for the variation of the functional as a function of the boundary Γ we have to express $\int_{\Gamma_\epsilon} f^\epsilon(u^\epsilon)ds$ in terms of an integral and quantities on Γ.

Consider a point $x \in \Gamma$ and the corresponding shift of it to $x^\epsilon \in \Gamma_\epsilon$ given by $x^\epsilon = x + \epsilon\alpha\mathbf{n}$. The integral depends on u which is a function of x, and

$$u(x^\epsilon) = u(x + \epsilon\alpha\mathbf{n}) = u(x) + \epsilon\alpha\frac{\partial u}{\partial n} + O(\epsilon^2) \tag{58}$$

$$u^\epsilon(x^\epsilon) = u(x + \epsilon\alpha\mathbf{n}) + \epsilon\tilde{u}(x + \epsilon\alpha\mathbf{n}) + O(\epsilon^2) = u(x) + \epsilon\alpha\frac{\partial u}{\partial n}(x) + \epsilon\tilde{u}(x) + O(\epsilon^2) \tag{59}$$

For simplicity, we assume that $f(u)$ does not depends explicitly on x, although this can be handled as well. Using the last two formulas we have

$$\begin{aligned} f(u^\epsilon)_{|\Gamma_\epsilon} &= f(u + \epsilon\tilde{u} + \epsilon\alpha\tfrac{\partial u}{\partial n})_{|\Gamma} + O(\epsilon^2) \\ &= f(u)_{|\Gamma} + \epsilon\alpha f_u(u)\tfrac{\partial u}{\partial n}_{|\Gamma} + \epsilon f_u(u)\tilde{u}_{|\Gamma} + O(\epsilon^2). \end{aligned} \tag{60}$$

Using this together with the formula for the line (area) element (56) we get

$$\begin{aligned} f(u^\epsilon)ds^\epsilon &= (f(u) + \epsilon\alpha f_u(u)\tfrac{\partial u}{\partial n} + \epsilon f_u(u)\tilde{u})(1 - \epsilon\tfrac{\alpha}{R})ds \\ &= f(u)ds + \epsilon[\alpha f_u(u)\tfrac{\partial u}{\partial n} - \tfrac{\alpha}{R}f(u)]ds + \epsilon f_u(u)\tilde{u}ds + O(\epsilon^2) \end{aligned} \tag{61}$$

Substituting (61) into (55) we have

$$\frac{1}{\epsilon}[\int_{\Gamma_\epsilon} f^\epsilon(u^\epsilon)ds - \int_\Gamma f(u)ds] = \int_\Gamma \alpha(-\frac{f(u)}{R} + f_u(u)\frac{\partial u}{\partial n})ds + \int_\Gamma f_u(u)\tilde{u}ds + O(\epsilon^2). \tag{62}$$

5 Applications to Fluid Dynamics

We use next the ideas developed in the previous sections to study shape optimization problems governed by two fluid dynamics equations. The first is the Full Potential equation and the second is the Euler equations. We derive in both case the optimality (necessary) conditions in details.

5.1 Shape Design Using The Full Potential Equation

Consider the Full Potential (FP) equation

$$\begin{array}{ll} \nabla\rho\nabla\phi = 0 & \Omega \\ \phi = \phi_\infty & \partial\Omega - \Gamma \\ \nabla\phi\cdot\mathbf{n} = 0 & \Gamma \end{array} \tag{63}$$

where $\rho = f(q)$ with $q = \frac{1}{2}|\nabla\phi|^2$ and the following shape optimization problem,

$$\min_{\Gamma} \frac{1}{2}\int_{\Gamma}(p - p^*)^2 ds \tag{64}$$

where $p = g(q)$. We derive the necessary conditions for this problem, and obtain a formula for the gradient for this functional subject to the FP equation (63).

As a result of changes in the shape Γ, the potential changes to $\phi + \epsilon\tilde{\phi} + O(\epsilon^2)$ and ρ into $\rho + \epsilon\tilde{\rho} + O(\epsilon^2)$. Moreover,

$$\tilde{\rho} = \frac{\partial f}{\partial q}\nabla\phi \cdot \nabla\tilde{\phi} \tag{65}$$

and the equation governing $\tilde{\phi}$ is

$$\nabla\tilde{\rho}\nabla\phi + \nabla\rho\nabla\tilde{\phi} = 0. \tag{66}$$

The functional variation with respect to Γ (see equation (62)) can be written as

$$\delta J = \epsilon\int_{\Gamma}(p - p^*)\tilde{p}ds + \epsilon\int_{\Gamma}\alpha[\frac{\partial p}{\partial n}(p - p^*) - \frac{(p - p^*)^2}{2R}]ds + O(\epsilon^2). \tag{67}$$

From the boundary condition $\frac{\partial\phi}{\partial n} = 0$ some terms are simplified, in particular $\frac{\partial p}{\partial n} = \frac{1}{2}\frac{\partial g}{\partial q}\frac{\partial}{\partial n}[(\frac{\partial\phi}{\partial n})^2 + \sum_{j=1}^{d-1}(\frac{\partial\phi}{\partial t_j})^2] = 0$. We also have the relation

$$\tilde{p} = \frac{\partial p}{\partial q}(\frac{\partial\phi}{\partial n}\frac{\partial\tilde{\phi}}{\partial n} + \frac{\partial\phi}{\partial t}\frac{\partial\tilde{\phi}}{\partial t}) = \frac{\partial g}{\partial q}\nabla_{\Gamma}\phi \cdot \nabla_{\Gamma}\tilde{\phi} \tag{68}$$

where ∇_{Γ} stands for the tangential gradient. Substituting these into δJ and using integration by parts for the $\nabla_{\Gamma}\tilde{\phi}$ terms gives

$$\delta J = -\int_{\Gamma}[\tilde{\phi}\sum_{j=1}^{d-1}\frac{\partial}{\partial t_j}\left(\frac{\partial g}{\partial q}(p - p^*)\frac{\partial\phi}{\partial t_j}\right) + \alpha\frac{(p - p^*)^2}{2R}]ds \tag{69}$$

This expression depends on $\tilde{\phi}$ which is to be eliminated using the same idea as before. To this end we use the identity

$$\int_{\Omega}\lambda(\nabla\tilde{\rho}\nabla\phi + \nabla\rho\nabla\tilde{\phi})dx = 0 \tag{70}$$

which follows from (66) and holds for an arbitrary λ. The relation $\tilde{\rho} = \frac{\partial f}{\partial q}\nabla\tilde{\phi} \cdot \nabla\phi$ and integration by parts of each of the terms in the above integral give

$$\int_{\Omega}\lambda\nabla\frac{\partial f}{\partial q}[\nabla\phi \cdot \nabla\tilde{\phi}]\nabla\phi = \int_{\Omega}\tilde{\phi}\nabla\frac{\partial f}{\partial q}[\nabla\lambda \cdot \nabla\phi]\nabla\phi dx \tag{71}$$

$$\int_\Omega \lambda \nabla \rho \nabla \tilde{\phi} dx = \int_\Omega \tilde{\phi} \nabla \rho \nabla \lambda dx + \int_{\partial\Omega} \rho (\lambda \frac{\partial \tilde{\phi}}{\partial n} - \tilde{\phi} \frac{\partial \lambda}{\partial n}) ds \tag{72}$$

where in the first integral we used the relation $\nabla \phi \cdot \mathbf{n} = 0$ on Γ as well as $\tilde{\phi} = 0$ and $\nabla_\Gamma \tilde{\phi} = 0$ on $\partial\Omega - \Gamma$. Thus,

$$\int_\Omega \tilde{\phi} (\nabla \rho \nabla \lambda + \nabla \frac{\partial f}{\partial q} [\nabla \lambda \cdot \nabla \phi] \nabla \phi) dx + \int_{\partial\Omega} \rho (\lambda \frac{\partial \tilde{\phi}}{\partial n} - \tilde{\phi} \frac{\partial \lambda}{\partial n}) ds = 0 \tag{73}$$

for an arbitrary smooth function λ. This is the analog of equation (10) of section (2.2).

Before we add this term to the functional we need to express certain terms in the boundary. The wall boundary condition for ϕ on Γ_ϵ

$$\nabla \phi^\epsilon \cdot \mathbf{n}^\epsilon{}_{|\Gamma^\epsilon} = \nabla (\phi + \epsilon \tilde{\phi}) \cdot \mathbf{n}^\epsilon{}_{|\Gamma^\epsilon} = 0 \tag{74}$$

will be transfered to Γ. It is easy to see that

$$\mathbf{n}^\epsilon = \mathbf{n} - \epsilon \sum_{j=1}^{d-1} \frac{\partial \alpha}{\partial t_j} \mathbf{t_j} + O(\epsilon^2) \tag{75}$$

by considering one dimension at a time. Therefore

$$\nabla (\phi + \epsilon \tilde{\phi} + \epsilon \alpha \frac{\partial \phi}{\partial n} + O(\epsilon^2))_{|\Gamma} \cdot (\mathbf{n} - \epsilon \sum_{j=1}^{d-1} \frac{\partial \alpha}{\partial t_j} \mathbf{t_j} + O(\epsilon^2))_{|\Gamma} = 0 \tag{76}$$

Using the boundary condition $\nabla \phi \cdot \mathbf{n}_{|\Gamma} = 0$ we get

$$\nabla \tilde{\phi} \cdot \mathbf{n} + \alpha \frac{\partial^2 \phi}{\partial n^2} - \sum_{j=1}^{d-1} \frac{\partial \alpha}{\partial t_j} \nabla \phi \cdot \mathbf{t_j} = 0 \qquad \Gamma \tag{77}$$

The expression for the change in the functional as given in (69) depends on α as well as on $\tilde{\phi}$. To eliminate the dependence on $\tilde{\phi}$ we add the left hand side of (73). We then collect terms involving $\tilde{\phi}$ separately from terms involving $\frac{\partial \tilde{\phi}}{\partial n}$, and use the boundary condition for $\frac{\partial \tilde{\phi}}{\partial n}$ on Γ, giving

$$\begin{aligned} \delta J = \; & - \int_\Gamma \tilde{\phi} [\textstyle\sum_{j=1}^{d-1} \frac{\partial}{\partial t_j} (\frac{\partial p}{\partial q} (p - p^*) \frac{\partial \phi}{\partial t_j}) + \rho \frac{\partial \lambda}{\partial n}] ds \\ & - \int_\Gamma \alpha [\rho \lambda \frac{\partial^2 \phi}{\partial n^2} + \frac{(p-p^*)^2}{2R} - \textstyle\sum_{j=1}^{d-1} \frac{\partial}{\partial t_j} (\lambda \rho \frac{\partial \phi}{\partial t_j})] ds \\ & + \int_{\partial\Omega - \Gamma} \rho (\lambda \frac{\partial \tilde{\phi}}{\partial n} - \tilde{\phi} \frac{\partial \lambda}{\partial n}) ds \\ & + \int_\Omega \tilde{\phi} (\nabla \rho \nabla \lambda + \nabla \frac{\partial f}{\partial q} [\nabla \lambda \cdot \nabla \phi] \nabla \phi) dx \end{aligned} \tag{78}$$

Now we choose λ such that it satisfies

`Adjoint Equation:`

$$\begin{array}{ll} \nabla \rho \nabla \lambda + \nabla (\nabla \lambda \cdot \nabla \phi \frac{\partial \rho}{\partial q} \nabla \phi) = 0 & \Omega \\ \rho \frac{\partial \lambda}{\partial n} + \sum_{j=1}^{d-1} \frac{\partial}{\partial t_j} [\frac{\partial g}{\partial q} (p - p^*) \frac{\partial \phi}{\partial t_j}] = 0 & \Gamma \\ \lambda = 0 & \partial\Omega - \Gamma \end{array} \tag{79}$$

and then the variation of the functional simplifies to

$$\delta J = -\int_{\Gamma} \alpha[\rho\lambda\frac{\partial^2\phi}{\partial n^2} + \frac{(p-p^*)^2}{2R} - \sum_{j=1}^{d-1}\frac{\partial}{\partial t_j}(\lambda\rho\frac{\partial\phi}{\partial t_j})]ds. \tag{80}$$

The gradient of the functional is given by

$$\nabla J = -\rho\lambda\frac{\partial^2\phi}{\partial n^2} - \frac{(p-p^*)^2}{2R} + \sum_{j=1}^{d-1}\frac{\partial}{\partial t_j}(\lambda\rho\frac{\partial\phi}{\partial t_j}) \qquad\qquad \Gamma. \tag{81}$$

5.2 Shape Design Using The Euler Equations

Our next example is a similar minimization problem but this time subject to the Euler equation. Namely,

$$\min_{\Gamma}\frac{1}{2}\int_{\Gamma}(p-p^*)^2 ds \tag{82}$$

where $p = p(U)$, and U is the solution of the Euler equation. Here U stands for the variables $(\rho, \rho\mathbf{u}, E)$ and $\mathbf{u} = (u, v, w)$. The Euler equations in conservation form are written as

$$f_x + g_y + h_z = 0 \tag{83}$$

where

$$f = AU \qquad g = BU \qquad h = CU, \tag{84}$$

and where the matrices A, B, C can be found, for example, in Hirsch [12]. An important property of the equation that we use here is

$$f_x = AU_x \qquad g_y = BU_y \qquad h = Cu_z. \tag{85}$$

The change $\tilde{f}$ in the flux vector f satisfies,

$$f(U+\epsilon\tilde{U}) = f(U) + \epsilon\frac{\partial f}{\partial U}\tilde{U} + O(\epsilon^2) = f(U) + \epsilon A\tilde{U} + O(\epsilon^2) = f + \epsilon\tilde{f} \tag{86}$$

and similar expressions for $\tilde{g}, \tilde{h}$. The equation for the perturbation quantities reads

$$\tilde{f}_x + \tilde{g}_y + \tilde{h}_z = 0 \tag{87}$$

or equivalently,

$$(A\tilde{U})_x + (B\tilde{U})_y + (C\tilde{U})_z = 0. \tag{88}$$

Now consider the following identity which follows from integration by parts,

$$\begin{array}{ll} \int_\Omega \Lambda \cdot (A\tilde{U})_x dV & = -\int_\Omega \Lambda_x \cdot A\tilde{U} dV + \int_{\partial\Omega} \Lambda \cdot A\tilde{U}\mathbf{n}\cdot\mathbf{i}ds \\ & = -\int_\Omega A^T\Lambda_x \cdot \tilde{U} dV + \int_{\partial\Omega} A^T\Lambda \cdot \tilde{U}\mathbf{n}\cdot\mathbf{i}ds \end{array} \tag{89}$$

and similar integrals for the g and h terms. Combining these identities we arrive at

$$\begin{array}{l} -\int_\Omega (A^T\Lambda_x + B^T\Lambda_y + C^T\Lambda_z)\cdot\tilde{U}dV \\ +\int_{\partial\Omega}(A^T\mathbf{n}\cdot\mathbf{i} + B^T\mathbf{n}\cdot\mathbf{j} + C^T\mathbf{n}\cdot\mathbf{k})\Lambda\cdot\tilde{U}ds \quad = 0, \end{array} \tag{90}$$

for an arbitrary Λ. We will use the notation

$$D = A\mathbf{n}\cdot\mathbf{i} + B\mathbf{n}\cdot\mathbf{j} + C\mathbf{n}\cdot\mathbf{k} \tag{91}$$

and note that DU is the normal flux at the boundary which has the form, see Hirsch [12],

$$DU = \begin{pmatrix} \rho\mathbf{u}\cdot\mathbf{n} \\ \rho(\mathbf{u}\cdot\mathbf{n})\mathbf{u} + p\mathbf{n} \\ (E+p)\mathbf{u}\cdot\mathbf{n} \end{pmatrix}, \tag{92}$$

and at a wall where $\mathbf{u}\cdot\mathbf{n} = 0$, it reduces to

$$DU_{|\Gamma} = \begin{pmatrix} 0 \\ p\mathbf{n} \\ 0 \end{pmatrix}. \tag{93}$$

We have $D\tilde{U} = \tilde{DU}$ following (84),(86) and its analog for the $\tilde{g}, \tilde{h}$ terms, and

$$\tilde{(p\mathbf{n})} = \tilde{p}\mathbf{n} + p\tilde{\mathbf{n}}. \tag{94}$$

Combining the last equalities and $\tilde{\mathbf{n}} = -\sum_{j=1}^{d-1}\frac{\partial\alpha}{\partial t_j}\mathbf{t}_j$ from (75), we get

$$\int_\Gamma \Lambda\cdot D\tilde{U}ds = \int_\Gamma \Lambda\cdot\tilde{DU}ds = \int_\Gamma \tilde{p}\lambda\cdot\mathbf{n}ds - \int_\Gamma p\sum_{j=1}^{d-1}\frac{\partial\alpha}{\partial t_j}(\lambda\cdot\mathbf{t}_j)ds \tag{95}$$

where we used the notation $\Lambda = (\lambda_1, \lambda, \lambda_5)$, and $\lambda = (\lambda_2, \lambda_3, \lambda_4)$. The wall boundary condition

$$\mathbf{u}\cdot\mathbf{n}_{|\Gamma} = 0 \tag{96}$$

becomes upon perturbation

$$\mathbf{u}^\epsilon\cdot\mathbf{n}^\epsilon{}_{|\Gamma^\epsilon} = 0, \tag{97}$$

and as before we transfer this boundary condition to the original boundary Γ,

$$(\mathbf{u}+\epsilon\tilde{\mathbf{u}})\cdot\mathbf{n}^{\epsilon}_{|\Gamma^{\epsilon}} = (\mathbf{u}+\epsilon\alpha\frac{\partial\mathbf{u}}{\partial n}+\epsilon\tilde{\mathbf{u}})_{|\Gamma}\cdot(\mathbf{n}-\epsilon\sum_{j=1}^{d-1}\frac{\partial\alpha}{\partial t_j}\mathbf{t_j})_{|\Gamma}+O(\epsilon^2). \tag{98}$$

Collecting only the ϵ terms we get

$$\tilde{\mathbf{u}}\cdot\mathbf{n}-\sum_{j=1}^{d-1}\frac{\partial\alpha}{\partial t_j}\mathbf{u}\cdot\mathbf{t_j}+\alpha\frac{\partial\mathbf{u}}{\partial n}\cdot\mathbf{n}=0 \qquad \Gamma. \tag{99}$$

The variation of the functional

$$\delta J=\int_\Gamma[(p-p^*)\tilde{p}+\alpha(p-p^*)\frac{\partial p}{\partial n}-\alpha\frac{(p-p^*)^2}{2R}]ds \tag{100}$$

will be simplified by adding (90) to it, but with a choice of Λ which makes the volume integral vanish. Thus, we assume that

$$A^T\Lambda_x+B^T\Lambda_y+C^T\Lambda_z=0 \qquad \Omega \tag{101}$$

Using (90),(95) it leads to

$$\begin{aligned}\delta J &= \textstyle\int_\Gamma[p-p^*+\lambda\cdot\mathbf{n}]\tilde{p}ds\\ &\quad+\textstyle\int_\Gamma\alpha[-\frac{(p-p^*)^2}{2R}+(p-p^*)\frac{\partial p}{\partial n}]ds\\ &\quad-\textstyle\int_\Gamma p\sum_{j=1}^{d-1}\frac{\partial\alpha}{\partial t_j}(\lambda\cdot\mathbf{t}_j)ds\\ &\quad+\textstyle\int_{\partial\Omega-\Gamma}D^T\Lambda\cdot\tilde{U}ds\end{aligned} \tag{102}$$

Now we come to use the boundary conditions for $\tilde{U}$. We begin with the far field $\partial\Omega-\Gamma$. We assume that the boundary conditions there are given in terms of characteristic variables and assume that T is the matrix such that $T\tilde{U}$ are the characteristic variables. We write the far field term as

$$\int_{\partial\Omega-\Gamma}D^T\Lambda\cdot\tilde{U}ds=\int_{\partial\Omega-\Gamma}D^T\Lambda\cdot T^{-1}T\tilde{U}ds=\int_{\partial\Omega-\Gamma}T^{-T}D^T\Lambda\cdot T\tilde{U}ds \tag{103}$$

We distinguish the following cases. *Supersonic inflow:* all variables are specified at inflow, and thus $\tilde{U}=0$. Thus, no boundary conditions are imposed on Λ. *Supersonic outflow:* No boundary conditions are specified for U, hence $\tilde{U}$ is arbitrary there and therefore we are led to the choice $\Lambda=0$ at supersonic outflow. *Subsonic inflow:* 4 conditions are specified (3 in 2D), and those are $(T\tilde{U})_{1,2,3,4}=0$, thus $(T\tilde{U})_5$ is arbitrary, leading to $(T^{-T}D^T\Lambda)_5=0$. *Subsonic outflow:* one condition is given for U which implies $(T\tilde{U})_5=0$ and therefore $(T^{-T}D\Lambda)_{1,2,3,4}=0$. On the *wall* Γ we choose

$$\lambda\cdot\mathbf{n}+p-p^*=0. \tag{104}$$

In summary, the boundary conditions for Λ are

$$\begin{array}{ll} \texttt{supersonic inflow} & \text{none} \\ \texttt{subsonic inflow} & (T^{-T}D^T\Lambda)_5 = 0 \\ \texttt{supersonic outflow} & \Lambda = 0 \\ \texttt{subsonic outflow} & (T^{-T}D^T\Lambda)_{1,2,3,4} = 0 \\ \texttt{Wall} & \lambda \cdot \mathbf{n} + p - p^* = 0 \end{array} \tag{105}$$

With this choice for Λ together with the interior equation (101) we get that δJ involves integrals depending on α and Λ and not on $\tilde{U}$ terms. Rearrangement by using integration by parts gives,

$$\delta J = \int_\Gamma \alpha[-\frac{(p-p^*)^2}{2R} + (p-p^*)\frac{\partial p}{\partial n} - div(p\lambda)]ds. \tag{106}$$

The gradient of the functional in this case is therefore given by

$$\nabla_\Gamma J = -\frac{(p-p^*)^2}{2R} + (p-p^*)\frac{\partial p}{\partial n} - div(p\lambda). \tag{107}$$

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