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Optimal Shape Design for Elliptic Systems

With 57 Figures

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"All life is yoga"—Sri Aurobindo

Preface

The study of optimal shape design can be arrived at by asking the following question: "What is the best shape for a physical system?" This book is an applications-oriented study of such physical systems; in particular, those which can be described by an elliptic partial differential equation and where the shape is found by the minimum of a single criterion function. There are many problems of this type in high-technology industries. In fact, most numerical simulations of physical systems are solved not to gain better understanding of the phenomena but to obtain better control and design. Problems of this type are described in Chapter 2.

Traditionally, optimal shape design has been treated as a branch of the calculus of variations and more specifically of optimal control. This subject interfaces with no less than four fields: optimization, optimal control, partial differential equations (PDEs), and their numerical solutions—this is the most difficult aspect of the subject. Each of these fields is reviewed briefly: PDEs (Chapter 1), optimization (Chapter 4), optimal control (Chapter 5), and numerical methods (Chapters 1 and 4).

If a computer program is used to yield the numerical solution of a PDE describing an optimal shape design problem, an optimization algorithm will have to be written (usually a gradient algorithm is used). Optimal control theory provides the basic techniques for computing the derivatives of the criteria functions with respect to the boundary. So in essence, optimal control and optimization may be applied when the "control" becomes associated with the shape of the domain (Chapter 6). However, problems are encountered with numerical discretization; thus two chapters are devoted to applications with finite elements (Chapter 7) and in a finite difference, or boundary element context (Chapter 8). Finally, two industrial applications are included (Chapter 9) for a practical illustration of the theory studied. Chapter 2 deals with the problem of the existence of solutions to PDEs. A study of this more theoretical question sheds some light on certain difficulties of convergence that are encountered in practice.

Optimal shape design has been studied in great depth by the French School of Applied Mathematics (at the Universities of Paris and Nice, in particular), and this book presents this approach. It represents a special blend of mathematics and engineering which some engineers may find too theoretical and applied mathematicians too computational. The best compromise between these two opposing points of view is difficult to find.

I am indebted to many of my colleagues whose work is presented in this book; in particular to Mrs. F. Angrand, A. Dervieux, H. Ghidouche, R. Glowinski, J. L. Lions, A. Marrocco, F. Murat, J. Periaux, E. Polak, and G. Poirier, L. Tartar, Sir James Lighthill and to Mrs. Barny for preparing the manuscript. I am also very grateful to my colleagues A. Angrand, D. Begis, J. Fray, Th. Labrujere, R. Glowinski, A. Marrocco, Ph. Morice, and J. Sloof for allowing their numerical results to be reproduced here. I wrote the book while on leave at the University of Tokyo, School of Applied Sciences (at the invitation of H. Kawarada through JSPS). The material was presented as a graduate course at the University of Paris 6 in 1981.

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Contents

Notation

Ω: open set of $\mathbb{R}^n$ (usually bounded), domain of definition of the PDE
D, $\mathbb{C}$: close subsets of Ω
$\mathring{\mathbb{C}}$: interior of $\mathbb{C}$
$\chi_{\mathbb{C}}$: characteristic function of $\mathbb{C}$
$\Omega - \mathbb{C}$: $\Omega \cap \mathbb{C}^c$, only if $\Omega \supset \mathbb{C}$
$\delta(D, \mathbb{C})$: Hausdorff distance [see Eq. (5) in Chapter 3]
Γ, S: whole or parts of the boundary of Ω
$\partial\Omega$: boundary of Ω
$x = (x_1, \ldots, x_n)$: point of Ω
$|x|$: Euclidian norm of $x \in \mathbb{R}^n$
$n(x)$: outward unit normal at $x \in \partial\Omega$ of Ω
$\mathbf{s}(x)$: one unit tangent vector at $x \in \partial\Omega$
$dx = dx_1\, dx_2 \ldots dx_n$: infinitesimal volume
$d\Gamma$: infinitesimal area
$L^2(\Omega)^m$: space of square integrable functions from Ω into $\mathbb{R}^m$.
$|\cdot|_0$: norm of $L^2(\Omega)^m$ [see Eq. (5) in Chapter 1]
$(\cdot,\cdot)$: scalar product of $L^2(\Omega)^m$ [see Eq. (4) in Chapter 1]
$L^\infty(\Omega)$: space of bounded functions on Ω
$W_p^m(\Omega) = \{\Phi \in L^p(\Omega): \partial^\alpha\Phi/\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n} \in L^p(\Omega), |\alpha| \le m\}$
$H^m(\Omega) = W_2^m(\Omega)$
$H_0^1(\Omega) = \{\Phi \in H^1(\Omega): \Phi|_\Gamma = 0\} \qquad (\Gamma = \partial\Omega)$
$H_{01}^1(\Omega) = \{\Phi \in H^1(\Omega): \Phi|_{\Gamma_1} = 0\} \qquad (\Gamma_1 \subset \partial\Omega, \Gamma_1 \neq \partial\Omega)$
$C^{m,k}$: = space of m-times differentiable functions whose mth derivative is Hölder continuous with exponent k.
C^m: space of m-times continuously differentiable function.
$\mathcal{T}^{k,\infty}$: set of regular mappings see (4) in Chapter 8.
supp Φ: support of Φ (largest closed set on which Φ is nowhere vanishing)
$\nabla\Phi = \{\partial\Phi/\partial x_1, \ldots, \partial\Phi/\partial x_n\}^t$
$\nabla \cdot \mathbf{u} = \partial u_1/\partial x_1 + \cdots + \partial u_n/\partial x_n$
$\nabla \times \mathbf{u}$: curl of $\mathbf{u}$
$\nabla \times \psi = \{\partial\psi/\partial x_2, -\partial\psi/\partial x_1\}$ in $\mathbb{R}^2$ only
$\psi^{i+\frac{1}{2},j}$: see Eq. (52) in Chapter 1
h: mesh size
$\mathcal{T}_h$: triangulation
$\mathcal{Q}_h$: quadrangulation
T_j: element of $\mathcal{T}_h$ or $\mathcal{Q}_h$

q^k: vertex of T_j
N: usually number of vertices or nodes not on a Dirichlet boundary
$\Phi_h, H_h, \Omega_h, \Gamma_h$: approximations of Φ, H, Ω, Γ
w^k: basis functions of H_h or V_h associated to q^k.
δ_{ik}: Kronecker symbol
$O(\lambda)$: small function $[O(\lambda) \to 0 \quad \text{if} \quad \lambda \to 0]$
$o(\lambda)$: very small function $[o(\lambda)/\lambda \to 0 \quad \text{if} \quad \lambda \to 0]$
$\mathcal{O}$: set of admissible shapes
$E(\Omega)$: value of the criteria at $\Omega \in \mathcal{O}$
$\partial_\alpha E$: Gateau derivative of E in the direction α with respect to Γ
arg min: see Eq. (4) in Chapter 4
$m = 1, \ldots, M$: m takes all integer values between 1 and M
For $m = 1, \ldots, M$ do

1. IP1(m)
2. IP2(m): perform IP1(1), then IP2(1), then IP1(2), IP2(2), $\cdots$ up to IP2(M).

CHAPTER 1

Elliptic Partial Differential Equations

1.1 Introduction

In this chapter we review the main tools used to study elliptic partial differential equations (PDE): Sobolev spaces, variational formulations, and continuous dependence on the data.

We also review the main numerical methods of solution that will be of use: finite element method, finite difference method with mappings into a simple domain, and boundary element method. Except for Section 1.7, the material of this chapter is classical in approach. For further details on Sobolev spaces, the reader is referred to [43], [1], for variational methods to [43], [51], [38], for the continuous dependence on the data to [39], [43], and for numerical methods to [59], [20], [11].

1.2 Green's Formula

Let Ω be a bounded open set of $\mathbb{R}^n$. Let Γ be its boundary. Assume that Ω is locally on one side of its boundary and that the outer normal $\mathbf{n}(x)$ at each point $x \in \Gamma$ is well defined at almost all points of Γ.

Proposition 1. *Let Φ and w be any functions of Ω into $\mathbb{R}$; let A be a mapping of Ω into $\mathbb{R}^{n \times n}$. For sufficiently regular A, Φ, w, and Ω, we have*

$$\int_\Omega -(\nabla \cdot (A\nabla\Phi))w \, dx = \int_\Omega (A\nabla\Phi) \cdot \nabla w \, dx - \int_\Gamma w(A\nabla\Phi) \cdot \mathbf{n} \, d\Gamma. \tag{1}$$

PROOF. See, for example, [43]. □

Consider a Dirichlet problem; for instance,

$$-\Delta\Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = 0. \tag{2}$$

The proof of the existence of Φ in the classical sense turns out to be quite difficult. Green's formula allows us to replace (2) by

$$\int_\Omega \nabla\Phi \cdot \nabla w \, dx = \int_\Omega f w \, dx \qquad \forall\, w \text{ "smooth"}, \ w|_\Gamma = 0, \ \Phi \text{ "smooth"}, \ \Phi|_\Gamma = 0, \tag{3}$$

which is much simpler when the "smoothness" is just sufficient for the integrals in (3) to exist. This provides the motivation for using Sobolev spaces.

1.3 Sobolev Spaces

Let $L^2(\Omega)^m$ denote square integrable functions from Ω into $\mathbb{R}^m$. Throughout the book, we denote by $(\cdot,\cdot)$ the scalar product of this space,

$$(\mathbf{a},\mathbf{b}) = \int_\Omega \sum_{i=1}^{m} a_i(x)b_i(x)\,dx, \tag{4}$$

and by $|\cdot|_0$ its norm

$$|\mathbf{a}|_0 = \sqrt{(\mathbf{a},\mathbf{a})}. \tag{5}$$

The Sobolev space of order 1 is defined by

$$H^1(\Omega) = \{w \in L^2(\Omega) : \nabla w \in L^2(\Omega)^n\}. \tag{6}$$

Provided that ∇ is understood in the distribution sense, (the derivative of a step function is a Dirac function), this space is a Hilbert space with respect to the scalar product

$$\langle \Phi, w\rangle_1 = (\Phi, w) + (\nabla\Phi, \nabla w), \qquad \Phi, w \in H^1(\Omega), \tag{7}$$

with norm

$$|w|_1 = (|w|_0^2 + |\nabla w|_0^2)^{\frac{1}{2}}, \qquad w \in H^1(\Omega). \tag{8}$$

The subspace

$$H_0^1(\Omega) = \{w \in H^1(\Omega) : w|_\Gamma = 0\} \tag{9}$$

is a closed subspace of $H^1(\Omega)$. From the Poincaré inequality it is a Hilbert space itself with respect to the scalar product

$$\langle \Phi, w\rangle_{01} = (\nabla\Phi, \nabla w) \qquad \Phi, w \in H_0^1(\Omega), \tag{10}$$

with norm $|\nabla w|_0$.[1] Similarly, higher-order Sobolev spaces may be defined as follows:

$$H^2(\Omega) = \{w \in H^1(\Omega) : \nabla(\nabla w) \in L^2(\Omega)^{n^2}\} \tag{11}$$

$$H^3(\Omega) = \{w \in H^2(\Omega) : \nabla(\nabla(\nabla w)) \in L^2(\Omega)^{n^3}\} \tag{12}$$

and so forth. The scalar product of $H^2(\Omega)$, for instance, is

$$\langle \Phi, w\rangle_2 = (\Phi, w) + (\nabla\Phi, \nabla w) + \sum_{i,j=1}^{n}\left(\frac{\partial^2\Phi}{\partial x_i\partial x_j}, \frac{\partial^2 w}{\partial x_i\partial x_j}\right). \tag{13}$$

From (8), we may consider $L^2(\Omega)$ to be $H^0(\Omega)$.

Each space is clearly included in the next one, and these inclusions are *compact*. This fact allows the following property to be valid.

---

[1] $|\Phi|_0 \le C|\nabla\Phi|_0 \quad \forall\,\Phi \in H_0^1(\Omega)$.

Proposition 2. *Let $\{w^i\}_{i \geq 0}$ be a bounded sequence of $H^m(\Omega)$ $(m \geq 1)$. Let $\{w^{i_j}\}_{j \geq 0}$ be any subsequence that converges weakly to w^* (there is at least one), thus*

$$w^{i_j} \to w^* \quad \text{strongly in } H^{m-1}(\Omega).$$

PROOF. See, for example, [1] or [43]. □

Sobolev spaces with a negative exponent can be defined by duality. For instance, we use

$$H^{-1}(\Omega) = \text{dual of } H_0^1(\Omega). \tag{14}$$

Identifying the dual of $L^2(\Omega)$ with itself then allows us to give meaning to the integral (Φ, w) where $w \in H_0^1(\Omega)$ and $\Phi \in H^{-1}(\Omega)$.

Sobolev spaces with a noninteger exponent may be defined by the Fourier transform. Let $H^m(\Omega)$ be defined for any real m. These 'new' spaces have the same properties as those above, namely, the inclusion $H^m(\Omega) \subset H^p(\Omega), m > p$, is compact.

Furthermore, if $C^s(\Omega)$ denotes the space of s-times continuous differentiable functions, the following proposition holds.

Proposition 3. $(\Omega \subset \mathbb{R}^n)$

$$H^m(\Omega) \subset C^s(\Omega) \qquad \forall m > \frac{n}{2} + s. \tag{15}$$

Another important property deals with regularity with the restriction $\Phi|_S$ of $\Phi \in H^m(\Omega)$ to a surface $S \subset \bar{\Omega}$.

Proposition 4 (The Trace Theorem). *If $\Phi \in H^m(\Omega)$ and S is a smooth surface in Ω, then $\Phi|_S \in H^{m-\frac{1}{2}}(S) \quad \forall m \geq \frac{1}{2}$.*

Similarly, $\partial\Phi/\partial n$ is equivalent to $\mathbf{n} \cdot \nabla\Phi$, we have

$$\left.\frac{\partial \Phi}{\partial n}\right|_S \in H^{m-\frac{3}{2}}(S) \qquad \forall m \geq \tfrac{3}{2}. \tag{16}$$

Finally, we will occasionally have to use the spaces $W_p^m(\Omega)$. They are analogous to $H^m(\Omega)$ when $L^2(\Omega)$ is replaced by $L^p(\Omega)$. The reader is referred to [39] or [1].

1.4 Linear Elliptic PDE of Order 2

1.4.1 Definitions

Let Ω be a bounded open set of $\mathbb{R}^n$ with smooth boundary Γ and Φ a real-valued function on Ω. Let A be an $n \times n$ matrix-valued function on Ω, a and f two real-valued functions on Ω, and $\mathbf{B}$ a vector-valued function on Ω.

The identity

$$-\nabla\cdot[A(x)\nabla\Phi(x)]+\mathbf{B}(x)\cdot\nabla\Phi(x)+a(x)\Phi(x)=f(x)\qquad\forall x\in\Omega\tag{17}$$

is a linear elliptic partial differential equation of order 2 for Φ, if

$$\sum_{i,j=1}^{n}A_{ij}(x)\,z_iz_j\geq 0\qquad\forall z\in\mathbb{R}^n,\forall x\in\Omega.\tag{18}$$

If $\mathbf{B}=0$, then the equation is in divergence form. If there exists $\alpha>0$ such that

$$a\geq\alpha,\qquad\sum_{i,j=1}^{n}A_{ij}(x)\,z_iz_j\geq\alpha\sum z_i^2\qquad\forall x\in\Omega,\tag{19}$$

and $\mathbf{B}=0$, the equation is said to be *strongly elliptic.*[2]

In (19) $\nabla\cdot$ is the divergence operator. By an appropriate change of variables, we can usually put a linear PDE of order 2 into divergent form.

Standard boundary conditions associated with (17) are

Dirichlet conditions:

$$\Phi|_\Gamma=\Phi_\Gamma\tag{20}$$

Neumann conditions:

$$A\nabla\Phi\cdot n|_\Gamma=g\tag{21}$$

Or both, i.e., mixed conditions:

$$\Phi|_{\Gamma_1}=\Phi_\Gamma;\qquad A\nabla\Phi\cdot n|_{\Gamma_2}=g,\qquad\Gamma_1\cup\Gamma_2=\Gamma,\overset{\text{o}}{\overline{\Gamma_1\cap\Gamma_2}}=\varnothing\tag{22}$$

1.4.2 Variational formulation

Consider the following problem: Find $\Phi\in H^1(\Omega)$ such that

$$(A\nabla\Phi,\nabla w)+(a\Phi,w)=(f,w)+\int_{\Gamma_2}gw\,d\Gamma\qquad\forall w\in V,\Phi|_{\Gamma_1}=\Phi_\Gamma,\tag{23}$$

where

$$V=\{w\in H^1(\Omega):w|_{\Gamma_1}=0\}.\tag{24}$$

Theorem 1. *If (19) holds, $f\in H^{-1}(\Omega)$, $g\in H^{-\frac{1}{2}}(\Gamma)$, $\Phi_\Gamma\in H^{\frac{1}{2}}(\Gamma)$, $\mathbf{B}\equiv 0$, $A\in L^\infty(\Omega)^{n\times n}$, $a\in L^\infty(\Omega)$, then (23) has a unique solution.*

If Φ is twice differentiable, then it satisfies (17) and (22).

For a proof of the general case the reader is referred to [43]. We assume that A is symmetric. Then (23) has a *variational principle.* There, Φ is also the solution of

[2] With a Dirichlet condition, $a\geq\alpha$ maybe replaced by $a\geq 0$.

$$\min E(\Phi), \qquad \Phi \in H^1(\Omega), \Phi|_{\Gamma_1} = \Phi_\Gamma, \tag{25}$$

where

$$E(\Phi) = \tfrac{1}{2}(A\nabla\Phi, \nabla\Phi) + \tfrac{1}{2}(a\Phi, \Phi) - (f, \Phi) - \int_{\Gamma_2} g\Phi \, d\Gamma. \tag{26}$$

Proof of Theorem 1 and of (26). E is quadratic, and (19) makes it strictly convex; therefore, if the solution exists, it is unique.

The solution of (25) must satisfy

$$\left.\frac{d}{d\lambda} E(\Phi + \lambda w)\right|_{\lambda=0} = 0 \qquad \forall w \in V. \tag{27}$$

It is easy to check that (27) is equivalent to (23); thus the solution of (25) satisfies (23).

Problem (25) has a unique solution. Indeed, let $\{\Phi^i\}_{i\geq 0}$ be a minimizing sequence of (26):

$$\lim_{i\to\infty} E(\Phi^i) = \inf\{E(\Phi) : \Phi \in H^1(\Omega), \Phi|_\Gamma = \Phi_\Gamma\}, \tag{28}$$

$$\Phi^i \in H^1(\Omega), \qquad \Phi^i|_{\Gamma_1} = \Phi_\Gamma. \tag{29}$$

From (19) and (28), we find that for large i,

$$\alpha(|\nabla\Phi^i|_0^2 + |\Phi^i|_0^2) - (f, \Phi^i) - \int_{\Gamma_2} g\Phi^i \, d\Gamma \leq E(0) = 0; \tag{30}$$

therefore, there exists C_1 such that

$$\|\Phi^i\|_{H^1(\Omega)} \leq C_1. \tag{31}$$

This implies the existence of $\Phi^* \in H^1(\Omega)$, the limit in the weak sense of a subsequence of $\{\Phi^i\}_i$. However, E is convex and quadratic; thus it is lower semicontinuous:

$$E(\Phi^*) \leq \lim_{i\to\infty} E(\Phi^i). \tag{32}$$

The trace application $\Phi \to \Phi|_\Gamma$ is continuous; thus $\Phi^*|_\Gamma = \Phi_\Gamma$ and therefore Φ^* must be the minimum.

The equivalence of (23) and (17) is a direct consequence of Green's formula:

$$(-\nabla \cdot (A\nabla\Phi) + a\Phi - f, w) + \int_{\Gamma_2} w(A\nabla\Phi \cdot n - g) \, d\Gamma = 0 \qquad \forall w \in V; \tag{33}$$

first taking $w|_{\Gamma_2} = 0$ yields (17) almost everywhere (a.e.), and then $w|_{\Gamma_2} \neq 0$ yields (22). $\square$

1.5 Numerical Solutions of Linear Elliptic Equations of Order 2

1.5.1 Numerical solution by the finite element method

If Ω is not simple, the easiest way to solve (23) is to use the Galerkin method, whereby H^1 is replaced by a finite--dimensional space H_h and Φ is approximated by Φ_h in H_h, the solution becomes

$$(A\nabla\Phi_h, \nabla w_h) + (a\Phi_h, w_h) = (f, w_h) + \int_{\Gamma_2} g w_h \, d\Gamma \qquad \forall w_h \in H_h,\ w_h|_{\Gamma_1} = 0, \tag{34}$$

$$\Phi_h|_{\Gamma_1} = \Phi_{\Gamma h}, \qquad \Phi_h \in H_h. \tag{35}$$

If N is the dimension of $H_h \cap V$ and $\{w^i\}_{i=1}^N$ is a basis of $H_h \cap V$, then (34) is equivalent to the linear system

$$C\Phi = F, \tag{36}$$

where $\Phi = (\Phi_1, \ldots, \Phi_N)$

$$C_{ij} = \int_\Omega (A\nabla w^i) \cdot \nabla w^j \, dx + \int_\Omega a w^i w^j \, dx, \tag{37}$$

$$F_j = \int_\Omega f w^j \, dx + \int_{\Gamma_2} g w^j \, d\Gamma - \int_\Omega (A\nabla\Phi_{\Gamma h}) \cdot \nabla w^j \, dx - \int_\Omega a\Phi_{\Gamma h} w^j \, dx, \tag{38}$$

$$\Phi_h(x) = \sum_{i=1}^N \Phi_i w^i(x) + \Phi_{\Gamma h}. \tag{39}$$

To make (36) easy to solve and (37) and (38) easy to compute, divide Ω into nonoverlapping triangles $\{T_k\}_k$ such that

$$T_k \cap T_l = \emptyset \quad \text{or} \quad \text{one vertex} \quad \text{or} \quad \text{one entire side } (k \neq l). \tag{40}$$

Then take

$$H_h = \{w_h \text{ continuous}: w_h|_{T_k} \text{ affine } \forall k\}. \tag{41}$$

This is known as the finite element method of order 1 on triangles.

A basis for H_h is easy to construct once it is noted that all functions of H_h are completely determined from their values at the vertices $\{q^i\}_1^M$ of the triangulation; thus $\{w^i\}$ is defined by

$$w^i(q^j) = \delta_{ij} \qquad \forall j = 1, \ldots, M;\ w^i \in H_h. \tag{42}$$

In terms of h, the length of the largest side of the triangles, the precision of the method is $O(h)$ for regular data,

$$|\nabla(\Phi_h - \Phi)|_0 + |\Phi_h - \Phi|_0 \leq Ch, \tag{43}$$

and when Ω is convex, $O(h^2)$ for $|\Phi_h - \Phi|_0$. Higher-order methods can be obtained by taking

$$H_h = \{w_h \text{ continuous}: w_h|_{T_k} \text{ polynomial of degree } m \;\forall k\}. \tag{44}$$

1.5.2 Numerical solution by finite difference methods

Consider again problems (17) and (23):

$$\begin{aligned} &-\nabla \cdot (A\nabla\Phi) + a\Phi = f \quad \text{in } \Omega, \\ &\Phi|_{\Gamma_1} = \Phi_\Gamma, \qquad A\nabla\Phi \cdot n|_{\Gamma_2} = g. \end{aligned} \tag{45}$$

Assume for clarity that the problem is bidimensional ($n = 2$). If $\mathbf{n}(x)$ is parallel to one of the axes of an orthonormal reference frame at all $x \in \Gamma$, it is well-known [59] that centered difference approximations of the derivatives yield a linear system in terms of

$$\Phi_{ij} = \Phi(ih, jh). \tag{46}$$

So suppose that Ω is the unit square $]0, 1[^2$ and that Γ_2 is the bottom side. Then (45) can be approximated by

$$\begin{aligned} &-\frac{1}{h}\left[A_{11}^{i+\frac{1}{2},j}\frac{\Phi_{i+1,j}-\Phi_{i,j}}{h} - A_{11}^{i-\frac{1}{2},j}\frac{\Phi_{i,j}-\Phi_{i-1,j}}{h}\right] \\ &\qquad -\frac{1}{h}\left[A_{22}^{i,j+\frac{1}{2}}\frac{\Phi_{i,j+1}-\Phi_{i,j}}{h} - A_{22}^{i,j-\frac{1}{2}}\frac{\Phi_{i,j}-\Phi_{i,j-1}}{h}\right] \\ &-\frac{1}{h}\left[A_{12}^{i+\frac{1}{2},j}\frac{\Phi_{i+\frac{1}{2},j+\frac{1}{2}}-\Phi_{i+\frac{1}{2},j-\frac{1}{2}}}{h} - A_{12}^{i-\frac{1}{2},j}\frac{\Phi_{i-\frac{1}{2},j+\frac{1}{2}}-\Phi_{i-\frac{1}{2},j-\frac{1}{2}}}{h}\right] \\ &-\frac{1}{h}\left[A_{21}^{i,j+\frac{1}{2}}\frac{\Phi_{i+\frac{1}{2},j+\frac{1}{2}}-\Phi_{i-\frac{1}{2},j+\frac{1}{2}}}{h} - A_{21}^{i,j-\frac{1}{2}}\frac{\Phi_{i+\frac{1}{2},j-\frac{1}{2}}-\Phi_{i-\frac{1}{2},j-\frac{1}{2}}}{h}\right] \\ &\qquad + a^{ij}\Phi_{ij} = f_{ij} \qquad \forall i,j = 1,\ldots,\mathrm{N}-1. \end{aligned} \tag{47}$$

$$A_{21}^{i+\frac{1}{2},\frac{1}{2}}\frac{\Phi_{i+1,\frac{1}{2}}-\Phi_{i,\frac{1}{2}}}{h} + A_{22}^{i-\frac{1}{2},\frac{1}{2}}\frac{\Phi_{i-\frac{1}{2},1}-\Phi_{i-\frac{1}{2},0}}{h} = g^i \qquad \forall i = 1,\ldots,N-1; \tag{48}$$

$$\Phi_{0,j} = \Phi_\Gamma^{0,j}; \qquad \Phi_{N,j} = \Phi_\Gamma^{N,j}; \qquad \Phi_{i,N} = \Phi_\Gamma^{i,N}\;\forall i,j = 0,\ldots,N. \tag{49}$$

The following notation has been used:

$$N = \text{integer part of } \frac{1}{h}, \tag{50}$$

$$\Psi^{i+\frac{1}{2},j} = \Psi\big((i+\tfrac{1}{2})h, jh\big). \tag{51}$$

If equality is not available, use linear interpolation:

$$\Psi^{i+\frac{1}{2},j} \simeq \tfrac{1}{2}(\Psi^{i+1,j} + \Psi^{i,j}). \tag{52}$$

When the problem is strongly elliptic, the linear system (47) to (49) is positive definite, and the precision is of order h^2.

1.5.3 Finite differences on domains of arbitrary shapes

In optimal shape design problems, however, the boundaries are almost never entirely parallel to the axes. For this case, one approach to the solution is to find a mapping T such that

$$T(]0,1[^2) = \Omega, \qquad T \text{ bijective,} \tag{53}$$

and then apply finite differences in the new frame.

Let $X = (X_1, X_2)$ denote the new variables

$$X = T^{-1}(x), \qquad x \in \Omega. \tag{54}$$

We obtain

$$\frac{\partial \Phi}{\partial x_i} = \sum_j \frac{\partial \Phi}{\partial X_j}\frac{\partial X_j}{\partial x_i} = \sum_j \frac{\partial \Phi}{\partial X_j}\frac{\partial T_j^{-1}}{\partial x_i}, \tag{55}$$

or equivalently [recall that in this case $(\nabla_X T)^{-1} = \nabla_x(T^{-1})$],

$$\nabla_x \Phi = (\nabla_X T)^{-1}\nabla_X \Phi. \tag{56}$$

Similarly,

$$|dx_1 \times dx_2| = \left|\frac{\partial T_1}{\partial X_i}\,dX_i \times \frac{\partial T_2}{\partial X_j}\,dX_j\right| = \det[\nabla_X T]\,dX_1\,dX_2. \tag{57}$$

Formulation (23) now becomes

$$\int_\Omega [A(\nabla_X T)^{-1}\nabla_X \Phi]\cdot(\nabla_X T)^{-1}\nabla w + a\Phi w - fw]\det[\nabla_X T]\,dX_1\,dX_2$$
$$= \int_{\Gamma_2} gw\left|\frac{\partial T}{\partial X_1}\right| dX_1 \qquad \forall w \in H^1(\hat\Omega);\ w|_{\hat\Gamma_1} = 0 \tag{58}$$

where $\hat\Omega =]0,1[^2$ and $\hat\Gamma_2 =]0,1[\times\{0\}$, as before. Equation (58) is equivalent to

$$-\nabla\cdot[(\nabla_X T)^{-t}\hat A(\nabla_X T)^{-1}\nabla\hat\Phi\det[\nabla_X T]] + \hat a\det[\nabla_X T]\hat\Phi = \hat f\det[\nabla_X T] \quad \text{in }]0,1[^2; \tag{59}$$

$$\Phi|_{\hat\Gamma_1} = \hat\Phi_\Gamma; \qquad (\nabla_X T)^{-t}\,\hat A(\nabla_X T)^{-1}\nabla\hat\Phi\cdot\hat n|_{\Gamma_2} = \hat g\frac{|\partial T/\partial X_1|}{|\det|\nabla_X T|}, \tag{60}$$

where ^ means that all functions are evaluated at $T(X)$; for example,

$$\hat\Phi(X) = \Phi(T(X)).$$

Now the finite difference method as described previously can be applied to (59) and (60).

1.5.4 Numerical solutions by boundary elements

The boundary element method is not as general because it requires Green's function of the operator, but it does not require any discretization of Ω.

Consider, for example, the Neumann problem

$$-\Delta\Phi = f \quad \text{in } \Omega \subset \mathbb{R}^3, \tag{62}$$

$$\left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = g.$$

If $\delta(x - x_0)$ is the Dirac function at x_0, the solution of

$$-\Delta G = \delta(x - x_0) \quad \text{in } \mathbb{R}^3, \qquad \lim_{|x|\to\infty} G(x) = 0, \tag{63}$$

is well-known:

$$G(x - x_0) = \frac{1}{4\pi|x - x_0|}. \tag{64}$$

Let

$$\hat{\Phi}(x) = \Phi(x) - \frac{1}{4\pi}\int_{\mathbb{R}^3} f(y)\frac{dy}{|x - y|}. \tag{65}$$

Then

$$-\Delta\hat{\Phi} = -\Delta\Phi - \int_{\mathbb{R}^3} \delta(x - y)f(y)\,dy = 0, \tag{66}$$

$$\left.\frac{\partial\hat{\Phi}}{\partial n}\right|_\Gamma = g - \frac{1}{4\pi}\int_{\mathbb{R}^3} f(y)\frac{\partial}{\partial n(x)}\left(\frac{1}{|x - y|}\right)dy. \tag{67}$$

Without loss of generality, we may assume that f is zero in (62). Then Green's formula (1) applied to (62) and (63) yields the following equalities:

$$\begin{aligned}\Phi(x_0) &= \int_\Omega -\Phi(x)\,\Delta G(x - x_0)\,dx = \int_\Gamma (-\Delta\Phi)G\,dx + \int_\Gamma \left(\frac{\partial\Phi}{\partial n}G - \Phi\frac{\partial G}{\partial n}\right)d\Gamma \\ &= \frac{1}{4\pi}\int_\Gamma \left[g|x - x_0|^{-1} - \Phi\frac{\partial}{\partial n}|x - x_0|^{-1}\right]d\Gamma. \end{aligned}\tag{68}$$

When $x_0 \in \Gamma$, the last integral is singular, but it can be shown that its limit when $x_0^* \to x_0 \in \Gamma$ is computable in terms of its principal value (see, for example, [11]):

$$\begin{aligned}&\lim_{\substack{x_0^* \to x_0 \in \Gamma \\ x_0 - x_0^* \parallel \mathbf{n}}} \frac{1}{4\pi}\int_\Gamma -\Phi\frac{\partial}{\partial n}|x - x_0^*|^{-1}\,d\Gamma \\ &\quad= \frac{1}{2}\Phi(x_0) - \frac{1}{4\pi}\lim_{\varepsilon\to 0}\int_{\Gamma\cap\{x:|x - x_0| > \varepsilon\}} \phi\frac{\partial}{\partial n}|x - x_0|^{-1}\,d\Gamma; \end{aligned}\tag{69}$$

so for points x_0 on Γ, (68) becomes

$$\frac{1}{2}\Phi(x_0) + \int_\Gamma \frac{1}{4\pi}\Phi\frac{\partial}{\partial n}|x - x_0|^{-1}\,d\Gamma = \int_\Gamma \frac{1}{4\pi}g|x - x_0|^{-1}\,d\Gamma \qquad \forall x_0 \in \Gamma. \tag{70}$$

To make this formula discrete, we assume that Γ is made of flat elements $\{T_k\}_1^N$ and that Φ is constant on T_k. We have

$$\frac{1}{2}\Phi_k + \sum_{l=1}^N \Phi_l \int_{T_l} \frac{1}{4\pi}\frac{\partial}{\partial n}|x - x^k|^{-1}\,d\Gamma = \int_\Gamma \frac{1}{4\pi}g|x - x^k|^{-1}\,d\Gamma \qquad \forall k = 1,\ldots,N, \tag{71}$$

where x^k is a point in T_k and Φ_k is $\Phi(x^k)$. The integrals are computed by Gauss' formula when $l \neq k$ and exactly when $l = k$.

A similar formula holds in two dimensions with $(1/4\pi)|x - x^k|^{-1}$ replaced by $(1/2\pi)\log|x - x^k|$.

1.6 Other Elliptic Equations

We deal later with a few other important PDEs from physics for which we briefly review here certain properties.

1.6.1 The biharmonic equation

The following problem is an elliptic equation of order 4:

$$\Delta^2\Phi = f \quad \text{in } \Omega, \tag{72}$$

$$\Phi|_\Gamma = \Phi_\Gamma; \qquad \left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = g. \tag{73}$$

Its variational form is found by multiplying (72) by w and applying Green's formula twice:

$$\int_\Omega \Delta\Phi\,\Delta w\,dx = \int_\Omega fw\,dx + \int_\Gamma gw\,d\Gamma \qquad \forall w \in H_0^2(\Omega), \tag{74}$$

$$\Phi - \tilde{\Phi}_\Gamma \in H_0^2(\Omega) = \left\{w \in H^2(\Omega) : w|_\Gamma = \left.\frac{\partial w}{\partial n}\right|_\Gamma = 0\right\}, \tag{75}$$

where $\tilde{\Phi}_\Gamma$ is an extension in $H^2(\Omega)$ of Φ_Γ such that its normal derivative is g. Equations (72) and (73) illustrate the vertical deflection of a plate subject to volumic forces f or the stream function of a two-dimensional Stokes problem (creeping flow).

Proposition 5. *Assume that* $f \in L^2(\Omega)$, $g \in L^2(\Gamma)$, *and* $\tilde{\Phi}_\Gamma \in H^2(\Omega)$; *then the problem given in (74) and (75) has a unique solution.*

PROOF. The argument is very similar to that of Proposition 1; we consider a similar problem

$$\min_{\Phi - \tilde{\Phi}_\Gamma \in H_0^2(\Omega)} \int_\Omega \tfrac{1}{2}(\Delta\Phi)^2\, dx - \int_\Omega f\Phi\, dx - \int_\Gamma g\Phi\, d\Gamma.$$

This problem has a unique solution because the function minimized is strictly convex weakly, lower semicontinuous with respect to the topology of $H_0^2(\Omega)$; therefore, the same argument applies. □

For finite element approximations of (74) and (75), the reader is referred to [20], [31].

1.6.2 The compressible potential flow equation

In two or three dimensions the velocity field for a compressible potential flow is computed as the gradient of a potential Φ satisfying a nonlinear equation of the following type:

$$\nabla \cdot (\rho(|\nabla\Phi|^2)\nabla\Phi) = f \quad \text{in } \Omega, \tag{76}$$

$$\rho(|\nabla\Phi|^2)\frac{\partial\Phi}{\partial n}\bigg|_{\Gamma_2} = g, \qquad \Phi|_{\Gamma_1} = \Phi_\Gamma. \tag{77}$$

In most cases f is zero and

$$\rho(|\nabla\Phi|^2) = |1 - |\nabla\Phi|^2|^{1/(\gamma-1)} \tag{78}$$

where γ is the adiabatic constant of the fluid ($\gamma = 1.4$ in air). This equation, in variational form, is

$$\int_\Omega \rho(|\nabla\Phi|^2)\nabla\Phi \cdot \nabla w\, dx = \int_\Omega fw\, dx + \int_{\Gamma_2} gw\, d\Gamma \qquad \forall w \in H_{01}^1(\Omega), \tag{79}$$

$$\Phi - \tilde{\Phi}_\Gamma \in H_{01}^1(\Omega) = \{w \in H^1(\Omega): w|_{\Gamma_1} = 0\}. \tag{80}$$

Proposition 6. *If, for some* $\alpha > 0$, *we have*

$$\rho(\lambda) + 2\lambda \min\left\{\frac{d\rho}{d\lambda}(\lambda), 0\right\} \geq \alpha > 0 \qquad \forall \lambda > 0 \tag{81}$$

If $\rho(+\infty) = +\infty$ *and if the data are smooth, then (79) and (80) have a unique solution, and it is an elliptic equation.*

PROOF. When a PDE is nonlinear, we say that it is elliptic if its linearized form is elliptic. Here the linearized equation is

$$\nabla \cdot (\rho\nabla\Psi) + \nabla \cdot (2\dot{\rho}\nabla\Phi \cdot \nabla\Psi\nabla\Phi) = 0. \tag{82}$$

Thus according to (21), we must check that for some $\alpha > 0$,

$$\rho \sum_i z_i^2 + 2\dot{\rho} \sum_{i,j} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_j} z_i z_j \geq \alpha \sum_i z_i^2 \qquad \forall z \in \mathbb{R}^n. \tag{83}$$

This is true when (81) holds because

$$\min_{|z|=1} \{\rho + 2(\nabla\Phi \cdot z)^2 \dot{\rho}\} = \rho + 2|\nabla\Phi|^2 \min\{\dot{\rho}, 0\}. \tag{84}$$

To prove that the solution exists, consider the problem

$$\min_{\Phi - \Phi_\Gamma \in H^1_{01}(\Omega)} \int_\Omega E(|\nabla\Phi|^2)\, dx - \int_\Omega f\Phi\, dx - \int_{\Gamma_1} g\Phi\, d\Gamma, \tag{85}$$

where

$$E(\mu) = \tfrac{1}{2} \int_0^\mu \rho(\lambda)\, d\lambda. \tag{86}$$

If (81) holds, this problem has a unique solution because E is strictly convex weakly lower semicontinuous in $H^1(\Omega)$ and $+\infty$ at ∞. It is equivalent to (79) and (80) because the solution we have

$$\frac{d}{d\lambda} \left\{ E(|\nabla(\Phi + \lambda w)|^2) - \int_\Omega f(\Phi + \lambda w)\, dx - \int_{\Gamma_2} g(\Phi + \lambda w)\, d\Gamma \right\} \bigg|_{\lambda = 0} = 0. \tag{87}$$

For further details, see Theorem 1 of Section 1.5.2 in [39]. □

1.6.3 Electromagnetic potential equation

Let **H** be the magnetic field, **J** the current density, **B** the flux density, and μ the magnetic permeability. Maxwell's equations

$$\nabla \times \mathbf{H} = \mathbf{J}, \qquad \mathbf{B} = \mu \mathbf{H}, \qquad \nabla \cdot \mathbf{B} = 0 \tag{88}$$

can be rewritten in terms of a vector potential **A**:

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} \right) = \mathbf{J}. \tag{89}$$

(Recall that μ may depend upon **A**). For two-dimensional problems $\mathbf{A} = (0, 0, A)$ and $\mathbf{J} = (0, 0, j)$, and thus (89) becomes

$$\nabla \cdot \left(\rho(|\nabla \mathrm{A}|^2, x) \nabla A\right) = j \quad \text{in } \Omega, \tag{90}$$

where j are the current densities (orthogonal to the plane of Ω) and where $\rho = 1/\mu$ may be tabulated as a function of $|\nabla A|$ and $x \in \Omega$. Feasible boundary conditions are

$$A|_{\Gamma_1} = 0 \qquad \frac{\partial A}{\partial \mathbf{n}}\bigg|_{\Gamma_2} = 0. \tag{91}$$

Thus, Proposition 5 is also an existence theorem for (90) and (91).

1.6.4 The stokes equations

Let $\mathbf{u}$ be a vector-valued mapping from $\Omega \subset \mathbb{R}^n$ into $\mathbb{R}^n$. Let p be a scalar function from Ω into $\mathbb{R}$ and consider the following system of PDEs:

$$\Delta \mathbf{u} = \nabla p + \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega, \tag{92}$$

$$\mathbf{u}|_\Gamma = \mathbf{u}_\Gamma. \tag{93}$$

An elliptic variational formulation of this problem can be given if (92) is multiplied by $\mathbf{v}$ in $J_0(\Omega)$ with

$$J_0(\Omega) = \{\mathbf{v} \in H^1(\Omega)^n : \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega; \mathbf{v}|_\Gamma = 0\}. \tag{94}$$

Indeed from Green's Formula,

$$\sum_1^n \int_\Omega v_i(\Delta u_i)\, dx = -\sum_1^n \int_\Omega \nabla v_i \cdot \nabla u_i\, dx \qquad \forall \mathbf{v} \in J_0(\Omega), \tag{95}$$

and it is easy to show that

$$\int_\Omega \mathbf{v}\, \nabla p\, dx = -\int_\Omega p \nabla \cdot \mathbf{v}\, dx + \int_\Gamma p \mathbf{v} \cdot \mathbf{n}\, d\Gamma \qquad \forall \mathbf{v} \in H^1(\Omega)^n, \forall p \in L^2(\Omega). \tag{96}$$

Therefore, (92) and (93) imply

$$\int_\Omega \nabla \mathbf{u} \cdot \nabla \mathbf{v}\, dx = \int_\Omega \mathbf{f} \cdot \mathbf{v}\, dx \qquad \forall \mathbf{v} \in J_0(\Omega), \mathbf{u} - \tilde{\mathbf{u}}_\Gamma \in J_0(\Omega), \tag{97}$$

where $\tilde{\mathbf{u}}_\Gamma$ is a divergence-free extension of $\mathbf{u}_\Gamma$ in $H^1(\Omega)^n$.

Proposition 7. *Assume that* $\mathbf{f} \in L^2(\Omega)^n$, $\tilde{\mathbf{u}}_\Gamma \in H^1(\Omega)^n$, *and* $\nabla \cdot \tilde{\mathbf{u}}_\Gamma = 0$. *Then problem (97) has a unique solution.*

PROOF. Again we consider the problem

$$\min_{\mathbf{u} - \tilde{\mathbf{u}}_\Gamma \in J_0(\Omega)} \int_\Omega \tfrac{1}{2} |\nabla \mathbf{u}|^2\, dx - \int_\Omega \mathbf{f}\mathbf{u}\, dx. \tag{98}$$

The functional minimized is strictly convex, weakly lower semicontinuous for $H^1(\Omega)^n$, and $J_0(\Omega)$ is a closed subspace of $H^1(\Omega)^n$. Thus the argument of Proposition 1 carries over to this case. □

For further details, see [38].

Remark. When $n = 2$ the divergence equation for $\mathbf{u}$ implies

$$\mathbf{u} = \nabla \times \Psi, \qquad \Psi \in H^2(\Omega); \tag{99}$$

therefore by taking the rotational of (92), we get a biharmonic equation for Ψ:

$$\Delta^2 \Psi = \nabla \times \mathbf{f} \quad \text{in } \Omega. \tag{100}$$

1.7 Continuous Dependence on the Boundary

In this section we review some technical results on the regularity of the solution of a PDE as a function of the regularity of the boundary. These results can be found in [39], [51], [38], [43], [27].

1.7.1 Regularity of the boundary

Let $\Phi(\Omega)$ be the solution in $H^1(\Omega)$ of

$$-\nabla \cdot A\nabla\Phi + a\Phi = f \quad \text{in } \Omega; \qquad \Phi|_\Gamma = \Phi_\Gamma \quad \text{or} \quad \left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = g, \tag{101}$$

where A and a satisfy the ellipticity condition (21).

If the boundary condition is a Dirichlet condition, and if it is replaced by

$$\Phi - \tilde{\Phi}_\Gamma \in H_0^1(\Omega), \tag{102}$$

where $\tilde{\Phi}_\Gamma$ is an extension of Φ_Γ in $H^1(\Omega)$, then the only conditions for the existence of Φ in $H^1(\Omega)$ are, for example,

$$\Omega \text{ open bounded}, \qquad f \in H^{-1}(\Omega), \qquad A, a \in L^\infty(\Omega), \qquad \tilde{\Phi}_\Gamma \in H^1(\Omega).$$

In particular, no regularity assumptions on Γ are needed. However, the trace of Φ or $\partial\Phi/\partial n$ on Γ requires some assumptions, for example, $\Gamma \in C^{0,\alpha}$. We state the conditions as given in [39]:

Definitions. Γ is *piecewise smooth* if there exists $\{\Omega_i\}_1^\mu$ such that

$$\bar{\Omega} = \cup\bar{\Omega}_i, \qquad \cap\Omega_i = \varnothing,$$

and a set of continuous mappings $\{Z^i\}_1^\mu$ such that Z^i maps $\bar{\Omega}_i$ homeomorphically onto the unit sphere of $\mathbb{R}^n$ and such that the determinants of ∇Z^i are bounded from below by a positive constant.

Γ satisfies *condition* (A) if there exists a_0, θ_0 positive such that

$$\operatorname{mes}\{\Omega_i \cap B(x,\rho)\} \le (1-\theta_0)\operatorname{mes} B(x,\rho) \qquad \forall x \in \Gamma, \forall \rho \le a_0,$$
$$B(x,\rho) = \{y : |x-y| \le \rho\}. \tag{103}$$

A local Cartesian coordinate system about $x^\circ \in \Gamma$ is $\{y_i\}_1^n$, where for some orthogonal matrix $\mathbf{A}$, $y = \mathbf{A}(x - x^\circ)$ and the y_n-axis is in the outer normal direction to Ω.

Γ is of class $C^{l,\alpha}$ (respectively, W_q^2) if there exists $\rho > 0$ such that for all x°, $S = \Gamma \cap B(x^0, \rho)$ is a connected surface and there exists $w \in C^{l,\alpha}$ (respectively, W_q^2) such that the equation of S is

$$y_n = w(y, \ldots, y_{n-1}) \tag{104}$$

in some local Cartesian coordinate system.

1.7.2 Regularity of the solution

Theorem 2 (See Theorem 3.14.1 in [39].) *If Γ satisfies condition (A), $\Phi_\Gamma \in C^{0,\beta}(\Gamma)$, A_{ij}, a, $f \in L^{q/2}(\Omega)$ $(q > n)$, then (101) with the Dirichlet condition has a unique solution in $C^{0,\alpha}(\bar{\Omega})$, for some α.*

Theorem 3 (See Theorem 3.15.1 in [39].) *If, in addition, $\Gamma \in W_q^2$, $\Phi_\Gamma \in W_q^2(\Omega)$, and f, $\partial f/\partial x_k$, $\partial A_{ij}/\partial x_k$, $\partial a/\partial x_k \in L^q(\Omega)$, then $\Phi \in C^{1,\alpha}(\bar{\Omega})$ with $\alpha = 1 - n/q$ and*

$$\|\Phi\|_{C^{1,\alpha}} \leq C(\|\Gamma\|_{W_q^2})(\|\tilde{\Phi}_\Gamma\|_{W_q^2} + \|f\|_{W_q^1}) \tag{105}$$

Theorem 4 (See Theorem 3.3.1 in [39].) *Assume Γ of class $C^{2,\alpha}$, $A_{ij} \in C^{1-\delta,\alpha}(\bar{\Omega})$, $a, f \in C^{0,\alpha}(\bar{\Omega})$, $g \in C^{1,\alpha}(\Gamma)$,* and *$\Phi_\Gamma \in C^{2,\alpha}(\Gamma)$.* Then *$\Phi \in C^{2,\alpha}(\bar{\Omega})$, and for some constant C which depends only on Γ through the $C^{2,\alpha}$ norm of Γ, we have*

$$\|\Phi\|_{C^{2,\alpha}} \leq C(\|\Gamma\|_{C^{2,\alpha}})(\delta\|\Phi_\Gamma\|_{C^{2,\alpha}(\Gamma)} + \|f\|_{C^{0,\alpha}} + \|g\|_{C^{1,\alpha}}(1-\delta)) \tag{106}$$

where Φ is the solution of the Dirichlet problem ($\delta = 1$) or the Neumann problem ($\delta = 0$).

1.7.3 Convergence with respect to the boundary

Denote by $\Phi(\Omega)$ the solution of (101). The following theorems address the convergence of $\Phi(\Omega^m)$ to $\Phi(\Omega)$ when $\Omega^m \to \Omega$.

Theorem 5. *Assume that Γ^m, $\Gamma \in C^{0,\alpha}$ and that $\Gamma^m \to \Gamma$ in $C^{0,\alpha}$; then for the Dirichlet or Neumann problem (101),*

$$\Phi(\Omega^m) \to \Phi(\Omega) \quad \textit{strongly in } H^1(\Omega). \tag{107}$$

PROOF. See Proposition 1 in Chapter 3 for the Dirichlet problem and [19] for the Neumann problem. □

Theorem 6. *Assume that the conditions of Theorem 4 are satisfied for Γ^m and Γ and that $\Gamma^m \to \Gamma$ in $C^{2,\alpha}$; then*

$$\|\Phi(\Omega^m) - \Phi(\Omega)\|_{C^{2,\alpha}} \to 0.$$

PROOF. Let $\tilde{\Phi}(\Omega)$ be a $C^{2,\alpha}$ extension of $\Phi(\Omega)$ in Ω^m. By substracting (101) with Γ from (101) with Γ^m, we find that $\Phi(\Omega^m) - \tilde{\Phi}(\Omega)$ satisfies a PDE in Ω^m and that by Theorem 4,

$$\|\Phi(\Omega^m) - \Phi(\Omega)\|_{C^{2,\alpha}(\Omega^m)} \leq C(\|\Gamma^m\|_{C^{2,\alpha}})\Bigg(\delta\|\tilde{\Phi} - \Phi_\Gamma\|_{C^{2,\alpha}(\Gamma^m)}$$

$$+ (1-\delta)\left\|\frac{\partial\tilde{\Phi}}{\partial n} - g\right\|_{C^{1,\alpha}(\Gamma^m)} + \|-\nabla\cdot A\nabla\tilde{\Phi} + a\tilde{\Phi}\|_{C^{0,\alpha}(\Omega^m - \Omega\cap\Omega^m)}\Bigg). \quad \square$$

CHAPTER 2

Problem Statement

2.1 Introduction

In this chapter we

- Define what is meant by optimal shape design and give examples.
- Review some historical developments of the subject.
- Give an informal argument to illustrate the method used here to solve these problems.

Concurrently, we introduce some concrete examples of optimal shape design problems, and we give some indication of the likely future developments of this field in industry.

2.2 Definition

Let Φ be the solution of a partial differential equation in a domain Ω;

$$\Phi(x) \in \mathbb{R}^m \qquad \forall x \in \Omega \subset \mathbb{R}^n. \tag{1}$$

Let $E(\Phi, \Omega)$ be a real-valued function of Φ and Ω. We may say that we have an *optimal shape design* problem to solve if we find Ω, in a class O of allowable domains, to minimize E.

Symbolically, we may write

$$\min_{\Omega \in O} \{E(\Phi, \Omega) : A(\Omega, \Phi) = 0\}, \tag{2}$$

where A is an unbounded operator that, for every $\Omega \in O$, defines a unique Φ.

In reality, this definition is too restrictive; broadly speaking, we use the term *optimal shape design* whenever a function is to be minimized with respect to a particular geometric element appearing in a PDE. Here we deal only with cases where A is an elliptic operator, either linear or nonlinear. Most of our discussion also applies to other operators, but their numerical solutions are usually much harder to solve.

2.3 Examples

2.3.1 Optimization of a nozzle

The velocity $u(x)$ at a point x of a nonviscous, incompressible potential flow (such as air or water at moderate speed) may be approximated by

$$\mathbf{u}(x) = \nabla\Phi(x) \qquad \forall\, x \in \Omega, \tag{3}$$

where Φ satisfies

$$\Delta\Phi = 0 \quad \text{in } \Omega; \tag{4}$$

Ω is the region occupied by the fluid.

Then the flow in a nozzle Ω with a prescribed pressure drop $\Phi_{\Gamma_0} - \Phi_{\Gamma_i}$ is obtained by solving

$$\Delta\Phi = 0 \quad \text{in } \Omega; \tag{5}$$

$$\Phi|_{\Gamma_0} = \Phi|_{\Gamma_0}; \qquad \Phi|_{\Gamma_i} = \Phi|_{\Gamma_i}; \qquad \left.\frac{\partial\Phi}{\partial n}\right|_{\Gamma_w} = 0. \tag{6}$$

The last condition states that the flow is tangent to the walls.

We may be interested in designing a nozzle that gives a prescribed velocity u_d near the exit, say in some given region D (see Figure 2.1). One way to obtain the design is to solve

$$\min_{\Omega \in O} E(\Omega) = \int_D |\nabla\Phi(\Omega) - \mathbf{u}_d|^2 \, dx, \tag{7}$$

where $\Phi(\Omega)$ is the solution of (5) and (6) and

$$O = \{\Omega : \Omega \supset D;\ \Gamma_0, \Gamma_i \text{ fixed}\}. \tag{8}$$

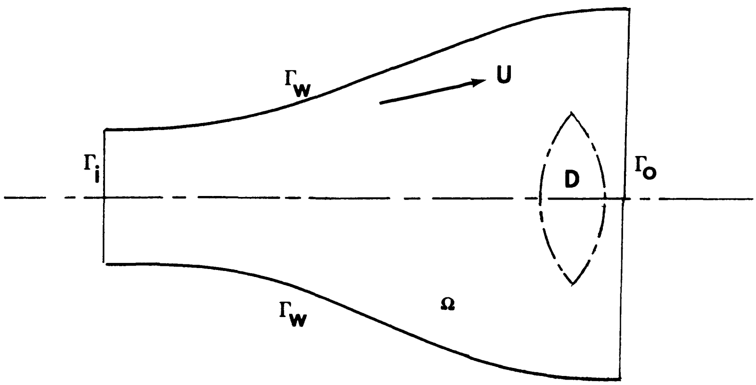


Fig. 2.1 Optimization of a nozzle. The unknowns are Γ_w; these walls are to be designed such that u is as near as possible to a prescribed value in D.

There are two special conditions of this problem:

1. The unknown boundaries Γ_w have *Neumann conditions.*
2. The criterion E does not involve Ω explicitly.

In this class of problems we also deal with the more practical case of *compressible* flows where (5) is replaced by a *non-linear* equation.

2.3.2 Minimum drag problems

At low Reynolds number *viscous* Newtonian flows have velocity $u(x)$ and pressure $p(x)$ that satisfy

$$\Delta \mathbf{u} = \nabla p; \qquad \nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega. \tag{9}$$

In this case, we may ask the following question: "What is the shape of a body S of given volume v having the smallest drag when moved at a uniform speed u_0 (see Figure 2.2)?" The minimization of the drag can be replaced by the minimization of the dissipated energy; so we consider the problem

$$\min_{\Omega \in O} E(\Omega) = \int_\Omega \tfrac{1}{2} |\nabla \mathbf{u}(\Omega) + (\nabla \mathbf{u}(\Omega))^t|^2 \, dx$$

where $\mathbf{u}(\Omega)$ is the solution of (9) plus (10),

$$\mathbf{u}|_{\partial S} = \mathbf{u}_0, \qquad \mathbf{u}|_{\partial C} = 0, \tag{10}$$

and where

$$O = \left\{ \Omega = C - S : S \subset C, C \text{ fixed} \int_S dx = v \right\}. \tag{11}$$

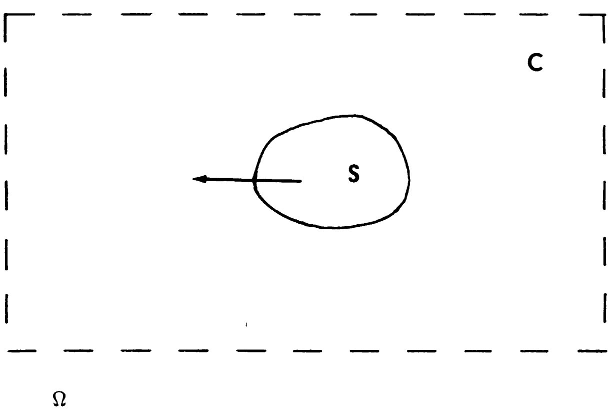


Fig. 2.2 Optimization of the shape of S with a given volume such that its drag in a flow at low speed is minimal.

Besides the fact that the PDE is a system of equations, this problem has the following features:

- Dirichlet conditions on the unknown boundary
- Criteria where Ω appears explicitly

We are also dealing with a minimum drag problem where (9) is replaced by the Navier–Stokes equation.

2.3.3 Optimization of an electromagnet

Can an electromagnet produce a constant magnetic field? To solve this problem, we call Ω the domain occupied by the iron parts and compute

$$\min_{\Omega \in O} E(\Omega) = \int_D |\nabla \times \mathbf{A} - \mathbf{B}_d|^2 \, dx, \tag{12}$$

where D is the region (possibly depending on Ω) where the magnetic field is required to be equal to $\mathbf{B}_d$ (see Figure 2.3).

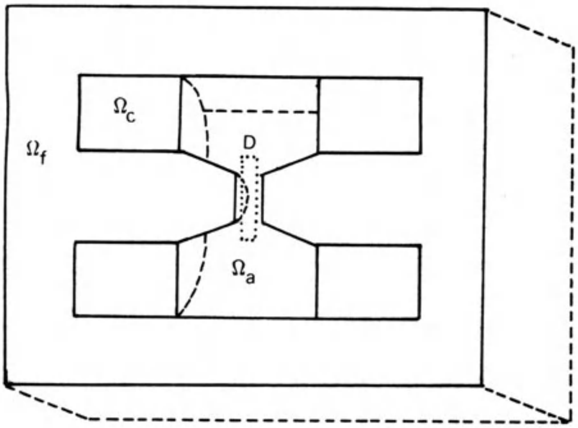


Fig. 2.3 Optimization of the shape of the poles of an electromagnet. D is the region where the magnetic field is desired to be constant. Ω_f is the ferrous material, Ω_c the copper (wire), and Ω_a the air. The geometry of half the magnet after a cut through the plane of symmetry.

In two dimensions the electromagnetic potential $\mathbf{A}$ is a scalar and is computed from

$$-\nabla \cdot (\nu \nabla \mathbf{A}) = j \quad \text{in } \mathbb{R}^2, \qquad \mathbf{A}|_\infty = 0, \tag{13}$$

where ν, the magnetic reluctivity, is a nonlinear function of $\mathbf{A}$ in Ω, $\nu(|\nabla \times \mathbf{A}|^2)$, and is a constant, ν_c (respectively, ν_a), in copper (respectively, air); j is the density of the currents (known).

The special condition of this problem is that Ω does not appear explicity in the boundary conditions but only in the coefficient of the PDE. Because of (14), however, we decompose (13) into three equations (one per medium); then Ω appears as *transmission boundary conditions.* More precisely (13) and (14) are equivalent to

$$\nabla \cdot \big(\nu(|\nabla \times \mathbf{A}|^2)\nabla \mathbf{A}\big) = 0 \qquad \text{in iron,} \tag{14}$$

$$\nu_a \, \Delta \mathbf{A} = 0 \qquad \text{in air,} \tag{15}$$

$$\nu_c \, \Delta \mathbf{A} = j \qquad \text{in copper,} \tag{16}$$

$$\text{Jump of } \nu \frac{\partial \mathbf{A}}{\partial \mathbf{n}} \text{ continuous at the interfaces;} \qquad \mathbf{A}|_\infty = 0. \tag{17}$$

2.3.4 Optimization of a wing

Let S be a wing profile and Ω the region occupied by air (complement of S). At moderate speed the pressure on the wing is

$$p(x) = k_1 - k_2|\nabla \times \Psi|^2(x), \tag{18}$$

where Ψ is the solution of

$$\Delta\Psi = 0 \quad \text{in } \Omega, \qquad \Psi|_{\partial S} = 0, \qquad \Psi|_\infty = u_{01}x_2 - u_{02}x_1 + \lambda. \tag{19}$$

Here $\mathbf{u}_0 = (u_{01}, u_{02})$ is the velocity of the wing, and λ is determined from the Joukowski condition: there is only one λ for which the flow does not turn around the trailing edge of S.

The lift factor of the wing profile is proportional to λ. Good wings have a boundary layer that separates from the profile very close to the trailing edge. Since this property is related to the flatness of p, we may study the following problem:

$$\min_{\Omega\in O} E(\Omega) = \left(\int_{\partial S} [k - |\nabla\Psi(\Omega)|^2]^m \, d\Gamma\right)^{1/m}, \tag{20}$$

where $\Psi(\Omega)$ is the solution of (19) for $k = k_1/k_2$ and

$$O = \{\Omega = \mathbb{R}^2 - S : S \text{ has a trailing edge and a given chord}\}.$$

Here $E(\Omega)$ is the $L^m(\partial S)$ norm of p, and ideally one would set $m = +\infty$, but then E becomes *nondifferentiable.*

Furthermore, since the lift factor is treated as data, one may introduce the incidence angle α (see Figure 2.4) and study the following for a given λ:

$$\min_{S,\alpha} \left\{ \left(\int_{\partial S} [k - |\nabla\Psi|^2]^m \, d\Gamma\right)^{1/m} : \Delta\Psi = 0 \text{ in } \mathbb{R}^2 - S \right.$$
$$\Psi|_{\partial S} = 0,\ \Psi|_\infty = -|\mathbf{u}_0|\cos\alpha x_2 + |\mathbf{u}_0|\sin\alpha x_1 + \lambda, \tag{21}$$
$$\left. \nabla \times \Psi \text{ continuous at the trailing edge} \right\}.$$

In the terminology of optimal control design, this problem has *state constraints.* The last equation is a constraint between Ψ and α.

Another condition of this problem is that the criteria involve a *boundary integral* on the unknown boundary. Again, the industrial applications use the transonic equations for the potential rather than the Laplace equation for the stream function Ψ.

2.3.5 Optimal shape problem with parabolic operator

In what way does a stretched-out body S swim (or fly)? Referring to Section 2.3.2 for notation, at high Reynolds number, the velocity and pressure in the flow

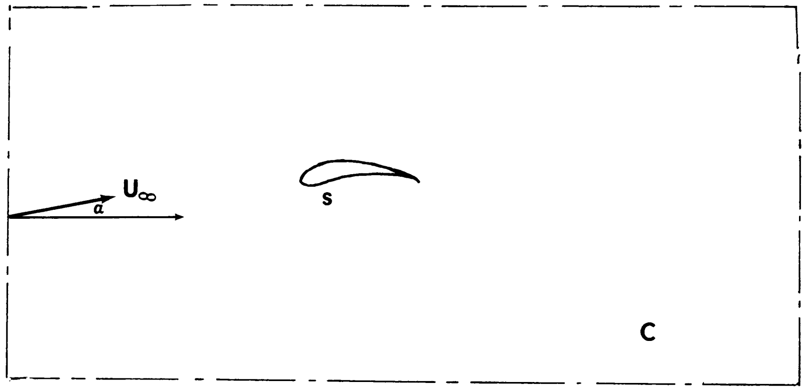


Fig. 2.4 Wing optimization. A two-dimensional airfoil S at incidence α and flying at speed u_∞. C approximates infinity.

satisfy the Navier–Stokes equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\,\nabla\mathbf{u} - \nu\,\Delta\mathbf{u} + \nabla p = 0, \qquad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \times]0,T[. \tag{22}$$

Let $\mathbf{x}(\cdot, t)$ be the position of ∂S at time t (see Figure 2.5). The motion of $\mathbf{x}$ is decomposed into a rigid-body motion plus a local deformation $\mathbf{l}(\cdot, t)$, which become the control parameters:

$$\frac{d\mathbf{x}}{dt}(s,t) = \frac{d\mathbf{x}_c}{dt}(t) + \mathbf{w}(t) \times \mathbf{x}(s,t) + \frac{d\mathbf{l}}{dt}(s,t), \qquad s \in \partial S, \tag{23}$$

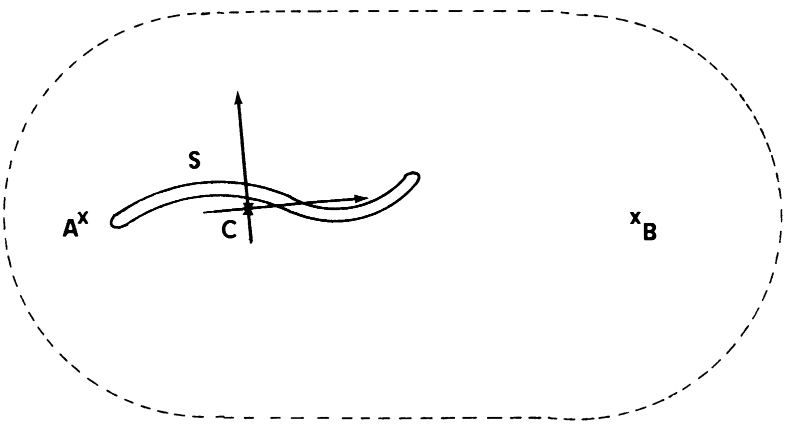


Fig. 2.5 Optimal swim from A to B of a deformable body; x_c is the center of gravity.

where $\mathbf{x}_c$ is the center of gravity of S and $\mathbf{w}(t)$ is the instantaneous rotation. Then Newton's laws for the equilibrium of S are

$$\int_{\partial S} (\boldsymbol{\sigma} + \mathbf{I}p)\, d\Gamma = m \frac{d\mathbf{x}_c}{dt} \qquad \text{(conservation of forces)}, \tag{24}$$

$$\int_{\partial S} (\boldsymbol{\sigma} + \mathbf{I}p)\, d\Gamma \times \mathbf{x} = m\mathbf{w} \qquad \text{(conservation of momentum)}, \tag{25}$$

where m is the mass of S, $\mathbf{I}$ is the identity tensor, and $\boldsymbol{\sigma}$ is the stress tensor

$$\sigma_{ij} = \frac{v}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{26}$$

An efficient swim is one that brings $\mathbf{x}_c$

$$\mathbf{x}_c(0) = \mathbf{a} \quad \text{to} \quad \mathbf{x}_c(T) = \mathbf{b} \tag{27}$$

into minimum energy:

$$\min_{\mathbf{l}} \left\{ E(\mathbf{l}) = \int_{\Omega \times]0,T[} \tfrac{1}{2}|\nabla \mathbf{u} + \nabla \mathbf{u}^t|^2\, dx\, dt \colon \int_S dx = m, (22) \text{ to } (27) \right\}. \tag{28}$$

These problems are quite important in practice to solve, but too time-consuming to solve using computers available at present. Except for the very special case of Stokes flow ($v \gg 1$) (see [56]), computer solutions to these problems are still being investigated.

2.3.6 Optimal shape problem with hyperbolic operator

Many shape optimization problems arise from the study of acoustics. For example, the best design of a soundproof wall may lead to the problem

$$\min_{C \in O} \left\{ \int_{D \times]0,T[} |\nabla \Phi|^2\, dx\, dt \colon \frac{\partial^2 \Phi}{\partial t^2} - \Delta \Phi = f \text{ in } (\Omega - C) \times]0,T[\right.$$
$$\left. \Phi(t=0) = \frac{\partial \Phi}{\partial t}(t=0) = 0, \left.\frac{\partial \Phi}{\partial n}\right|_{\Gamma} = 0 \right\}. \tag{29}$$

where C is the wall, D is the region of space where silence is desired, and f is the noise source, presumably of compact support S (see Figure 2.6).

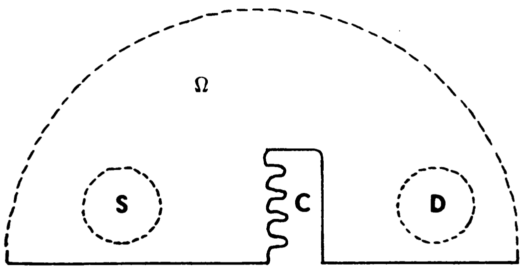


Fig. 2.6 Accoustic optimization. The design parameter is the wall C; S is the noise source, and D is the region which needs to be insulated.

2.3.7 Free boundary problem

Optimum shape design is related to free boundary problems, as illustrated by the following example. Suppose we wish to find $\{\Psi, S\}$ such that

$$\Delta\Psi = 0 \text{ in } \Omega, \qquad \Psi|_\Gamma = \Psi_\Gamma, \qquad \left.\frac{\partial\Psi}{\partial n}\right|_S = 1, \qquad S \subset \Gamma = \partial\Omega. \tag{30}$$

This problem is similar to determining the boundary surface of water running down a slope (see Figure 2.7). To solve this problem, one may consider one of the equivalent optimal shape problems:

$$\min_\Omega \left\{ \int_S \left| \frac{\partial\Psi}{\partial n} - 1 \right|^2 d\Gamma : \Delta\Psi = 0 \text{ in } \Omega \ \Psi|_\Gamma = \Psi_\Gamma \right\}, \tag{31}$$

$$\min_\Omega \left\{ \int_S \left| \Psi - \Psi_\Gamma \right|^2 d\Gamma : \Delta\Psi = 0 \text{ in } \Omega, \left.\frac{\partial\Psi}{\partial n}\right|_S = 1, \Psi|_{\Gamma - S} = \Psi_\Gamma \right\}, \tag{32}$$

$$\min_\Omega \left\{ \int_\Omega |\nabla(\Psi - \Phi)|^2 \, dx : \Delta\Psi = 0 \text{ in } \Omega, \left.\frac{\partial\Psi}{\partial n}\right|_S = 1, \Psi|_{\Gamma - S} = \Psi_\Gamma, \right.$$
$$\left. \Delta\Phi = 0 \text{ in } \Omega, \Phi|_\Gamma = \Psi_\Gamma \right\}, \tag{33}$$

or even, for some m,

$$\min_\Omega \left\{ \int_\Omega \left| \nabla\Psi \right|^2 dx : \Delta\Psi = 0 \text{ in } \Omega, \Psi|_\Gamma = \Psi_\Gamma, \int_\Omega dx = m \right\}. \tag{34}$$

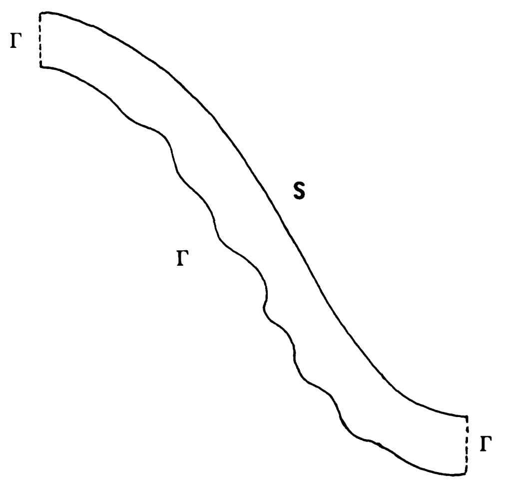


Fig. 2.7 Computation of a spillway. The unknown is the free surface S.

2.4 Principles of Solution

There are several ways of solving optimal shape design problems using a computer. Most of them are based on applications of the principles of the calculus of variations.

We present one of these techniques informally in the following problem model:

$$\min_{\Omega \in O} E(\Omega) = \int_\Omega |\nabla(\Phi(\Omega) - \Phi_d)|^2 \, dx, \tag{35}$$

where $\Phi(\Omega)$ is the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega, \qquad \left.\frac{\partial \Phi}{\partial n}\right|_\Gamma = 0, \tag{36}$$

and D and C are bounded:

$$O = \{\Omega : C \supset \Omega \supset D, \Omega \text{ open}, \Gamma \text{ Lipschitz}\}. \tag{37}$$

To ensure that (36) has a solution, we assume that f is zero outside D and f has zero mean. Assuming that a solution Ω^* exists, we wish to compute it as a limit of $\{\Omega^n\}$, where Ω^{n+1} is generated from Ω^n by a process to be defined.

Thus the problem becomes the following: Knowing an approximation Ω of Ω^*, how can we choose Ω' such that

$$E(\Omega') < E(\Omega)? \tag{38}$$

If Ω' is "close" to Ω, then

$$\delta\Phi = \Phi(\Omega') - \Phi(\Omega) \tag{39}$$

is small, and we may write

$$\begin{aligned} E(\Omega') - E(\Omega) \simeq & \int_\Omega 2\nabla(\Phi(\Omega) - \Phi_d) \cdot \nabla\delta\Phi \, dx \\ & + \int_{\Omega' - \Omega \cap \Omega'} |\nabla(\Phi(\Omega') - \Phi_d)|^2 \, dx \\ & - \int_{\Omega - \Omega' \cap \Omega} |\nabla(\Phi(\Omega) - \Phi_d)|^2 \, dx. \end{aligned} \tag{40}$$

Now, from (36),

$$\int_\Omega \nabla\Phi \cdot \nabla w \, dx = \int_\Omega f w \, dx \qquad \forall w \in H^1(C), \tag{41}$$

where $H^1(C)$ is the set of square integrable functions with square integrable first derivatives. To find $\delta\Phi$, we differentiate (41):

$$\int_{\delta\Omega} \nabla\Phi \cdot \nabla w \, dx + \int_{\Omega} \nabla\delta\Phi \cdot \nabla w \, dx = 0 \qquad \forall\, w \in H^1(C) \tag{42}$$

The right hand side is zero because f is zero outside D, and Ω always contains D. By $\delta\Omega$, we mean the strip $\Omega' - \Omega' \cap \Omega$, where the integrand is taken with a plus sign, and $\Omega - \Omega' \cap \Omega$, where it is taken with a minus sign (see Figure 2.8). If $\alpha(s)$

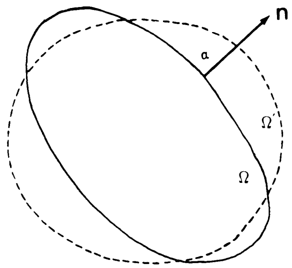


Fig. 2.8 The domain Ω' is close to Ω in the sense that the distance α is small.

denotes the distance between Γ and Γ' at $x(s) \in \Gamma$ measured positively on $\Omega' - \Omega' \cap \Omega$ and negatively in $\Omega - \Omega' \cap \Omega$, then from the mean value theorem, we have

$$\int_{\delta\Omega} \nabla\Phi \cdot \nabla w \, dx \simeq \int_{\Gamma} \alpha \nabla\Phi \cdot \nabla w \, d\Gamma. \tag{43}$$

Thus, by taking $w = \Phi - \Phi_d$, we are able to write

$$\int_{\Omega} \nabla\delta\Phi \cdot \nabla(\Phi - \Phi_d) \, dx \simeq \int_{\Gamma} - \alpha\nabla\Phi \cdot \nabla(\Phi - \Phi_d) \, d\Gamma. \tag{44}$$

Applying once again the mean value theorem to (40), we find that

$$E(\Omega') - E(\Omega) \simeq \int_{\Gamma} [-2\nabla\Phi \cdot \nabla(\Phi - \Phi_d) + |\nabla(\Phi - \Phi_d)|^2]\alpha \, d\Gamma + o(\alpha). \tag{45}$$

If we choose

$$\alpha(x) = \rho[2\nabla\Phi \cdot \nabla(\Phi - \Phi_d) - |\nabla(\Phi - \Phi_d)|^2], \tag{46}$$

then (45) yields

$$E(\Omega') - E(\Omega) = -\rho \int_{\Gamma} [-2\nabla\Phi \cdot \nabla(\Phi - \Phi_d) + |\nabla(\Phi - \Phi_d)|^2]^2 \, d\Gamma + o(\rho). \tag{47}$$

So $\rho \ll 1$ necessarily results in (38) since the integrand is positive. This means that Ω' is constructed from Ω by moving Γ normal a small distance proportional to (46) at every point.

This is not a rigorous calculation, and we must clarify the meaning of the following statements such as

Is $\Phi(\Omega')$ "close" to $\Phi(\Omega)$ when Ω' is "close" to Ω?
What is the meaning of "close"?
Is Ω' constructed by (46) admissible?
Is (38) sufficient for the convergence of $\{\Omega^n\}$?

Besides these mathematical questions, it remains to provide a discrete version of this calculation which may be implemented on a computer.

Remark. From (45), we also find that

$$|\nabla(\Phi(\Omega^*) - \Phi_d)|^2 - 2\nabla\Phi(\Omega^*) \cdot \nabla(\Phi(\Omega^*) - \Phi_d)_{x\in\Gamma^*} \begin{cases} = 0 & \forall x \in \Gamma^*, x \notin \partial D \cup \partial C, \\ \geq 0 & \forall x \in \Gamma^* \cap \partial D, \\ \leq 0 & \forall x \in \Gamma^* \cap \partial C. \end{cases}$$

This is known as a *necessary optimality condition* for Ω^*.

2.5 Future of Optimal Design Applications in Industry

It should be clear from the examples considered that optimal shape design is an applications-oriented subject. The systems described in PDEs have practical shape design applications in industry. At present the most critical applications are for the design of airplanes and of structures using mechanical engineering; but other applications will arise with the development of more numerical simulations applied to in industrial design work.

We examine the drawbacks of solving design problems by optimization techniques. A good engineer, familiar with any approach to problem solving is, as everyone knows, an intuitive optimizer; he or she knows how to adjust the parameters to reach within, say, 5% of a physically meaningful objective model, with the following restrictions:

i. He or she must have worked for a long time with the system.
ii. The number of parameters should not be greater than, say, five.

Thus if i and ii are not met, there are unlikely to be alternative solutions other than optimization. This is especially true of three-dimensional designs.

Let us examine another problem: the choice of the criterion E and the choice of the constraint set. For optimization problems, the design engineer usually aims at an optimum for one criterion which is adequate for the needs of the other criteria. These so-called pareto-optimum problems are very difficult to deal with from the analysis point of view. Furthermore, even if the engineer has decided to optimize with respect to one criterion only, he or she may find that the mathematical answer to the problem is not feasible due to some constraints which are seen *a posteriori* only.

The author's experience confirms that the business of defining beforehand what is good and what is feasible or admissible is difficult. Thus the algorithm of Figure 2.9 is too simple to be used in practice; optimization cannot be a

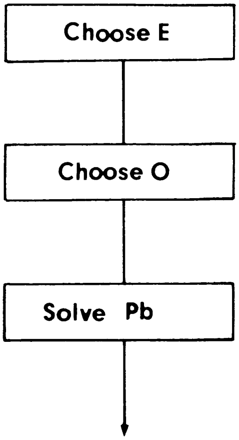


Fig. 2.9 An oversimplified view of optimal shape design in industry.

substitute for the engineer's know-how. Therefore one should aim at a dialogue between the engineer and the optimizer, for example, the algorithm of Figure 2.10. But then shape optimization using a computer becomes a rather expensive business because anytime E or O are changed, the formulas for the gradients must be reprogrammed into the computer.

Therefore, we conclude that optimum shape design analysis cannot replace a good design engineer, but rather it should be used as a tool; it is costly, but for systems with many degrees of freedom there is no other approach. The following comments deal with how and by whom the optimal shape design should be done.

There are two obvious prerequisites for optimization:

i. The industry must have computing facilities.
ii. The industry must be knowledgable in the numerical simulation of its own systems.

If these prerequisites are met, then there are on-the-spot numerical analysts who can either themselves optimize or can direct external optimizers.

This book demonstrates that optimal shape design is easiest to follow using the finite element method (FEM), but it can also be done with other numerical

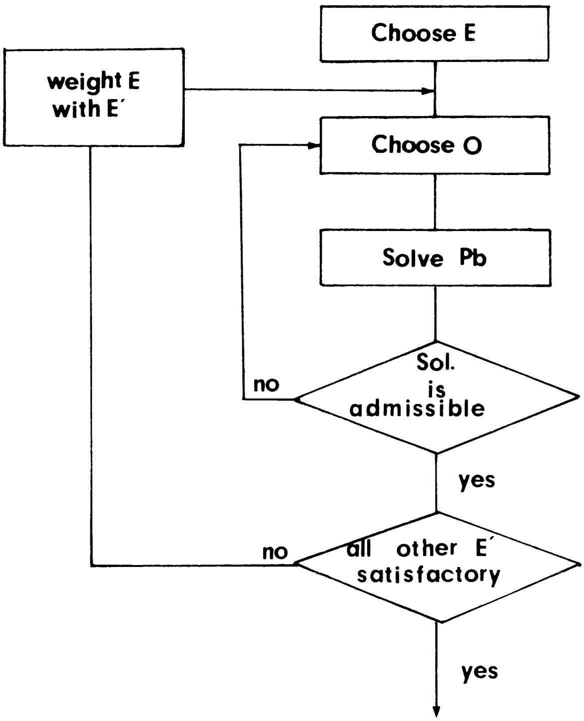


Fig. 2.10 A more reallistic view of optimal shape design in industry.

methods. Because of prerequisite ii, the industry has usually invested several years making efficient numerical software describing its own systems. Thus, it would be foolish to start from scratch again just because the FEM approach is recommended, and indeed, this author advises not to do so. Whenever possible, the optimizer should use the industry's own know-how and previous choices of applied numerical methods.

2.6 Historical Background and References

Optimal shape design has been studied in a wide variety of fields; so it is difficult to give a complete account of the previous work. This section contains a few comments on articles and books.

Shape optimization is a branch of optimal control theory, which is based on the calculus of variation. Under this topic Hadamard (1910) [32] gave a formula to compute the derivative of Green's function of the Laplace operator with respect to the normal variations of the domain. Namely, let Ω_0 of boundary Γ_0

and Ω_λ be such that

$$\Gamma_\lambda = \{x + \mathbf{n}(x)\alpha(x)\lambda : x \in \Gamma_0\}, \tag{48}$$

where α is a given function of $L^2(\Gamma)$ and $\mathbf{n}(x)$ is the normal at x. Let $G(x, y, \Gamma_0)$ be Green's function of the Laplace operator, then Hadamard finds

$$\partial_\alpha G(x, y, \Gamma_0) = \frac{d}{d\lambda} G(x, y, \Gamma_\lambda)\bigg|_{\lambda=0} = \int_{\Gamma_0} -\frac{\partial G}{\partial n_z}(z, x, \Gamma_0)\frac{\partial G}{\partial n_z}(z, y, \Gamma_0)\alpha(z)\, d\Gamma(z).$$

This important step does not seem to have been pursued further, possibly because computers were not present then to facilitate such studies. Later on, studies were made only for those problems with an explicit solution for the PDE. Among the later work we note Miele (1965) [47] on the optimization of wing profiles at supersonic speed. Eventually the method was extended to problems of structural engineering; in particular those where it is possible to convert the shape design problem into one of an optimal control problem with control governed by the coefficients of the PDE (see, for example, Armand (1974) [6], Gallagher and Zienkiewicz (1973) [29], and Banichuk (1980) [7]).

The direct treatment in its generality using the techniques of optimal control of distributed systems seems to have begun in 1972 with Lions [42] and with Cea, Gioan, and Michel (1973) [18], where the first algorithm is found. Optimality conditions were found concurrently by Pironneau (1973) [53] and (1976) [55] and Murat and Simon (1976) [49] for problems with Dirichlet conditions, by Dervieux and Palmerio (1975) [25] for the Neumann problem, and by Murat and Simon (1977) [50] and Rousselet (1976) [60] for the eigenvalue problem. The existence of solutions was then studied by Murat and Simon (1976) [49], Chenais (1975) [19], and Zolezio (1979) [67]. Numerical methods based on the above results were devised and tested by Begis and Glowinski (1975) [8] and Morice (1974) [48] for the technique of mappings (see Chapter 8) and by Marrocco and Pironneau (1978) [46] and Angrand (1980) [4] for the finite element method. Several of these results are available in Cea [16] and Banichuk [7].

Related works include Dervieux and Palmerio (1972) [24] for an extension of Hadamard's method, Cea (1976) [15] for a dynamical interpretation of optimal design algorithms, and Dervieux (1981) [23] for the relation to free boundary problems.

CHAPTER 3

Existence of Solutions

3.1 Introduction

To study the existence and uniqueness of solutions of optimal shape design problems, is interesting from the point of view of theory. However, at the present time, this problem has not been solved entirely; so we can only present some partial results.

The type of boundary conditions existing in the PDE plays an important role; therefore, we examine the results of two representative examples: one with Dirichlet conditions and one with Neumann conditions. The first results of this type were obtained by Murat and Simon [49] and several authors from the University of Nice [19], [14], [67]. Later, it was found that this problem is related to the study of PDEs with oscillating coefficients (homogenization), and further results can be found in [21], [12], [57], [63], [36].

3.2 Dirichlet Conditions

3.2.1 General case

Consider the problem model

$$\min_{\Omega \in O} E(\Omega) = \int_D |\nabla \Phi(\Omega) - \mathbf{u}_d|^2 \, dx \tag{1}$$

where O is a given set of admissible domains (bounded open sets of $\mathbb{R}^n$ containing D) D is a given bounded open set of $\mathbb{R}^n$, $\mathbf{u}_d$ is a given square integrable vector-valued function on D, and $\Phi(\Omega)$ is the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega; \qquad \Phi|_\Gamma = 0. \tag{2}$$

We wish to find under which conditions on O does (1) have a solution.

Definition. Let A, B be two subsets of $\mathbb{R}^n$ and define

$$d(x, \mathrm{B}) = \inf_{y \in B} |x - y|, \tag{3}$$

$$\rho(A, B) = \sup_{x \in A} d(x, \mathrm{B}), \tag{4}$$

$$\delta(A, B) = \max\{\rho(A, B), \rho(B, A)\}; \tag{5}$$

δ is the *Hausdorff distance* between A and B; it defines a topology on the closed bounded sets of $\mathbb{R}^n$ (see Figure 3.1):

$$A_m \to A \quad \text{in the Hausdorff sense if } A_m, A \text{ are closed and bounded and if } \delta(A_m, A) \to 0. \tag{6}$$

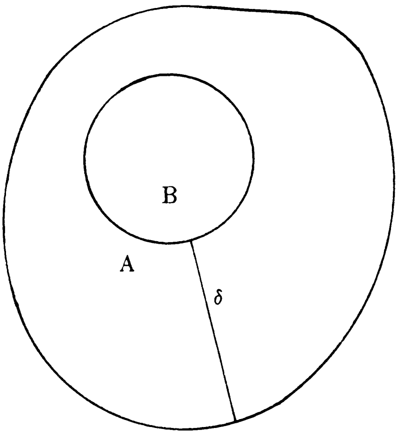


Fig. 3.1 The Hausdorff distance $\delta(A, B)$.

Lemma 1. *The Hausdorff limit A of $\{A_m\}$ is also the set of all accumulation points of the sequences $\{x^m\}$ such that $x^m \in A_m \; \forall m$.*

PROOF. Assume $A_m \to A$, Hausdorff. Let $\{x^m\}$ converge to x and $x^m \in A_m \; \forall m$. By (4)

$$d(x^m, A) \to 0.$$

Since A is compact, $x = \lim x^m \in A$. Conversely, since A is the set of accumulation points of $\{x^m\}$, $x^m \in A_m$, we have

$$d(x, A_m) \to 0 \qquad \forall x \in A; \qquad d(x^m, A) \to 0 \qquad x^m \in A.$$

Therefore $A_m \to A$, Hausdorff. □

Lemma 2. *The set inclusion is continuous for the Hausdorff topology:*

$$A_m \to A, \qquad B_m \to B, \qquad A_m \subset B_m \Rightarrow A \subset B.$$

PROOF.

$$x \in A \Rightarrow \exists\, x^m \to x,\; x^m \in A_m \Rightarrow x^m \in B_m \Rightarrow x \in B.$$ □

Theorem 1. *Let $\{A_m\}$ be a sequence of closed sets of $\mathbb{R}^n$ such that for some bounded C of set $\mathbb{R}^n$,*

$$A_m \subset C \qquad \forall m. \tag{7}$$

Then there exists a set A closed and contained in C and a subsequence $\{A_{m_i}\}_i$ of $\{A_m\}$ such that $A_{m_i} \to A$, in the Hausdorff sense, as $i \to \infty$.

PROOF. See [22].

Remark. Hausdorff convergence should not be confused with the two other types of convergence of domain: the convergence in L^∞ weak star of

$$\chi_{A_m} \to \chi_A \qquad \text{(convergence of the characteristic functions)} \tag{8}$$

and the pointwise convergence of the boundaries

$$\Gamma_{A_m} \to \Gamma_A, \tag{9}$$

Although (9) implies (6), the connection between (6) and (8) is not simple. As χ_{A_m} is bounded in L^∞, there always exists an l with

$$\chi_{A_{m_i}} \to l \quad \text{in } L^\infty \text{ weak star,} \tag{10}$$

but l may not be a characteristic function.

Proposition 1. *Given a sequence $\{\Omega^m\}$ of open sets included in C bounded, let Φ^m be the solution of*

$$-\Delta\Phi^m = f \quad \text{in } \Omega^m, \qquad \Phi^m|_{\Gamma^m} = 0, \tag{11}$$

where Γ^m is the boundary of Ω^m. Assume that

i. $C - \Omega^m \to C - \Omega$ *in the sense of Hausdorff.* (12)
ii. $\chi_{C-\Omega^m} \to l$ *in L^∞ weak star, $l > 0$ a.e. in $C - \Omega$.* (13)
iii. $w \in H^1(C)$, $w\chi_{C-\Omega} = 0 \Rightarrow w|_\Omega \in H_0^1(\Omega)$.

Then $\Phi^m \to \Phi$ in H^1, where *Φ is the solution of*

$$-\Delta\Phi = f \quad \text{in } \Omega; \qquad \Phi|_\Gamma = 0. \tag{14}$$

Comment. If Ω is open, $H_0^1(\Omega)$ is defined as the closure in H^1 of the set of C^∞ functions with compact support; so iii is not implied. By (11) we mean the solution in $H_0^1(\Omega^m)$ of

$$\int_{\Omega^m} \nabla\Phi \cdot \nabla w \, dx = \int_{\Omega^m} fw \, dx \qquad \forall w \in H_0^1(\Omega).$$

In order to prove Proposition 1, we establish the following property.

Lemma 3. *Let $\{F^m\}$ be a sequence of closed sets of $\mathbb{R}^n$, contained in C bounded, which converges in the sense of Hausdorff to F closed and bounded. Then*

$$\forall w \in H_0^1(\Omega) \qquad \exists \{w^m\},\ w^m \to w \quad \text{in } H^1 \text{ and } w^m \in H_0^1(\Omega^m), \tag{15}$$

where $\Omega^m = C - F^m$ and $\Omega = C - F$.

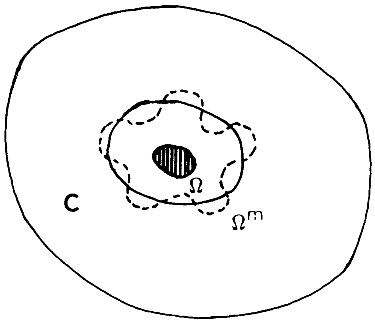


Fig. 3.2 If $C - \Omega^m \to C - \Omega$, Hausdorff, supp w (shaded) in Ω will eventually be included in Ω^m.

PROOF. (See Figure 3.2.) Let $\mathscr{D}(\Omega)$ be the set of C^∞ functions with compact supports in Ω. Assume for the time being that $w \in \mathscr{D}(\Omega)$; then

$$\operatorname{supp} w \subset \Omega, \tag{16}$$

or equivalently,

$$F \cap \operatorname{supp} w = \varnothing, \qquad F = C - \Omega. \tag{17}$$

Suppose that there exists a subsequence for which

$$F^{m_j} \cap \operatorname{supp} w \neq \varnothing \qquad \forall j. \tag{18}$$

Then there exists $\{x_{m_j}\}$ and x^* such that

$$x_{m_j} \in F^{m_j} \cap \operatorname{supp.} w, \qquad x_{m_j} \to x^* \in \operatorname{supp} w \tag{19}$$

because supp w is compact, but that is not possible because

$$F \cap \operatorname{supp} w = \varnothing \Rightarrow \exists\, \varepsilon : d(x^*, F) \geq 2\varepsilon > 0 \Rightarrow d(x_{m_j}, F^{m_j}) \geq \varepsilon \qquad \forall j \geq j_0. \tag{20}$$

Therefore, there exists m_0 such that

$$\operatorname{supp} w \subset \Omega^m \qquad \forall m > m_0; \tag{21}$$

hence $w \in H_0^1(\Omega^m)$. So let $w^m = w$ for $m > m_0$.

Now $\mathscr{D}(\Omega)$ is dense in $H_0^1(\Omega)$; therefore, by density the property holds for $H_0^1(\Omega)$:

$$\int_C |\nabla(\tilde{w}^m - \tilde{w})|^2 \, dx \to 0, \tag{22}$$

where the $\tilde{}$ denotes the extension by 0 in C. □

PROOF OF PROPOSITION 1. In variational form, (11) is

$$\int_{\Omega^m} \nabla\Phi^m \cdot \nabla w \, dx = \int_{\Omega^m} fw \, dx \qquad \forall\, w \in H_0^1(\Omega^m). \tag{23}$$

Extending Φ^m by zero in C yields

$$\int_C \nabla\tilde{\Phi}^m \cdot \nabla\tilde{w}\,dx = \int_C \tilde{f}\tilde{w}\,dx \qquad \forall\,\tilde{w} \in H_0^1(C), \qquad \tilde{w}|_{\Omega^m} \in H_0^1(\Omega^m). \tag{24}$$

Taking $\tilde{w} = \tilde{\Phi}^m$ yields

$$|\nabla\tilde{\Phi}^m|_0^2 \leq |\tilde{f}|_0|\tilde{\Phi}^m|_0, \tag{25}$$

and the Poincaré inequality shows that $\{\tilde{\Phi}^m\}$ is bounded in $H_0^1(C)$. Therefore there exists an accumulation point Φ^* of $\{\tilde{\Phi}^m\}$ with respect to the weak topology of H^1.

From Lemma 3, for a fixed $w \in H_0^1(\Omega)$, we have

$$\tilde{w}^m \to \tilde{w} \quad \text{in } H_0^1(C),\ \tilde{w}^m \in H_0^1(C) \tag{26}$$

and from (24)

$$\int_C \nabla\tilde{\Phi}^m \cdot \nabla\tilde{w}^m\,dx = \int_C \tilde{f}\tilde{w}^m\,dx. \tag{27}$$

Approaching the limit yields

$$\int_C \nabla\tilde{\Phi} \cdot \nabla\tilde{w}\,dx = \int_C f\tilde{w}\,dx, \tag{28}$$

Thus, it remains to show that

$$\tilde{\Phi} \in H_0^1(\Omega). \tag{29}$$

By hypothesis

$$\chi_{C-\Omega^m}\tilde{\Phi}^m = 0. \tag{30}$$

Therefore, at the limit,

$$l\tilde{\Phi}^m = 0 \Rightarrow \tilde{\Phi}^m = 0 \quad \text{in } C - \Omega^m \qquad \square \tag{31}$$

Proposition 1 gives a set of sufficient conditions for the convergence of the solutions of Dirichlet problems when the domains converge in the Hausdorff sense.

Now we proceed by giving some conditions that will enable us to apply Proposition 1 to the minimizing sequence of an optimum design problem.

Definition. (See [19]; see also [3], [26]). Let $C(\varepsilon, \xi, x)$ be the half-cone of angle ε, direction ξ, and vertex x (see Figure 3.3) intersected with the ball $B(x, \varepsilon)$ of center x and radius ε.

Then Ω has the *ε-cone property* if for all $x \in \Gamma$ there exists a direction $\xi(x)$ such that

$$C(\varepsilon, \xi(x), y) \subset \Omega \qquad \forall\,y \in B(x, \varepsilon) \cap \Omega \tag{32}$$

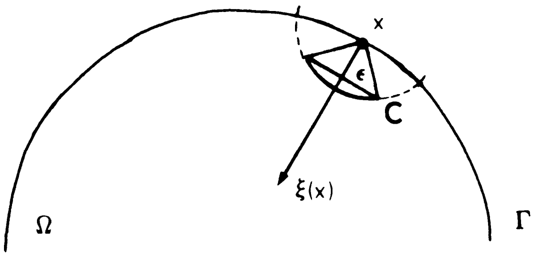


Fig. 3.3 The truncated cone C, with direction ξ, angle ε, and vertex x.

Proposition 2. *(See [19].) Ω has the ε-cone property if and only if Γ is Lipschitz continuous with constant $k(\varepsilon) > 0$.*

Theorem 2. *Assume that for some ε, $\mathcal{O}$ is taken to be*

$$\mathcal{O}_\varepsilon = \{\Omega \text{ open}: C \supset \Omega \supset D, \Omega \text{ has the } \varepsilon\text{-cone property}\}. \tag{33}$$

Then problem (1) *has at least one solution.*

To prove this result, we need the following lemmas.

Lemma 4. *If $\Omega^m \in \mathcal{O}_\varepsilon$, $\Omega \in \mathcal{O}$, and $\bar{\Omega}^m \to \bar{\Omega}$ or $C - \Omega^m \to C - \Omega$, Hausdorff, then $\Omega \in \mathcal{O}_\varepsilon$ and*

$$\chi_{\Omega^m} \to \chi_\Omega \quad \text{in } L^\infty \tag{34}$$

Proof. Take $x \in \Omega$ and let $x^m \in \Omega^m$ converge to x. Since the truncated half-cone $C(\varepsilon, \xi^m, x^m) \subset \Omega^m$ is defined by $2n$ parameters (direction and vertex), a subsequence converges to a truncated half-cone $C(\varepsilon, \xi, x)$; from Lemma 2 it is included in Ω, as is $C(\varepsilon, \xi, y)$ for all $y \in B(x, \varepsilon - \delta) \cap \Omega$, $\forall \delta > 0$. Therefore Ω satisfies the ε-cone property.

Now let l be such that

$$\chi_{\Omega^m} \to l \quad \text{in } L^\infty \text{ weak star.}$$

Then

$$\int_{C(\varepsilon,\xi,x)} dx = \lim \int_{C(\varepsilon,\xi^m,x^m)} dx = \lim \int_{C(\varepsilon,\xi^m,x^m)} \chi_{\Omega^m}\, dx$$
$$= \int_{C(\varepsilon,\xi,x)} l\, dx. \tag{35}$$

This in turn implies that $l = 1$ in $C(\varepsilon, \xi, x)$, hence in Ω also.

To prove that $l = 0$ in $C - \Omega$, we use exactly the same argument on the complementary set Ω^c of Ω. First we use the result of Proposition 2. This implies that $(\Omega^m)^c$ and its accumulation points Ω_c have the ε'-cone property for some $\varepsilon' > 0$. Thus

$$l = 0 \quad \text{on } \Omega_c. \tag{36}$$

However, by construction $\Omega_c \supset \Omega^c$; so the proof is completed. □

Proof of Theorem 2. Let $\{\Omega^m\}$ be a minimizing sequence for E. From Theorem 1 there exists Ω such that $C - \Omega^m \to C - \Omega$, Hausdorff, for some subsequence. Now let us check that the assumptions of Proposition 1 are satisfied.

Hypothesis i holds by construction.
Hypothesis ii is shown by Lemma 4.
Hypothesis iii is a result of the Lipschitz continuity of $\partial\Omega$. □

Remark. This also proves that the ε-cone property plus $\bar{\Omega}^m \to \bar{\Omega}$, Hausdorff, implies

$$\Phi^m \to \Phi \quad \text{strongly in } H^1 \tag{37}$$

Comments. Theorem 2 is an example of the type of conditions that are sufficient for the existence of solutions; but such conditions are clearly too strong. Their purpose is to forbid the oscillation of the boundaries; however, some oscillations are compatible with ii, as demonstrated by the following example.

$$\Omega^m = \{x, y : y \leq 2 + \sin mx\} \cap]0, 3[^2, \tag{38}$$

$$\Omega =]0, 3[\times]0, 1[, \tag{39}$$

$$\chi_{C-\Omega^m} \to \begin{cases} 0 & \text{if } y \leq 1, \\ \frac{1}{2} & \text{if } 1 \leq y \leq 3, \\ 1 & \text{if } y \geq 3, \text{ in } L^\infty \text{ weak*}. \end{cases} \tag{40}$$

3.2.2 Minimum energy problem

As noted in [52], [55], there is at least one case where we can prove the existence of a solution without any restriction of regularity on the boundaries. Consider the problem

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \frac{1}{2} \int_\Omega |\nabla\Phi(\Omega)|^2 \, dx - \int_\Omega f\Phi \, dx, \tag{41}$$

where $\Phi(\Omega)$ is the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega; \qquad \Phi|_\Gamma = 0; \tag{42}$$

$$\mathcal{O} = \left\{\Omega \subset C : \Omega \text{ open}, \int_{C-\Omega} dx = 1\right\}. \tag{43}$$

The special condition of this problem is that $E(\Omega)$ is the energy of the system. The constraints in (43) on the measure of Ω are necessary to make the problem nontrivial. We assume, obviously, that the measure of C is greater than 1.

Theorem 3. *The problem given in (41) to (43) has at least one solution; it can be found by solving*

$$\min_{\Phi \in V} E(\Phi) = \tfrac{1}{2} \int_C |\nabla \Phi|^2 \, dx - \int_C f\Phi \, dx, \tag{44}$$

where

$$V = \{\Phi \in H_0^1(C) : \text{mes}\{x : \Phi(x) = 0\} \geq 1\}, \tag{45}$$

and by setting

$$\Omega = C - \bigcap_{\Psi = \Phi \, a.e.} \overline{\{x : \Psi(x) = 0\}}. \tag{46}$$

PROOF. Let Ω^* be the solution of (41) and $\Phi(\Omega^*)$ the corresponding solution of (42). Extending Φ by zero outside Ω^* yields an admissible function for (43); so if $\hat{\Phi}$ is a solution of (43), we have

$$E(\hat{\Phi}) \leq E(\Omega^*). \tag{47}$$

Conversely, denote by $\hat{\Omega}$ the set defined by (46) with $\hat{\Phi}$. As $W = \{\Phi \in H_0^1(C) : \Phi = 0 \text{ in } C - \hat{\Omega}\}$ is a subset of V, we have

$$E(\hat{\Phi}) = \min_V E(\Phi). \tag{48}$$

Now $E(\Phi)$ is the energy of (42); so $\hat{\Phi}$ satisfies (42). This proves the equivalence between (44) and (41).

Now let us prove that (44) has a solution. Since E is strictly convex weakly semicontinuous in $H^1(C)$, all we have to do is to prove that V is weakly close, i.e.,

$$\Phi^n \to \Phi \quad \textit{weak } H^1, \qquad \text{mes}\{x : \Phi^n(x) = 0\} \geq 1 \Rightarrow \text{mes}\{x : \Phi(x) = 0\} \geq 1. \tag{49}$$

From Murat–Tartar in [41], for example, we know that

$$|\Phi^n - \Phi|_0 \to 0 \Rightarrow \limsup \text{mes}\{x : \Phi^n(x) = 0\} \leq \text{mes}\{x : \Phi(x) = 0\}. \tag{50}$$

So (49) holds, and V is weakly closed.

3.2.3. Counterexample

An interesting example is presented in [21]. It illustrates very well that when the boundaries are allowed to oscillate, the limit of a sequence that minimizes the criteria may have nothing to do with the original problem.

Let $\{\Omega^m\}$ be a sequence of bounded open sets of $\mathbb{R}^2$. Consider $\{\Phi^m\}$, where Φ^m is the solution of

$$-\Delta\Phi^m = f \quad \text{in } \Omega^m, \qquad \Phi^m|_{\Gamma_m} = 0. \tag{51}$$

Assume Ω^m is

$$\Omega^m = \Omega - \Omega \cap D^m, \tag{52}$$

where D^m is a regular array of circles of radius

$$r^m = e^{-dm^2} \tag{53}$$

and centers at $\{2i/m, 2j/m\}$, i, j integers (see Figure 3.4).

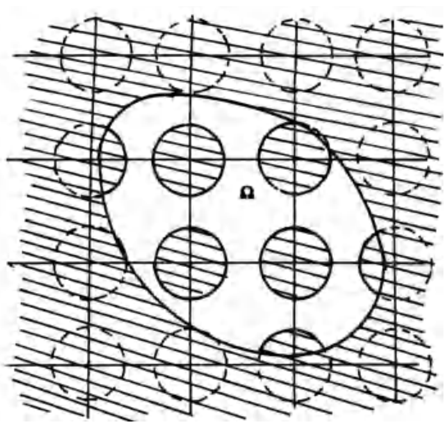


Fig. 3.4 A counterexample: $\bar{\Omega}^m \to \bar{\Omega}$, Hausdorff, but $\Phi^m \not\rightarrow \Phi$. Ω^m is $\Omega - \Omega \cap$ holes.

Theorem 4.

$$\Phi^m \rightarrow \Phi \quad \textit{weakly in } H^1,$$

and Φ is the solution of

$$-\Delta\Phi + \frac{d}{2\pi}\Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = 0. \tag{54}$$

Corollary: *Let Φ_d be the solution of (54); then the problem*

$$\min_{\Omega \subset C}\left\{\int_\Omega |\Phi - \Phi_d|^2\,dx: -\Delta\Phi = f \text{ in } \Omega \qquad \Phi|_\Gamma = 0\right\} \tag{55}$$

has no solution ($f \neq 0$).

PROOF: If Theorem 4 holds, then Φ^m is a minimizing sequence for (55); so the criterion can be as close to zero as required, but in the limit (51) is replaced by (54)! These two equations have different solutions if $f \neq 0$. □

Remark. A similar counterexample can be constructed in $\mathbb{R}^3$ with simply connected domains; it suffices to take a sequence of domains with cross section equal to Ω^m for $z \le z^0$ and Ω for $z > z^0$.

PROOF OF THEOREM 4. The detailed proof is rather involved, and we refer the reader to [21]. Let w^m be the function which satisfies the properties of Figure 3.5 in each small squares of Ω^m. Then one can show that

$$-\Delta w^m = \mu^m - \nu^m, \tag{56}$$

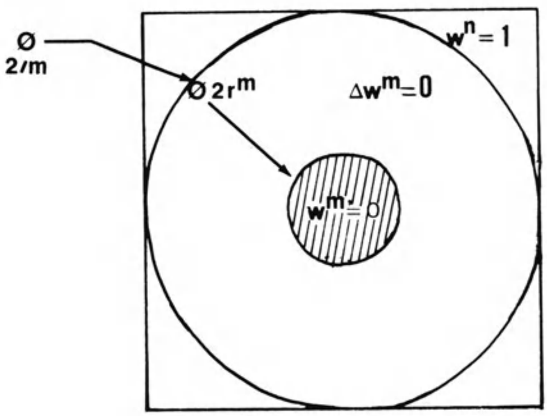


Fig. 3.5 The radius of holes (shaded) tend to zero very fast.

where μ^m is a measure on the big circles and ν^m is a measure on the small ones. Both w^m and μ^m are zero on the holes, but because the holes are very small, we have

$$w^m \to 1 \quad \text{in } H^1 \text{ weakly}, \tag{57}$$

$$\mu^m \to d/2\pi \quad \text{in } H^{-1} \tag{58}$$

Now for any $\Phi \in \mathscr{D}(\Omega)$, $\Phi w^m \in H_0^1(\Omega_m)$ (because w^m is zero on the holes); (51) can be written as

$$\int_\Omega w^m \nabla \tilde{\Phi}^m \cdot \nabla \Phi \, dx - \int_\Omega \tilde{\Phi}^m \Phi \, \Delta w^m \, dx + \int_\Omega \tilde{\Phi}^m \nabla w^m \cdot \nabla \Phi \, dx = \int_\Omega f \Phi w^m \, dx, \tag{59}$$

where $\tilde{}$ stands for an extension by zero in Ω. As $\tilde{\Phi}^m \to \Phi$ in H^1 weakly and as $\tilde{\Phi}^m \nu^m = 0$, by (56) to (58) the limit can be taken in (59), and (54) is found. Furthermore, it can be shown that

$$|\Phi^m - \Phi w^m| \to 0 \text{ in } W_1^1 \text{ strongly}. \tag{60}$$

Remark. Proposition 1 fails in this example because ii does not hold.

3.3 Neumann Boundary Conditions

3.3.1 Sufficient Condition

Again let us work with problem model, for instance,

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_D |\nabla\Phi(\Omega) - u_d|^2 \, dx, \tag{61}$$

where $\Phi(\Omega)$ is the solution of

$$\Phi - \Delta\Phi = f \quad \text{in } \Omega, \qquad \left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = 0, \tag{62}$$

and since C is bounded,

$$\mathcal{O} = \{\Omega : D \subset \Omega \subset C, \Omega \text{ open}\}. \tag{63}$$

For irregular Ω what is meant by (62) is

$$\int_\Omega (\Phi w + \nabla\Phi \cdot \nabla w)\, dx = \int_\Omega f w \, dx \qquad \forall\, w \in H^1(\Omega);\ \Phi \in H^1(\Omega). \tag{64}$$

Unlike the Dirichlet problem (where Φ was always extended to zero outside Ω), equation (64) for the Neumann problem does not imply that $\|\Phi\|_1$ is uniformly bounded independently of Ω; some regularity is assumed.

We state, without proof, the result of Chenais [19]:

Proposition 3. *Let $\mathcal{O}_\varepsilon$ be the elements of $\mathcal{O}$ which have the ε-cone property. Then for all $\Omega \in \mathcal{O}_\varepsilon$,*

$$\forall\, u \in H^1(\Omega)\ \exists\, \tilde{u} \in H^1(C) \text{ such that } \|\tilde{u}\|_{H^1(C)} \le K(\varepsilon, C)\|u\|_{H^1(\Omega)}, \tag{65}$$

and $\tilde{u} = u$ in Ω, where $K(\varepsilon, C)$ is independent of Ω.

Theorem 5. *Let*

$$\mathcal{O}_\varepsilon = \{\Omega : D \subset \Omega \subset C, \Omega \text{ open}, \Omega \text{ has the } \varepsilon\text{-cone property}\} \tag{66}$$

with the notation defined in (61) and (62); then the problem

$$\min_{\Omega \in \mathcal{O}_\varepsilon} E(\Omega) \tag{67}$$

has at least one solution.

PROOF: As before, let $\{\Omega^m\}$ be a minimizing sequence for (67). From (62) we have

$$\|\Phi^m\|_{H^1(\Omega^m)} \le |f|_{L^2(\Omega^m)} \le |f|_{L^2(C)}.$$

Therefore, *by Proposition* 3, $\|\tilde{\Phi}^m\|_1$ is uniformly bounded. Thus, a subsequence for which $\{\bar{\Omega}^m\}$ converges to $\bar{\Omega}^*$ in the sense of Hausdorff and for which

$\{\tilde{\Phi}^m\}$ converges to Φ^* weakly in $H^1(C)$ will have the following properties (*cf.* Lemma 4):

$$\Omega^* \in \mathcal{O}_\varepsilon, \tag{68}$$

$$E(\Omega^*) \leq \inf_{\Omega \in \mathcal{O}_\varepsilon} E(\Omega). \tag{69}$$

Thus, it is necessary to show that Φ^* is the solution of (62) in Ω^*. Another way of writing (64) for Ω^m is

$$\int_C \chi_{\Omega^m}(\Phi^m w + \nabla\Phi^m \cdot \nabla w - fw)\, dx = 0 \qquad \forall\, w \in H^1(C). \tag{70}$$

From Lemma 4 and the definition of $\mathcal{O}_\varepsilon$,

$$\chi_{\Omega^m} \to \chi_\Omega \quad \text{strongly in } L^2(C);$$

so at the limit, (70) becomes

$$\int_C \chi_{\Omega*}(\Phi^* w + \nabla\Phi^* \cdot \nabla w - fw)\, dx = 0 \qquad \forall\, w \in H^1(C). \qquad \square \tag{71}$$

$$\|\Phi(\Omega^m)\|_1^2 = \int_{\Omega^m} f\Phi(\Omega^m)\, dx \to \int_\Omega f\Phi(\Omega^*)\, dx = \|\Phi(\Omega^*)\|_1^2. \tag{73}$$

3.3.2 Counterexample

The situation is similar to the Dirichlet case:

1. The conditions of Theorem 4 are too strong.
2. Too oscillatory boundaries may cause problems.

To illustrate the second point, let us recall the counterexample presented in [12].

Let h be a continuously differentiable periodic function of period T such that

$$h(x) \in [0, h_1] \qquad \forall\, x \in [0, T]; \qquad h(0) = h(T) = 0. \tag{74}$$

Then consider (see Figure 3.6)

$$\Omega^m = \{\{x, y\} : 0 < x < T,\ -1 < y < h(mx)\}, \tag{75}$$

$$\phi - \Delta\phi = f \quad \text{in } \Omega^m; \qquad \left.\frac{\partial\Phi}{\partial n}\right|_{\Gamma^m} = 0. \tag{76}$$

Proposition 4. *The solution Φ^m of (75) and (76) converges weakly in $H^1(\Omega)$ to the solution Φ of*

$$-\Delta\Phi + \Phi = f \quad \text{in } \Omega^- =]0, T[\times]-1, 0[\tag{77}$$

$$-\frac{l}{l}\frac{\partial}{\partial y} l(y)\frac{\partial\Phi}{\partial y} + \Phi = f \quad \text{in } \Omega^+ =]0, T[\times]0, h_1[\tag{78}$$

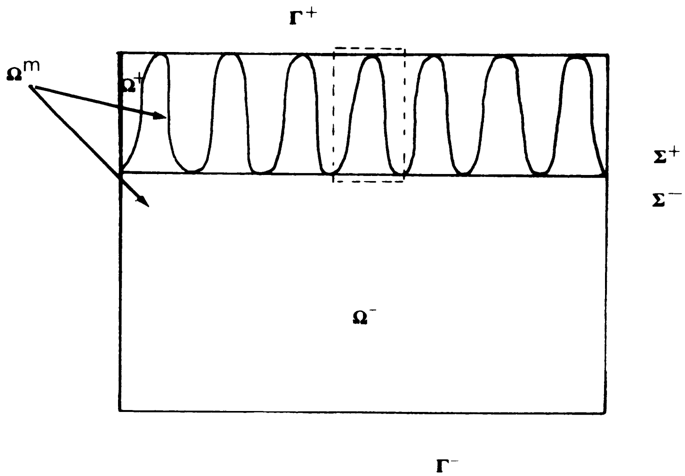


Fig. 3.6 The counterexample for the Neumann problem.

with the boundary conditions ($\sum =]0, T[\times \{0\}$)

$$\Phi|_{\Sigma^+} = \Phi|_{\Sigma^-}; \qquad l(0)\left.\frac{\partial \Phi}{\partial y}\right|_{\Sigma^+} = \left.\frac{\partial \Phi}{\partial y}\right|_{\Sigma^-} \tag{79}$$

$$l(h_1)\left.\frac{\partial \Phi}{\partial y}\right|_{\Gamma^+} = 0; \qquad \left.\frac{\partial \Phi}{\partial n}\right|_{\Gamma^-} = 0, \tag{80}$$

where $l(y) = (\beta(y) - \alpha(y))/T$ *and* α, β *are the reciprocal functions of* h *(Figure 3.7).*

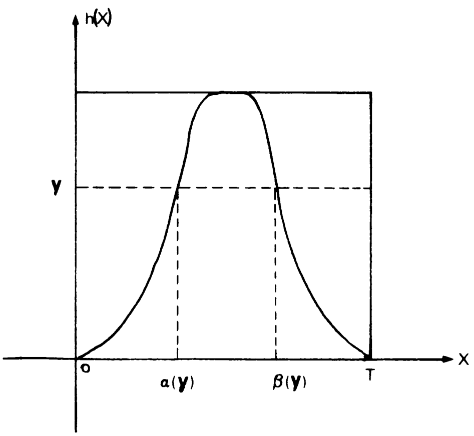


Fig. 3.7 The unit cell of the boundary of Figure 3.6 rescaled horizontally. The inverse functions α, β are shown.

Corollary. *Let Φ_d be the solution of (77) to (80); then for some f the problem*

$$\min_{\Omega \in \mathcal{O}} \left\{ \int_{]0,T[\times]-1,0[} (\Phi - \Phi_d)^2\, dx : \Phi - \Delta\Phi = f \text{ in } \Omega; \left.\frac{\partial \Phi}{\partial n}\right|_\Gamma = 0 \right\}, \tag{81}$$

$$\mathcal{O} = \{\Omega :]0,T[\times]-1,0[\subset \Omega \subset]0,T[\times]-1,h_1[\}, \tag{82}$$

has no solution.

Proof of Proposition 4: Again for more details the reader is referred to [12]. To study the limit of Φ^m, we must construct explicitly its extension $\tilde{\Phi}^m$ into $]0,T[\times]-1,h_1[$. For $\{x,y\} \notin \Omega^m$ define $\tilde{\Phi}^m$ by linear interpolation:

$$\tilde{\Phi}^m(x,y) = -\left[\Phi^m(x_1,y) - \Phi^m\left(x_1 + \frac{T}{m}, y\right)\right] \frac{mx - (\beta(y) + kT)}{T - [\beta(y) - \alpha(y)]} + \Phi^m(x_1, y), \tag{83}$$

where

$$x_1 = -\frac{l(y)x}{1 - l(y)} + \frac{1}{m}\frac{\beta(y) + kT}{1 - l(y)} \tag{84}$$

and where k is an integer such that $mx \in]\beta(y) + kT, \alpha(y) + (k+1)T[$. This defines a continuous extension of Φ^m such that $\|\Phi\|_1 \le C$ implies $\|\tilde{\Phi}\|_1 \le C$; therefore, for some subsequence,

$$\tilde{\Phi}^{m'} \to \Phi \quad \text{in } H^1 \text{ weakly}. \tag{85}$$

Also

$$\chi_{\Omega^{m'}} \to l \quad \text{in } L^\infty \text{ weak star},$$

where $l = 1$ in Ω^- and l is independent of x in Ω^+. As $\tilde{\Phi}^{m'}$ satisfies

$$\int_\Omega \chi_{\Omega^{m'}} \nabla\tilde{\Phi}^{m'} \cdot \nabla w\, dx + \int_\Omega \chi_{\Omega^{m'}} \tilde{\Phi}^{m'} w\, dx = \int_\Omega \chi_{\Omega^{m'}} f w\, dx \qquad \forall w \in H^1(\Omega), \tag{86}$$

we must find the limit of $\chi_{\Omega^{m'}} \nabla\tilde{\Phi}^{m'}$. As shown in [12], the limit is $l\nabla\Phi$; so (86) becomes

$$\int_\Omega l\nabla\Phi \cdot \nabla w\, dx + \int_\Omega l\Phi w\, dx = \int_\Omega l f w\, dx \qquad \forall w \in H^1(\Omega). \tag{87}$$

Conclusion

In the two cases studied—Neumann and Dirichlet conditions—we have found that

- Conditions of compactness such as the cone condition or uniform Lipschitz conditions, imply the existence of a solution.

- Without some restriction on the boundaries certain problems may not have a solution.

However, we would like to know what happens in between these two extremes, i.e., when the boundaries are not “thick” in the limit sense nor Lipschitz continuous.

CHAPTER 4

Optimization Methods

4.1 Orientation

In this chapter we review the classical algorithms of optimization which are used in the numerical solution of shape design problems. For unconstrained minimization problems, the most widely used algorithm is the conjugate gradient method; however, it is best to begin with the method of steepest descent and Newton's method.

In most cases there are restrictions to the allowable shapes; therefore optimization problems have imposed constraints. For this reason we review the reduced and projected gradient algorithms. There are several books on optimization to which the reader is referred for more details, for example, [58], [44], [66], [45].

4.2 Problem Statement

Let Z be a Hilbert space with scalar product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$:

$$\|z\| = \langle z, z \rangle^{\frac{1}{2}} \qquad \forall z \in Z. \tag{1}$$

Let E be real valued a function of z, i.e.,

$$E: Z \to \mathbb{R}, \tag{2}$$

we wish to find $z^* \in Z$ such that

$$E(z^*) = \inf_{z \in Z} E(z) \tag{3}$$

For such a z^* we write

$$z^* = \arg\min_{z \in Z} E(z). \tag{4}$$

Problem (3) is an unconstrained optimization problem in contrast with problem (5),

$$\min_{z \in Z_{ad}} E(z), \tag{5}$$

which is a constrained optimization problem when Z_{ad} is a subset of Z. Naturally, (3) is a particular case of (5) in which Z_{ad} equals Z. Because Z may be of infinite dimension, the problem of proving the existence of solutions for (5) is difficult. We start with the following result.

Theorem 1. *Assume that*

i. E is lower semicontinuous for the weak topology of Z.
ii. $E(z) \to +\infty$ when $\|z\| \to +\infty$.
iii. Z_{ad} is a closed convex subset of Z.

Then (5) has at least one solution z^*. Furthermore, if E is strictly convex, the solution is unique.

PROOF. Let $\{z^i\}_{i \geq 0}$ be a minimizing sequence for E, i.e.,

$$\lim_{i \to \infty} E(z^i) = \inf_{z \in Z_{\mathrm{ad}}} E(z). \tag{6}$$

By hypothesis ii the set $\{z : E(z) \leq E(z^0)\}$ is bounded, and $\{z^i\}_{i \geq 0}$ belongs to that set; therefore there exists C_1 with

$$\|z^i\| \leq C_1 \qquad \forall i \geq 0. \tag{7}$$

Consequently, there exists $z^* \in Z$ such that

$$z^i \to z^* \text{ weakly in } Z. \tag{8}$$

Now hypothesis i implies that

$$E(z^*) \leq \lim_{i \to \infty} E(z^i); \tag{9}$$

so if $z^* \in Z_{\mathrm{ad}}$, then z^* must be a solution of (5).
This is so from assumption iii.

Assume now that E is strictly convex, and let z^* and $z^{*\prime}$ be two solutions of (5). By the strict convexity of E, we have

$$E(\tfrac{1}{2}(z^* + z^{*\prime})) < \tfrac{1}{2}E(z^*) + \tfrac{1}{2}E(z^{*\prime}) = \min_{z \in Z_{\mathrm{ad}}} E(z), \tag{10}$$

which is a contradiction. □

Comments. The hypothesis of Theorem 1 are usually too restrictive; so we may wonder what happens in practice if we attempt to compute a solution for which an optimization algorithm does not exist.

As an example, consider the design problem

$$\min_{\Omega \subset]0,1[^2} \frac{1}{l(\Gamma_1)} \tag{11}$$

where $\Omega = \{(x_1, x_2) : x_2 \leq y(x_1)\} \cap]0,1[^2$ (see Figure 4.1), and where Γ_1 is the upper boundary of Ω and $l(\Gamma_1)$ is the length of that boundary.

The minimum does not exist, but the criteria tends to zero when Γ_1 oscillates more and more inside the area $]0,1[^2$.

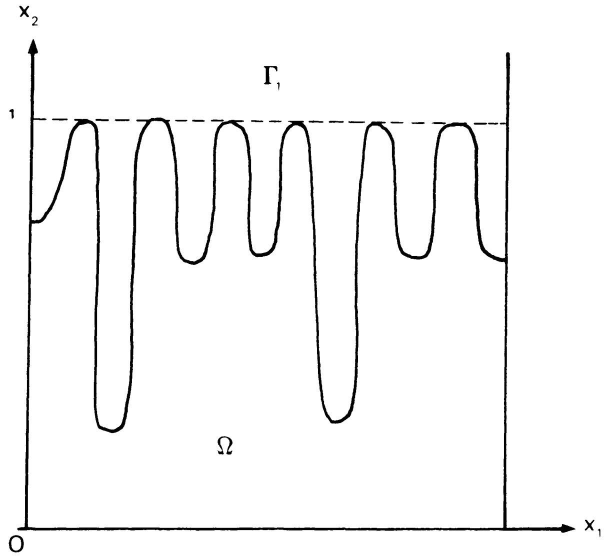


Fig. 4.1 An optimization problem without solution: maximization of the length of the curve.

4.3 Gradients

Before stating the gradient algorithms, it is useful to study the difference between gradients and derivatives.

4.3.1 Definition

If E is differentiable in Z, the *gradient* of E, denoted grad $E(z)$, is the unique element of Z which satisfies

$$\langle \text{grad } E(z), t\rangle = \lim_{\lambda \to 0} \frac{1}{\lambda}[E(z + \lambda t) - E(z)] \qquad \forall t \in Z. \tag{12}$$

The gradient is not to be confused with the *derivative* $E'(z)$, which is a linear map from Z into $\mathbb{R}$ (and therefore not an element of Z). Naturally, grad $E(z)$ and $E'(z)$ are related by the formula

$$\langle \text{grad } E(z), t\rangle = E'(z)t \qquad \forall t \in Z.$$

4.3.2 Notation

A "little o" function is any function from $\mathbb{R}$ into $\mathbb{R}$ such that

$$\lim_{\lambda \to 0^+} \frac{1}{\lambda} o(\lambda) = 0. \tag{13}$$

Therefore, (12) may be rewritten in a more convenient form:

$$E(z + \delta z) = E(z) + \langle \text{grad } E(z), \delta z\rangle + o(\|\delta z\|) \qquad \forall \delta z \in Z. \tag{14}$$

This identity also defines grad $E(z)$ in a unique fashion.

4.3.3 Examples

1. $E(z) = f(z)$; $z \in \mathbb{R}^n \Rightarrow \operatorname{grad} f(z) = \nabla f(z)$.
2. $E(\phi) = \int_\Omega \phi(x)^{\frac{3}{2}}\,dx$; $Z = L^2(\Omega) \Rightarrow \operatorname{grad} E(\phi) = \frac{3}{2}\phi^{\frac{1}{2}}$.

   Indeed we have

$$E(\phi + \delta\phi) = E(\phi) + \tfrac{3}{2}\int_\Omega \phi^{\frac{1}{2}}\delta\phi\,dx + o(\|\delta\phi\|). \tag{15}$$

3. $E(\phi) = \int_\Omega \phi(x)^{\frac{3}{2}}\,dx$; $Z = H^1(\Omega)$.

In that case, the scalar product of Z is different:

$$\int_\Omega (\operatorname{grad} E(\phi))\,\delta\phi\,dx + \int_\Omega \nabla(\operatorname{grad} E(\phi)) \cdot \nabla\delta\phi\,dx = \langle \operatorname{grad} E(\phi), \delta\phi \rangle. \tag{16}$$

Therefore, from Eq. (15) in Chapter 2, grad $E(\phi)$ is the unique element of $H^1(\Omega)$ with

$$\int_\Omega \operatorname{grad} E(\phi)\,\delta\phi\,dx + \int_\Omega \nabla(\operatorname{grad} E(\phi)) \cdot \nabla\delta\phi\,dx = \tfrac{3}{2}\int_\Omega \phi^{\frac{1}{2}}\delta\phi\,dx \qquad \forall\,\delta\phi \in H^1(\Omega); \tag{17}$$

i.e., we must solve the PDE

$$\Psi - \Delta\Psi = \tfrac{3}{2}\phi^{\frac{1}{2}} \quad \text{in } \Omega; \qquad \left.\frac{\partial\Psi}{\partial n}\right|_\Gamma = 0 \tag{18}$$

to find $\Psi = \operatorname{grad} E(\phi)$.

EXERCISE

Let Z^1 be $\mathbb{R}^n$ with the Euclidean scalar product and Z^2 be $\mathbb{R}^n$ with the scalar product

$$\langle z, z' \rangle_2 = z^t \mathbf{A} z'$$

where $\mathbf{A}$ is a positive definite matrix. Show that the gradient $\operatorname{grad}_2 E(z)$ with respect to Z^2 is related to the gradient $\nabla E(z)$ with respect to Z^1 by

$$\operatorname{grad}_2 E(z) = \mathbf{A}^{-1}\nabla E(z) \tag{19}$$

4.4 Method of Steepest Descent

Henceforth, we assume that the following problem has a unique solution:

$$\min_{z \in Z} E(z). \tag{20}$$

The gradient methods of solution are based on the following observation: In (14) if we replace δz by

$$\delta z = -\rho \operatorname{grad} E(z), \tag{21}$$

where ρ is a small positive number, then (14) becomes

$$E(z + \delta z) = E(z) - \rho \|\operatorname{grad} E(z)\|^2 + o(\rho \|\operatorname{grad} E(z)\|). \tag{22}$$

Therefore, (21) provides us with a way to construct from z a new point $z + \delta z$ such that

$$E(z + \delta z) < E(z). \tag{23}$$

Indeed, the second term in the right-hand member of (22) is strictly negative, and the third term can be made very small.

4.4.1 The method of steepest descent with fixed step size

Algorithm 1

[0. Choose z^0, ρ, M, ε.
For $m = 0, \ldots, M$ do

$$\begin{bmatrix} 1.\ z^{m+1} = z^m - \rho \operatorname{grad} E(z^m). \\ 2.\ \text{If } \|\operatorname{grad} E(z^m)\| \le \varepsilon, \quad \text{stop.} \end{bmatrix} \tag{24}$$

Theorem 2. *Assume Z of finite dimension. Assume that E is twice differentiable and such that*

$$\lambda |y|^2 \le E''(z)yy \le \Lambda |y|^2 \qquad \forall z \in Z, \forall y \in Z, \tag{25}$$

for some positive λ, Λ. *Then, if* $\rho = 2/(\lambda + \Lambda)$, *the sequence* $\{z^m\}$ *generated by Algorithm 1 converges to the solution* z^* *(when* $M = +\infty$, $\varepsilon = 0$) *and*

$$\|z^m - z^*\| \le \|z^0 - z^*\| \left(\frac{\Lambda - \lambda}{\Lambda + \lambda}\right)^m. \tag{26}$$

Proof. Let z^* be a solution so that grad $E(z^*)$ is zero.

$$\|z^{m+1} - z^*\| = \|z^m - \rho \operatorname{grad} E(z^m) - z^*\| \tag{27}$$

$$= \left\| z^m - z^* - \rho \int_0^1 E''(z^* + t(z^m - z^*))(z^m - z^*)\, dt \right\| \tag{28}$$

$$\le \|z^m - z^*\| \left\| I - \rho \int_0^1 E''(z^* + t(z^m - z^*))\, dt \right\| \tag{29}$$

$$\le \|z^m - z^*\| \max\{1 - \rho\lambda, \rho\Lambda - 1\}$$

$$= \|z^m - z^*\| \frac{\Lambda - \lambda}{\Lambda + \lambda}. \tag{30}$$

Comments.

- Inequality (26) shows that $\{z^m\}$ converges similar to a geometric progression; in such a case, it is said that the *rate* of convergence is *linear.*
- In practice Λ and λ are the largest and smallest eigenvalues of E; so the method is quite a fast one when Λ is not too far from λ.
- Unfortunately Λ and λ are usually not known, and it is difficult to choose a good value for ρ in Algorithm 1.

4.4.2 Method of steepest descent with optimal step size

Algorithm 2. Method of Steepest Descent

[0. Choose z^0, M, ε

For $m = 0, \ldots, M$, do

1. Compute $h^m = -\text{grad } E(z^m)$. (31)
2. Compute $\rho^m = \arg\min_{\rho > 0} E(z^m + \rho h^m)$. (32)
3. Set $z^{m+1} = z^m + \rho^m h^m$. (33)
4. If $\|\text{grad } E(z^m)\| < \varepsilon$, stop.

Theorem 3. *Assume that E is continuously differentiable and bounded from below, then all accumulation points $\hat{z}$ of $\{z^m\}$ satisfy*

$$\text{grad } E(\hat{z}) = 0. \tag{34}$$

Proof [58] Let $\{z^{m_i}\}_{i \geq 0}$ be a subsequence which converges to $\hat{z}$. Because $\{E(z^m)\}$ is decreasing we have

$$E(z^{m_{i+1}}) - E(z^{m_i}) \leq E(z^{m_i+1}) - E(z^{m_i}). \tag{35}$$

However, since z^{m_i+1} is computed from (32), we also have

$$\begin{aligned} E(z^{m_i+1}) - E(z^{m_i}) &\leq E(z^{m_i} + \rho h^{m_i}) - E(z^{m_i}) \\ &\leq \rho \langle \text{grad } E(z^{m_i} + \theta h^{m_i}), h^{m_i} \rangle, \qquad \forall \rho > 0 \end{aligned} \tag{36}$$

for some $\theta \in]0, \rho[$.

Now we use the continuity of grad E and the definition of h^{m_i}:

$$z^{m_i} \to \hat{z}, \qquad h^{m_i} \to -\text{grad } E(\hat{z});$$

Thus,

$$\forall \alpha \in]0, \tfrac{1}{2}[, \exists\, i(\alpha), \hat{\rho} > 0, \text{ such that}$$

$$\rho \langle \text{grad}(z^{m_i} + \theta h^{m_i}), h^{m_i} \rangle \leq -\alpha \|\text{grad } E(\hat{z})\|^2 \qquad \forall \rho \langle \hat{\rho}, i \rangle\, i(\alpha). \tag{37}$$

Hence,

$$E(z^{m_{i+1}}) - E(z^{m_i}) \leq -\alpha \|\text{grad } E(\hat{z})\|^2 \qquad \forall i > i(\alpha), \tag{38}$$

which is a contradiction to the boundedness from below of E if (34) does not hold. □

EXERCISE

Show that when Eq. (25) of Chapter 2 holds, $\rho^m \in]1/\Lambda, 1/\lambda[$ and

$$|z^m - \hat{z}| \leq C\left|1 - \frac{\lambda}{\Lambda}\right|^m. \tag{39}$$

4.4.3 One-dimensional minimization

In general, it is not possible to compute exactly the ρ^m solution of (32); so step 2 in Algorithm 2 must be approximated. There are several iterative methods to compute the minimum of a one-dimensional function $E(\rho)$; most of them are governed by trial and error. We learn that for optimal shape design problems, it is as expensive on a computer to compute $E(z^m)$ as it is to compute the grad $E(z^m)$. Thus, step 2 above should be carried out with the least number of evaluations of E possible.

We present another algorithm that gives reasonable results for the problems considered; this algorithm is a combination of dichotomy and parabolic fit. Let

$$E(\rho) = E(z^m + \rho h^m) - E(z^m). \tag{40}$$

Notice that $E(0) = 0$ and

$$\frac{dE}{d\rho}(0) = \langle \text{grad } E(z^m), h^m \rangle = -\|\text{grad } E(z^m)\|^2. \tag{41}$$

Therefore, when E is bounded from below and continuous, there is at least one local minimum of $E(\rho)$.

Algorithm 3. One-Dimensional Minimization
Assume $\partial E(0)/\partial\rho < 0$, $E(+\infty) = +\infty$, $E(\rho) \neq -\infty\ \forall \rho$.:

0. Choose ρ and set $d = \rho > 0$.
1. Set $\rho_2 = \rho + d$, $\rho_{\frac{1}{2}} = \rho - d$.
2. If $E(\rho) > E(\rho_2)$, then set $\rho = \rho + d$ and go to step 1.
   If $E(\rho_{\frac{1}{2}}) < E(\rho)$ then set $\rho = \rho - d/2$, $d = d/2$ and go to step 1; else go to step 3.
3. Compute the minimum of the parabola running through the three points $\{\rho_{\frac{1}{2}}, E(\rho_{\frac{1}{2}})\}$, $\{\rho, E(\rho)\}$, and $\{\rho_2, E(\rho_2)\}$, i.e., set

$$\rho = \rho + \tfrac{1}{2}(\rho - \rho_{\frac{1}{2}})\frac{E(\rho_{\frac{1}{2}}) - E(\rho_2)}{E(\rho_2) + E(\rho_{\frac{1}{2}}) - 2E(\rho)}. \tag{42}$$

4. If more precision is required go back to step 1, $d/2$ substituting for d. (E convex)

Comments. *Step 2 finds a so-called "convex situation" where the exact minimum presumably lies within* $]\rho_{\frac{1}{2}}, \rho_2[$. *The parabolic fit of step 3 would not be precise if the minimum of the parabola did not reside in* $]\rho_{\frac{1}{2}}, \rho_2[$.

This algorithm is contained in all other algorithms, and thus the Fortran program for it is included at the end of the chapter.

4.5 Newton Method

Another algorithm is to replace (20) by the following:

$$\text{Find } z \in Z \quad \text{such that} \quad \operatorname{grad} E(z) = 0. \tag{43}$$

More generally, let F be a mapping from Z into Z that is continuously differentiable and solve

$$F(z) = 0. \tag{44}$$

Newton's algorithm is

$$z^{m+1} = z^m - F'(z^m)^{-1} F(z^m). \tag{45}$$

Formula (45) is based on the following expansion:

$$F(z^{m+1}) = F(z^m) + F'(z^m)(z^{m+1} - z^m) + o(\|z^{m+1} - z^m\|). \tag{46}$$

Thus, setting $F(z^{m+1}) = 0$ and ignoring the o function yields (45). Numerically, we never compute $F'^{-1}(z^m)$ but solve for h in the equation

$$F'(z^m)h = -F(z^m). \tag{47}$$

Theorem 4. *Let us assume Z to be of finite dimension, that F is twice differentiable, and F' has only positive eigenvalues, then Newton's method converges, and the rate of convergence is superlinear with* $\forall\, k \in]0, 1[, \exists\, m(k)$ *such that*

$$\|z^m - z^*\| \leq Ck^m \qquad \forall\, m > m(k). \tag{48}$$

PROOF [58] Let

$$a(z) = z - F'^{-1}(z) F(z).$$

Step 1. A Taylor expansion gives

$$F(a(z)) = F(z) - F'(z)F'^{-1}(z)F(z) + \int_0^1 (1-t)F''(z - tF'(z)^{-1}F(z))F'(z)^{-1}F(z)F'(z)^{-1}F(z)\,dt. \tag{49}$$

Hence,

$$F(a(z)) \leq \int_0^1 (1-t)|F''(y(t))|\,dt\, \|F'^{-1}(z)F(z)\|^2 \leq \frac{B}{\mu^2}\|F(z)\|^2, \tag{50}$$

where B is an upper bound of F'' and μ is the smallest eigenvalue of $F'(z)$.

Step 2. Since $F(z^*) = 0$, when z^* is a solution, a second Taylor expansion yields

$$\|F(z)\| = \|F(z^*) + F'(\xi)(z - z^*)\| \leq M\|z - z^*\|. \tag{51}$$

Step 3. Again taking into consideration the fact that $F(z^*) = 0$, the mean value theorem yields

$$F(a(z))(a(z) - z^*) = F'(\xi)(a(z) - z^*)(a(z) - z^*) \tag{52}$$

for some ξ. Hence,

$$\mu\|a(z) - z^*\| \leq \|F(a(z))\|. \tag{53}$$

Finally, (50), (51), and (53) gives

$$\|z^{m+1} - z^*\| \leq \frac{BM^2}{\mu^3}\|z^m - z^*\|^2, \tag{54}$$

which, in turn, implies (48). □

We can take advantage of the fact that (43) comes from (20); this gives the following algorithm.

Algorithm 4. Newton's Method

[0. Choose z^0, M, ε

For $m = 0, \ldots, M$ do

1. Compute h^m by solving

$$E''(z^m)h \cdot y = -\langle y, \text{grad } E(z^m)\rangle \qquad \forall y \in Z. \tag{55}$$

2. Compute ρ^m:

$$\rho^m = \arg\min_{\rho > 0} E(z^m + \rho h^m). \tag{56}$$

3. Set

$$z^{m+1} = z^m + \rho^m h^m. \tag{57}$$

4. If $\|\text{grad } E(z^m)\| < \varepsilon$, stop.

Naturally, in practice, we will have to use a method similar to Algorithm 3 to compute ρ^m.

Proposition 1. *If Z is a finite-dimensional space and E is twice continuously differentiable, then $\rho^m \to 1$ when $m \to \infty$.*

PROOF. From (56),

$$E'(z^{m+1})h^m = 0. \tag{58}$$

Therefore, for some ξ, we have

$$E'(z^m)h^m + \rho^m E''(\xi)h^m h^m = 0, \tag{59}$$

that implies

$$\rho^m = -\frac{E'(z^m)h^m}{E''(\xi)h^m h^m} = \frac{E''(z^m)^{-1}E'(z^m)E'(z^m)}{[E''(\xi)(E''^{-1}(z^m)E'(z^m))](E''^{-1}(z^m)E'(z^m))}. \tag{60}$$

If $z^m \to z^*$, then $\xi \to z^*$; and from (56)–(60) $\rho^m \to 1$. □

Corollary 1. The rate of convergence of Newton's method is superlinear; i.e., satisfies (48).

Remark. Newton's method is quite fast, but it has two drawbacks:

1. If E'' is singular, the algorithm might not converge.
2. The computation of $E''^{-1}E'$ is very costly on a computer when the dimension of Z is large (say more than a few hundred).

Thus, we usually prefer using the conjugate gradient method, which we now present.

4.6 Conjugate Gradient Method

Suppose for the moment that E is quadratic:

$$E(z) = -\langle a, z\rangle + \tfrac{1}{2}\langle \mathbf{B}z, z\rangle \tag{61}$$

with $\mathbf{B}$ a positive definite matrix. Then, the minimum satisfies

$$\mathbf{B}z^* = a. \tag{62}$$

So the problem is reduced to that of an $n \times n$ linear system.

Obviously, when $\mathbf{B}$ is diagonal, the solution of (62) is trivial. The Gramm–Schmidt orthogonalization procedure is used to find a basis in which $\mathbf{B}$ is the diagonal.

4.6.1 Gramm–Schmidt procedure

PROBLEM. Given $\mathbf{B} \in \mathbb{R}^{n\times n}$, find $\{g^i\}_0^{n-1}$, $\{h^i\}_0^{n-1}$ such that

$$\langle g^i, g^j\rangle = 0 \qquad \forall\, i,j = 0,\dots,n-1, \quad i \neq j, \tag{63}$$

$$\langle h^i, \mathbf{B}h^j\rangle = 0 \qquad \forall\, i,j = 0,\dots,n-1, \quad i \neq j. \tag{64}$$

PROCEDURE.

[0. Choose g^0; set $h^0 = g^0$.

For $m = 0,\dots,n-1$ do

1. $$\rho^m = \frac{\|g^m\|^2}{\langle g^m, \mathbf{B}h^m\rangle}. \tag{65}$$
2. $$g^{m+1} = g^m - \rho^m \mathbf{B}h^m. \tag{66}$$
3. $$\gamma^m = -\frac{\langle \mathbf{B}h^m, g^{m+1}\rangle}{\langle \mathbf{B}h^m, g^m\rangle}. \tag{67}$$
4. $$h^{m+1} = g^{m+1} + \gamma^m h^m. \tag{68}$$
5. If $g^{m+1} = 0$, stop.

This procedure is based on the fact that when $\mathbf{B}$ is positive definite, the vectors $\{h^0, \mathbf{B}h^0,\dots,\mathbf{B}^{n-1}h^0\}$ generate Z.

Therefore, assume that $\{g^i\}_0^m$ satisfies (63) for $i,j \leq m$ and that they are in the space generated by $\{h^0,\dots,\mathbf{B}^m h^0\}$. Define g^{m+1} by (65) and (66); then

$$\begin{aligned}\langle g^{m+1}, g^l\rangle &= \langle g^m, g^l\rangle - \rho^m\langle \mathbf{B}h^m, g^l\rangle \\ &= \langle g^m, g^l\rangle - \rho^m\langle \mathbf{B}h^m, h^l - \gamma^{l-1}g^{l-1}\rangle \\ &= \delta_{ml} - \rho^m\delta_{ml} - \gamma^l\delta_{ml-1} \\ &= 0 \qquad \forall\, l < m.\end{aligned} \tag{69}$$

Similarly,

$$\begin{aligned}\langle h^{m+1}, \mathbf{B}h^l\rangle = \gamma^m\langle h^m, \mathbf{B}h^l\rangle + \langle g^{m+1}, \mathbf{B}h^l\rangle &= \gamma^m\lambda\delta_{ml} + \langle g^{m+1}, g^{l+1} - g^l\rangle/\rho^l \\ &= 0 \qquad \forall\, l < m.\end{aligned} \tag{70}$$

So we have proved that the procedure works.

Remark. From (64), we also have

$$\gamma^m = \frac{\|g^{m+1}\|^2}{\|g^m\|^2} = \frac{\langle g^{m+1} - g^m, g^{m+1}\rangle}{\|g^m\|^2}. \tag{71}$$

4.6.2 Conjugate gradient algorithm

Algorithm 5.

[0. Choose z^0, M, ε; set $h^{-1} = 0, g^{-1} = -\text{grad } E(z^0)$.

For $m = 0, \ldots, M$, do

1. $g^m = -\text{grad } E(z^m); \gamma^m = \langle g^m - g^{m-1}, g^m \rangle / \| g^{m-1} \|^2;$ (72)

   $h^m = g^m + \gamma^m h^{m-1}.$ (73)

2. Compute $\rho = \arg \min_{\rho > 0} E(z^m + \rho h^m).$ (74)

3. Set $z^{m+1} = z^m + \rho h^m.$ (75)

4. If $\| g^m \| < \varepsilon$, stop.

Proposition 2. *If E is quadratic and Z of dimension n, Algorithm 5 converges in at most n iterations.*

PROOF. When E is quadratic, (74) gives

$$\rho^m = -\frac{\langle \text{grad } E(z^m), h^m \rangle}{\langle h^m, E'' h^m \rangle} = \frac{\langle g^m, h^m \rangle}{\langle h^m E'' h^m \rangle} = \frac{\| g^m \|^2}{\langle g^m, E'' h^m \rangle}. \tag{76}$$

So (72) and (74) are identical to the Gramm–Schmidt procedure. Therefore, at the nth iteration at the latest, we have

$$\text{grad } E(z^n) = g^n = 0, \tag{77}$$

which implies that z^n is a solution. □

Theorem 5. *Assume that Z is of finite dimension and that E is strictly convex and twice continuously differentiable. Then Algorithm 5 converges, and if E is $C^3(Z)$, its rate of convergence is superlinear.*

PROOF. See [58]. The convergence is easy to prove once it is shown that there exists a λ such that

$$-\langle \text{grad } E(z^m), h^m \rangle \geq \lambda \| \text{grad } E(z^m) \| \, \| h^m \| \qquad \forall m \geq m_0. \tag{78}$$

To prove (78), one first shows that

$$|\gamma^m| \leq \frac{M}{\mu} \frac{\| g^m \|}{\| h^{m-1} \|} \tag{79}$$

and hence that

$$\langle g^m, h^m \rangle \geq \| h^{m-1} \| \frac{\| g^{m-1} \|}{1 + M/\mu}. \tag{80}$$

4.7 Optimization with Equality Constraints

From now on let us assume $Z = \mathbb{R}^n$, and we wish to solve

$$\min\{E(z): f^j(z) = 0, \quad j = 1,\ldots,N\}. \tag{81}$$

Problems with constraints are usually more difficult from the computational point of view, except if all the f^j are linear.

We assume that $N < n$, and that the system

$$f^j(z) = 0, \qquad j = 1,\ldots,N, \tag{82}$$

allows us to express N variables $z'' = \{z_{n-N+1},\ldots,z_n\}$ in terms of the first $n - N$ variables:

$$z'' = z''(z'). \tag{83}$$

So, in particular, by differentiation of (82), we obtain

$$\nabla_{z'} f^j(z) + \nabla_{z'} z'' \, \nabla_{z''} f^j(z) = 0, \tag{84}$$

and $\nabla_{z''}\mathbf{F}(z)$ is a nonsingular matrix with $\mathbf{F} = \{f^1, f^2,\ldots,f^N\}$. Thus problem (81) is equivalent to the unconstrained problem

$$\min_{z' \in \mathbb{R}^p} E_1(z') = E(z', z''(z')), \qquad p = n - N. \tag{85}$$

The gradient of E_1 is

$$\nabla E_1 = \nabla_{z'} E + \nabla_{z'} z'' \, \nabla_{z''} E = \nabla_{z'} E - (\nabla_{z''}\mathbf{F})^{-1} \nabla_{z'}\mathbf{F} \, \nabla_{z''} E. \tag{86}$$

This formula is sufficient to use for applying one of the gradient methods, but since it is not symmetric with respect to all the components of z, let us derive an equivalent formulation.

Let D be the space spanned by $\nabla f^j, j = 1,\ldots,N$. Formula (84) multiplied by dz' indicates that the vector $\{dz', dz'' = \nabla z'' \, dz'\}$ is orthogonal to D. Thus, if we change the basis of Z so that D is now the set of vectors whose z' components are equal to zero, then $dz'' = 0$; i.e., the orthogonality is expressed as

$$(\nabla_{z''}\mathbf{F})^{-1} \nabla_{z'}\mathbf{F} = 0. \tag{87}$$

Hence, (86) now tells us that the gradient of E_1 is just $\nabla_{z'} E$, i.e., it is the projection of ∇E on $D^\perp$, the orthogonal complement of D. This is best illustrated in Figure 4.2, where $N = 1$, $n = 2$, and the new basis is (X_1, X_2). Since the projection of ∇E on D is

$$\nabla\mathbf{F}(\nabla\mathbf{F}^t\nabla\mathbf{F})^{-1}\nabla\mathbf{F}^t\nabla E, \tag{88}$$

we have

$$\nabla E_1 = \nabla E - \nabla\mathbf{F}(\nabla\mathbf{F}^t\nabla\mathbf{F})^{-1}\nabla\mathbf{F}^t\nabla E. \tag{89}$$

Thus, the following algorithm solves (81).

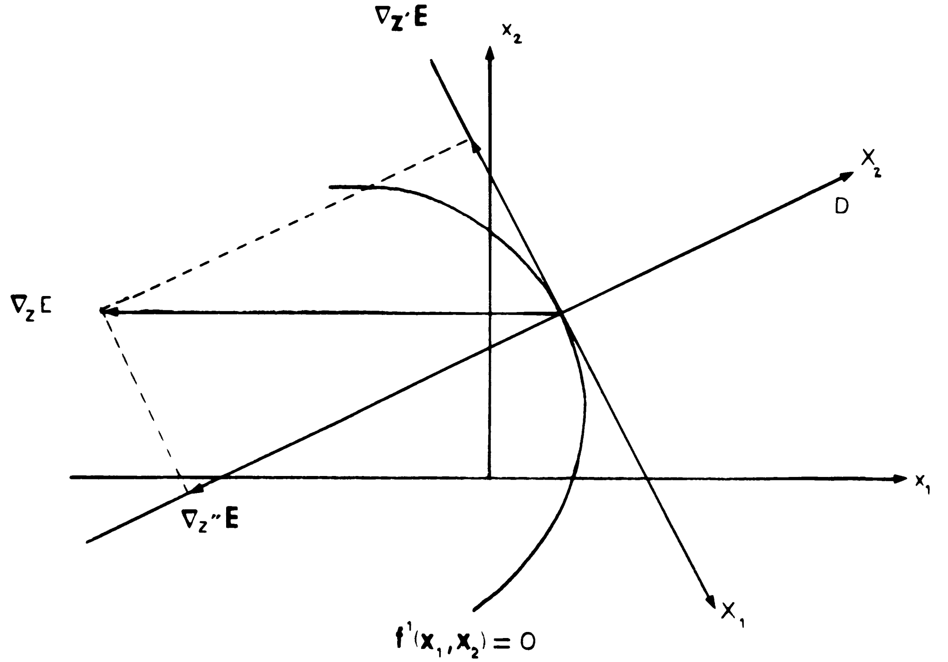


Fig. 4.2 The reduced gradient $\nabla_{z'}E$ is minus the direction of descent.

Algorithm 6. Reduced Gradient

[0. Choose z^0, M, ε.

For $m = 0,\ldots,M$, do

1. Compute

$$h^m = -\nabla E(z^m) + \nabla \mathbf{F}(z^m)(\nabla \mathbf{F}^t(z^m)\nabla \mathbf{F}(z^m))^{-1}\nabla \mathbf{F}^t(z^m)\nabla E(z^m). \tag{90}$$

2. Compute

$$\rho^m = \arg\min_{\rho>0} \{E(z^m + \rho h^m): f^j(z^m + \rho h^m) = 0, \qquad j = 1,\ldots,m\}. \tag{91}$$

3. Set $z^{m+1} = z^m + \rho^m h^m$, projected on the admissible set.
4. If $\|h^m\| < \varepsilon$, stop.

Theorem 6. *Let us assume that E and f^j are continuously differentiable, and that $\nabla \mathbf{F}^t \nabla \mathbf{F}$ is invertible at all points. Let us also assume that E tends to $+\infty$ when $\|z\| \to +\infty$. Then Algorithm 6 generates sequences whose accumulation points z^* all satisfy*

$$\nabla E(z^*) + \sum_{j=1}^{n} \lambda_j \nabla f^j(z^*) = 0 \qquad \textit{for some } \{\lambda_j\}_1^M, \tag{92}$$

$$f^j(z^*) = 0, \qquad j = 1,\ldots,M. \tag{93}$$

Proof. It is clear from the previous construction (89) and Theorem 2 that z^* satisfies

$$\nabla E(z^*) - \nabla \mathbf{F}(z^*)(\nabla \mathbf{F}^t(z^*) \nabla \mathbf{F}(z^*))^{-1} \nabla \mathbf{F}^t(z^*) \nabla E(z^*) = 0. \tag{94}$$

This formula is rewritten as in (92); it is not necessary that we know the values of λ because (93) yields M equations that determine λ, once z^* is known. □

Exercise

Prove (88) by considering the problem

$$\min_{z \in D} \|z - \tilde{z}\|^2, \tag{95}$$

where z is given and

$$D = \{\tilde{z} : \exists \mu_1, \ldots, \mu_M, \text{ such that } \tilde{z} = \sum_1^M \mu_1 \nabla f^j(z)\}. \tag{96}$$

4.8 Optimization with Inequality Constraints

Consider, as before, the finite-dimensional case $Z = \mathbb{R}^n$ and the problem

$$\min_{z \in \mathbb{R}^n} \{E(z) : f^j(z) \le 0, j = 1, \ldots, M\}, \tag{97}$$

where E and f^j are continuously differentiable real-valued functions. We assume that the constraint set has a nonempty interior:

$$C = \{z : f^j(z) \le 0, j = 1, \ldots, M\}; \qquad \mathring{C} \ne \varnothing. \tag{98}$$

As usual, we suppose that E tends to infinity at infinity.

By repeating the argument in Theorem 1, we can show that under these assumptions (97) has at least one solution.

4.8.1 Optimality conditions

All the algorithms we have examined cannot be used to compute the absolute minimum of the problems considered but only to suggest candidates for local minimums. For unconstrained optimization, all we can assert is that

$$\nabla E(z^*) = 0. \tag{99}$$

For equality constraints, we have

$$\nabla E(z^*) + \sum \lambda_j \nabla f^j(z^*) = 0. \tag{100}$$

These are called the first-order *optimality conditions* of any problem. These conditions are important because in many cases they give valuable information about the minimum.

For problem (97) the optimality conditions, also known as the Kuhn–Tucker conditions, are as given below.

Proposition 3. *Under the above assumptions, the solution z^* of (97) must satisfy*

$$-\nabla E(z^*) + \sum_1^M \lambda_j \nabla f^j(z^*) = 0 \tag{101}$$

for some $\{\lambda_j\}$, $\lambda_j \geq 0$ such that

$$\lambda_j f^j(z^*) = 0, \forall j. \tag{102}$$

PROOF. The general proof is complicated by all possible degenerate cases. So the reader is referred to [13], for example, and we give only the main argument.

1. If $z^* \in \mathring{C}$, then take $\lambda_j = 0$ for all j, and (101) and (102) are satisfied.
2. Let J be the set of j such that $f_j(z^*) = 0$, then there exists some open set V of z^* such that

$$\min_{z \in V} \{E(z) : f^j(z) = 0, j \in J\} \tag{103}$$

has z^* as a solution. So if $\{\nabla f^j\}_{j \in J}$ are linearly independent, then from the discussion on the equality constraints there exists $\{\lambda_j\}$ for which (101) and (102) are satisfied, and it we need only prove that these λ_j are positive.

Assume $\lambda_k < 0$, and let us consider

$$C_k = \{z : f^j(z) = 0, j \in J - \{k\}\}. \tag{104}$$

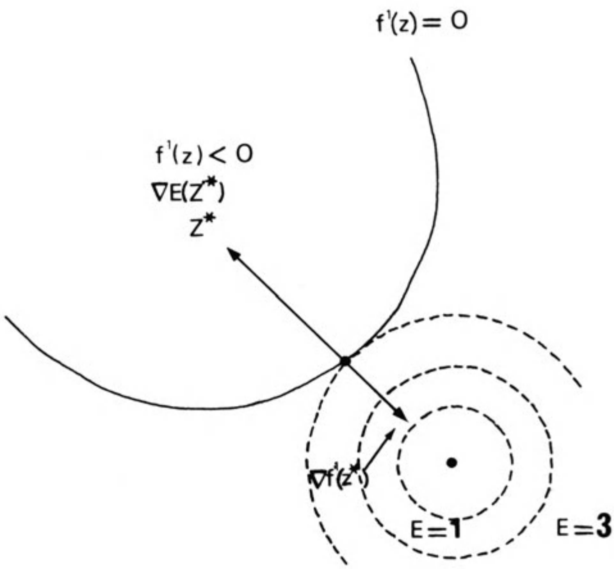


Fig. 4.3 At the minimum, $\nabla E(z^*)$ and $\nabla f^1(z^*)$ are parallel. The dotted lines are the level curves of E.

If $\nabla E(z^*) \neq 0$ and $z^* + \delta z \in C_k$ while $\delta z \cdot \nabla f^k(z^*) < 0$, then

$$E(z^* + \delta z) = \nabla E(z^*) \cdot \delta z + o(\|\delta z\|) = \lambda_k \, \delta z \cdot \nabla f^k(z^*) + o(\|\delta z\|) < 0,$$

where the last equality comes from (101). Thus, we are able to decrease the function while remaining within the allowable set C (see Figure 4.3). □

4.8.2 The projected gradient method

NOTATIONS. Let us denote by $J(z)$ the set of active constraints at z,

$$J(z) = \{j : f^j(z) = 0\}, \tag{105}$$

and $\mathbf{P}_J(z)$ the projection operator from $\mathbb{R}^n$ into the space generated by $\{\nabla f^j(z)\}_{j \in J}$. As before, the matrix associated with $\mathbf{P}_J(z)$ is

$$\mathbf{P}_J = \nabla \mathbf{F}_J(\nabla \mathbf{F}_J^t \nabla \mathbf{F}_J)^{-1} \nabla \mathbf{F}_J^t, \tag{106}$$

where $\nabla \mathbf{F}_J$ denotes the matrix whose columns are $\nabla f^j(z), j \in J$.

Algorithm 7. (Projected gradient, see Fig. 4.4)

[0. Choose $z^0 \in C$, M, ε. Compute $J = J(z^0)$

For $m = 0, \ldots, M$ do

1. Compute

$$h^m = (-\mathbf{I} + \mathbf{P}_J) \nabla E(z^m), \tag{107}$$

where $\mathbf{P}_J$ is given by (106).

2. While $h^m = 0$, do

set $J = J(z^m)$.

Compute $y^m = (\nabla \mathbf{F}_J^t \nabla \mathbf{F}_J)^{-1} \nabla \mathbf{F}_J \nabla E(z^m)$. (108)

Find $l \in J(z^m)$ such that

$$\max_{l \in J(z^m)} \{\|(-\mathbf{I} + \mathbf{P}_{J-l}) \nabla E(z^k)\|^2 : y_l^m > 0\}. \tag{109}$$

If there are no such l (i.e., $y_l^m < 0 \; \forall \, l$), stop;

else, change J into $J - \{l\}$. Set

$$h^m = (-\mathbf{I} + \mathbf{P}_J) \nabla E(z^m). \tag{110}$$

3. Compute

$$\rho^m = \arg\min_{\rho > 0} \{E(z^m + \rho h^m) : f^j(z^m + \rho h^m) \leq 0, j = 1, \ldots, M\}. \tag{111}$$

4. Set

$$z^{m+1} = z^m + \rho^m h^m.$$

5. If $\|h^m\| \leq \varepsilon$, stop.

Comments: This algorithm works in the following manner: It computes the direction of descent of the reduced gradient algorithm corresponding to the set of active constraints. If this direction is not zero, then it optimizes E within the set of active constraints until the minimum of E is found within this set (suboptimum condition). Then it changes the set J by removing, one by one, the constraints whose gradient points in the wrong direction, until a nonzero direction of descent is found. Then, it optimizes E again in the new set J. We note that Algorithm 7 is a *conceptual* outline. Some modifications are necessary in practice (see [58]).

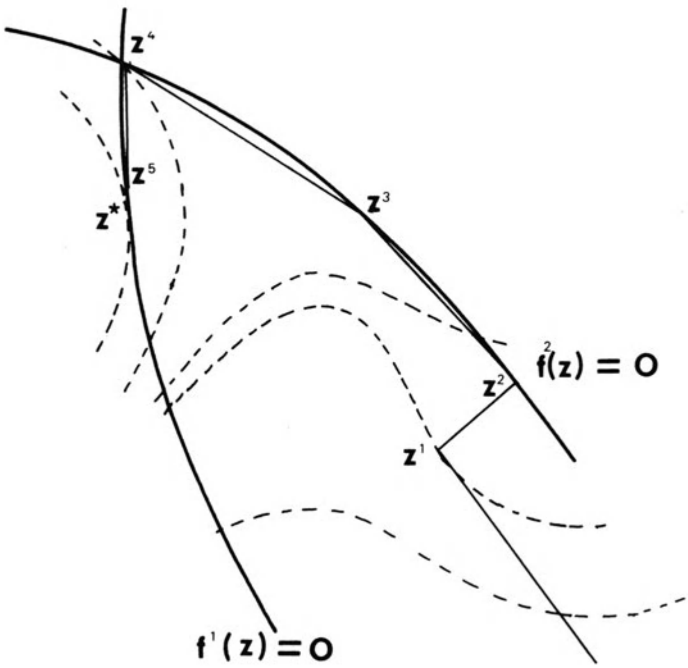


Fig. 4.4 A possible sequence $\{z^n\}$ generated by Algorithm 7. The doted lines are the level curves of E.

The set J should be defined as

$$J_\varepsilon(z) = \{j = f^j(z) \leq -\varepsilon'\} \qquad (\varepsilon' > 0) \tag{112}$$

because there are pathological cases where the algorithm jumps back and forth from one suboptimum point to another. Then ε is decreased as m increases.

- $\|h^m\|$ should be tested against ε' instead of 0 because a suboptimum point might require an infinite number of iterations.
- Then ε' must be divided by 2 instead of the "stop" in step 2.

Application to interval constraints: Very frequently the constraints are of the type

$$a_i \leq z_i \leq A_i. \tag{113}$$

In this case, the projected gradient algorithm is easy to apply. Indeed if, for example, the second constraint is active,

$$z_i = A_i, \tag{114}$$

then the projected gradient algorithm simply states that when

$$-\nabla E(z^m)_i > 0 \tag{115}$$

we must set

$$h_i = 0. \tag{116}$$

So the ith component of the projected gradient is

$$(\mathbf{P}\nabla E)_i = \min_{\{i:z_i=A_i\}} \{\nabla E(z^m)_i, 0\} + \max_{\{i:z_i=a_i\}} \{\nabla E(z^m)_i, 0\}. \tag{117}$$

A satisfactory adaptation of Algorithm 7 to the above case is the following rather simple algorithm.

Algorithm 8

[0. Choose z^0, M, ε

For $m = 0, \ldots, M$ do

[1. Compute $\nabla E(z^m)$ and $\mathbf{P}\nabla E$ according to (117).
2. Compute

$$\rho^m = \arg\min_{\rho>0} \{E(z^m - \rho\mathbf{P}\nabla E): a_i \le z_i - \rho\mathbf{P}\nabla E \le A_i\}.$$

3. Set $z^{m+1} = z^m - \rho^m\mathbf{P}\nabla E$.
4. If $\|\mathbf{P}\nabla E\| < \varepsilon$, stop.

Appendix to Chapter 4: Fortran Code for Algorithms 3 & 5

```
      SUBROUTINE cjgal5(z,e,g,h,gm2,n,mmax,eps,romin,itrace,iout)
C Conjugate gradiant algorithm to minimize E(z(1),...,z(n))
C  INPUT:
C              z(1..n):array 1..n of initial guess of solution
C              e      :value of E at z
C              n      :number of optimization variables
C              mmax:maximum number of iterations
C              eps    :precision; if norm**2 of grad E < eps, it stops
C              romin :minimum allowable step size
C              itrace : =0 no intermediate output, =2 with output,
C                       =1 check magic formula
C              iout   :logical number of output unit
C              cost(e,z,n,iout): subroutine to compute e from z
C              dcost(z,g,n): subroutine to compute g(1..n)= grad E at z
C  OUTPUT:
C              z      :computed solution
C              e      :value of E at the computed solution
```

```
C               g(1..n):value of grad E at computed solution
C               h(1..n):direction of descent at comp. sol.
C uses subroutine CRITER and SCALAR provided below.
  DIMENSION z(n),g(n),h(n)
C                                 initialization
  write(iout,5)
5 FORMAT('ITER',7X,'E',12X,'GM2',11X,'GAMA',11X,'RO')
  DO 1 i=1,n
1 h(i)= 0.
  gm12= 1.
C                                 iteration loop
  DO 2 m=1, mmax
    CALL dcost(z,g,n)
    CALL scalar(g,g,gm2,n)
    IF (gm2.LE.eps) RETURN
C                                 assumes E will decrease by 0.005*gm2
    IF (m.EQ.1) de= -0.005*gm2
    gama= gm2/gm12
    IF ((m.EQ.1).OR.(ro.LE.romin)) gama=0.
      DO 3 i= 1, n
3     h(i)= -g(i)+gama*h(i)
    el= e
    CALL minld(e,ro,romin,z,h,g,n,iout,itrace,de)
    de= e-el
      DO 4 i= 1, n
4     z(i)=z(i)+ ro*h(i)
    gm12= gm2
2 write(iout,6) m, e, gm2, gama, ro
6 FORMAT(1X,I4,4(1X,E12.5))
  RETURN
  END

  SUBROUTINE minld(e,ro,romin,z,h,g,n,iout,itrace,de)
  DIMENSION z(n), h(n), g(n)
C computes an approximate minimum of the one dimensional function of ro:
C e(z+ro*h)
C  INPUT:
C               e      :value of criter at ro= 0.
C               romin:smallest ro admissible
C               n      :dimension of arrays
C               iout   :logical number of output unit
C               itrace:see cjgal5
C               de     :estimate of e(ro=0)-emin
C  OUTPUT:
C               e      :value of e at computed minimum
C               ro     :computed minimum
C  WORKING variables: z,h,g: see cjgal5
C USES subroutine CRITER(ro,e,z,h,n,itrace,iout) to compute e at ro and
```

```
C       SCALAR(g,h,slope,n) to compute slope= d e/d ro at ro= 0.
      LOGICAL bol
      ed2= e
C                               test magic formula if itrace = 1
      CALL scalar(g,h,slope,n)
      IF(itrace.NE.1) GOTO 5
      CALL criter(romin,em,z,h,n,itrace,iout)
      derel= (em-ed2)/(romin*slope)-1.
      write(iout,3) derel,romin
3     FORMAT(62X,'magic formula: is',E11.4,'0 of',e11.4,'?')
C                               test ro=minimum of parabola achieving de, and
C                                        with slope at origin= slope
5     ro= de*2./slope
      IF (ro.LT.romin) ro= romin
      CALL criter(ro,e,z,h,n,itrace,iout)
C                               if decrease is sufficient return
      bol= ((e-e1).LE.(0.1*slope*ro)).AND.((e-el).GE.(0.9*slope*ro))
      IF (bol) RETURN
C                               else test minimum of parabola from slope and (e,ro)
      rol= -slope*ro*0.5/((e-ed2)/ro-slope)
      IF (rol.LT.romin) GOTO 1
      ro=ro1
      CALL criter(ro,e,z,h,n,itrace,iout)
      IF ((e-ed2).LE.0.1*slope*ro) RETURN
C                               Dichotomy until convex situation
1     e2= e
      ro= ro*0.5
      IF (ro.LT.romin) write(iout,4)
      IF (ro.LT.romin) RETURN
4     FORMAT('error in MIN1D: d e / d ro non negative at ro=0')
      CALL criter(ro,e,z,h,n,itrace,iout)
      IF (e.GT.ed2) GOTO 1
      ro1=ro
      e1=e
      ro= ro*(-e+e2*0.25+0.75*ed2)/(-e+e2*0.25+ed2*0.5)
      CALL criter(ro,e,z,h,n,itrace,iout)
      IF (e.GT.el) ro=rol
      IF (e.GT.el) e=el
      RETURN
      END
C
C
C
C
C
      SUBROUTINE scalar(a,b,c,n)
C computes the scalar product c= a.b
C the user may define his own scalar product (noneuclidean OK)
```

```
      DIMENSION a(n),b(n)
      c=0.
      DO 1 i= 1, n
1     c= c+ a(i)*b(i)
      RETURN
      END
C
C
C
C
C
      SUBROUTINE criter(ro,e,z,h,n,itrace,iout)
C     return e(z+ro*h)
      DIMENSION z(n),h(n)
      DO 1 i= 1, n
1     z(i)= z(i) +ro*h(i)
      CALL cost(e,z,n)
      DO 2 i= 1, n
2     z(i)= z(i)- ro*h(i)
      IF (itrace.GE.1) write(iout,3)e,ro
3     FORMAT(70X,'E= ',E11.4,' RO= ',E11.4)
      RETURN
      END
      PROGRAM test
      DIMENSION z(10),g(10),h(10)
      OPEN(6,FILE='PRINTER:')
      DO 1 i=1,10
1     z(i)=0.
      CALL cost(e,z,10)
      CALL cjgal5(z,e,g,h,gm2,10,7,1.0E-4,0.0001,1,6)
      write(6,2) (z(i),i=1,10)
2     FORMAT('z= ',10E11.5)
      END
      SUBROUTINE cost(e,z,n)
      DIMENSION z(n)
      e=0.
      DO 1 i=1, n
1     e=e+0.1*i*((z(i)-1.)**4)
      RETURN
      END
      SUBROUTINE dcost(z,g,n)
      DIMENSION z(n),g(n)
      DO 1 i= 1, n
1     g(i)=0.4*i*((z(i)-1.)**3)
      RETURN
      END
      RESULTS:
```

Sample output of test program:

```
ITER      E          GM2          GAMA          RO
                                                         E=   .5494E+01  RO=   .1000E-03
                                               magic formula: is -.4997E-03 0 of   .1000E-03  ?
                                                         E=   .4912E+01  RO=   .1000E-01
                                                         E=   .1486E+01  RO=   .1085E+00
   1  .14857E+01  .61600E+02  .00000E+00  .10846E+00
                                                         E=   .1485E+01  RO=   .1000E-03
                                               magic formula: is -.3572E-03 0 of   .1000E-03  ?
                                                         E=   .2322E+00  RO=   .9234E+00
                                                         E=   .5319E-01  RO=   .5471E+00
   2  .53185E-01  .66776E+01  .10840E+00  .54712E+00
                                                         E=   .5318E-01  RO=   .1000E-03
                                               magic formula: is  .1654E-02 0 of   .1000E-03  ?
                                                         E=   .1372E+04  RO=   .6138E+02
                                                         E=   .5026E-01  RO=   .6395E-01
   3  .50263E-01  .45116E-01  .67564E-02  .63946E-01
                                                         E=   .5026E-01  RO=   .1000E-03
                                               magic formula: is -.7092E-03 0 of   .1000E-03  ?
                                                         E=   .4467E-01  RO=   .7089E-01
                                                         E=   .1011E-01  RO=   .8166E+00
   4  .10113E-01  .41397E-01  .91755E+00  .81658E+00
                                                         E=   .1011E-01  RO=   .1000E-03
                                               magic formula: is -.1078E-02 0 of   .1000E-03  ?
                                                         E=   .1287E-01  RO=   .1435E+02
                                                         E=   .8024E-04  RO=   .6939E+01
   5  .80237E-04  .35481E-02  .85710E-01  .69388E+01
z=  .10094E+01 .10118E+01 .96096E+00 .91597E+00 .91291E+00 .95052E+00 .99842E+00 .10348E+01 .10555E+01 .10647E+01
```

CHAPTER 5

Design Problems Solved by Standard Optimal Control Theory

5.1 Introduction

A large number of optimum shape designs can be expressed or approximated in terms of the optimal control of distributed systems (see, for example, [47], [29]).

We give three examples of this type and use these examples as an opportunity to review the techniques of optimal control developed in [40]. This approach ought to be well understood before proceeding to the general case where the control is looked at as a geometric element of the system. For further details and examples, the reader is referred to [40].

5.2 Optimization of a Thin Wing

5.2.1 Problem statement

Let Ψ be the stream function of a flow around a symmetric airfoil S. Let the flow be uniform at infinity with velocity $\{u_\infty, 0\}$.

If we wish to design S in order that the pressure assumes a prescribed value on ∂S, then the following expression of the problem may be considered:

$$\min_{S \subset \mathbb{R}^2} \left\{ \int_{\partial S} f(\nabla \times \Psi)\, d\Gamma : \Delta\Psi = 0 \text{ in } \mathbb{R}^2 - S;\ \Psi_\infty = u_\infty x_2,\ \Psi|_{\partial S} = 0 \right\}$$

$$\left(\nabla \times \Psi = \left\{ \frac{\partial \Psi}{\partial x_2}, -\frac{\partial \Psi}{\partial x_1} \right\} \right). \tag{1}$$

If $S = \{\{x_1, x_2\} : |x_2| \le y(x_1),\ x_1 \in [a, b]\}$ is very thin, then the condition

$$\Psi(x_1, y(x_1)) = 0 \qquad x_1 \in [a, b] \tag{2}$$

may be approximated by

$$\frac{\partial \Psi}{\partial x_1} + tg\beta \frac{\partial \Psi}{\partial x_2} = 0, \tag{3}$$

where β is the angle of the tangent to ∂S relative to the first axis (see Figure 5.1). Then we set

$$v = -\frac{\partial \Psi}{\partial x_1}(tg\beta)^{-1}, \tag{4}$$

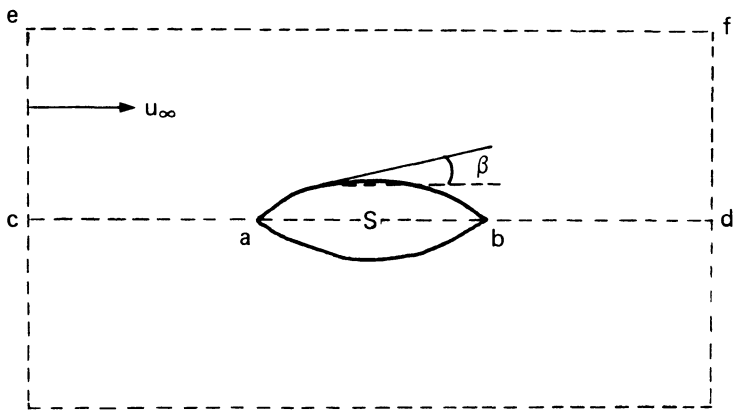


Fig. 5.1 Optimization of a thin axisymmetric profile S.

and we consider half of the domain because of symmetry and the finite region $]c,d[\times]c,e[$ to avoid dealing with the infinite domain. By (4) the unknown component of $\nabla\times\Psi|_\Gamma$ reduces to $\partial\Psi/\partial s$. If f in (1) is $|\partial\Psi/\partial s-\partial\Psi_d/\partial s|^2$, then we may simplify the problem and consider only

$$\min_{v\in V} E(v)=\int_a^b|\Psi(v)-\Psi_d|^2\,dx_1, \tag{5}$$

where Ψ_d is some desired distribution and $\Psi(v)$ is the solution of

$$\Delta\Psi=0 \quad \text{in}\,\Omega=]c,d[\times]c,e[; \tag{6}$$

$$\frac{\partial\Psi}{\partial n}=v \quad \text{on}\,\Gamma_2=[a,b]; \qquad \Psi=u_\infty x_2 \quad \text{on}\,\Gamma_1=\partial\Omega-\Gamma_2. \tag{7}$$

Now following the notation used in [40], this problem is an optimal control problem for a distributed system with Neumann boundary control and boundary observation.

There are a number of constraints on v. First, β must be small:

$$tg\beta=-\frac{\partial\Psi/\partial x_1}{v}\ll 1. \tag{8}$$

Second, the profile must not be open in b:

$$y(b)=\int_a^b\frac{dy}{dx_1}dx_1,=\int_a^b\frac{1}{v}\frac{\partial\Psi}{\partial x_1}dx_1=0. \tag{9}$$

Finally, some regularity on v is needed to define Ψ by (6) and (7), at least $v\in H^{-\frac{1}{2}}(\Gamma_2)$. For simplicity we ignore constraints (8), (9).

5.2.2 Optimality conditions

Using the usual technique for minimizing sequences, we can prove that with $V = H^{-\frac{1}{2}}(\Gamma_2)$, the problem given in (5) to (7) has at least one solution. If the constraints (8) and (9) are included in V, then the study of the existence of a solution becomes difficult.

Nevertheless, if v^* is a solution, we must have

$$E(v^* + \delta v) = \int_a^b |\Psi(v^* + \delta v) - \Psi_d|^2 \, dx_1 \geq \int_a^b |\Psi(v^*) - \Psi_d|^2 \, dx \qquad \forall v^* + \delta v \in V. \quad (11)$$

This (with self-explanatory notation) is also

$$\delta E = 2 \int_a^b (\Psi^* - \Psi_d) \delta \Psi \, dx_1 + \int_a^b |\delta \Psi|^2 \, dx; \quad (12)$$

$$\delta \Psi = \Psi(v^* + \delta v) - \Psi(v^*); \qquad \delta E = E(v^* + \delta v) - E(v^*). \quad (13)$$

From (6) and (13), we find that

$$\Delta \delta \Psi = 0 \quad \text{in } \Omega. \quad (14)$$

From (7),

$$\left.\frac{\partial \delta \Psi}{\partial n}\right|_{\Gamma_2} = \delta v, \qquad \delta \Psi|_{\Gamma_1} = 0. \quad (15)$$

For some C, this then allows us to write

$$\|\delta \Psi\|_1 \leq C \|\delta v\|_{H^{-\frac{1}{2}}(\Gamma_2)}. \quad (16)$$

Therefore, the last integral in (12) is a $o(\|\delta v\|)$ [for the definition of $o(\ )$, see eq. (13) and (15)].

To eliminate $\delta\Psi$ in (12), we have to use the *adjoint* method: let $p \in H^1(\Omega)$ be the solution of

$$\Delta p = 0 \quad \text{in } \Omega, \quad (17)$$

$$\left.\frac{\partial p}{\partial n}\right|_{\Gamma_2} = 2(\Psi^* - \Psi_d), \qquad p|_{\Gamma_1} = 0, \quad (18)$$

or equivalently,

$$\int_\Omega \nabla p \cdot \nabla w \, dx = 2 \int_a^b (\Psi^* - \Psi_d) w \, dx_1 \qquad \forall w \in H^1_{01} = H^1(\Omega) \cap \{w : w|_{\Gamma_1} = 0\}, \qquad p \in H^1_{01}. \quad (19)$$

Now (14) and (15) are also equivalent to

$$\int_\Omega \nabla \delta \Psi \cdot \nabla w \, dx = \int_b^a \delta v \, w \, dx_1 \qquad \forall w \in H^1_{01}, \delta \Psi \in H^1_{01}. \quad (20)$$

Thus, if we take $w = \delta\Psi$ in (19) and $w = p$ in (20), then we find that

$$2\int_a^b (\Psi^* - \Psi_d)\,\delta\Psi\,dx_1 = \int_a^b \delta v\,p\,dx_1. \tag{21}$$

Thus (12) becomes

$$\delta E = \int_a^b \delta v\,p\,dx_1 + o(\|\delta v\|_{H^{-\frac{1}{2}}(\Gamma_2)}). \tag{22}$$

Let us summarize this result.

Proposition 1. *With (5) and (7) the gradient of E with respect to the metric of $L^2(\Gamma_2)$ is*

$$\mathrm{grad}_{L^2(\Gamma_2)} E = p|_{\Gamma_2}, \tag{23}$$

where p is the solution of (17) and (18).

Remark 1. A consequence of (22) is also that

$$\frac{d}{d\lambda} E(v^* + \lambda v)\bigg|_{\lambda=0} = \int_a^b pv\,d\Gamma;$$

$$E(v + \delta v) = E(v) + \int_{\Gamma_2} p\,\delta v\,d\Gamma + o(\|\delta v\|_{H^{-\frac{1}{2}}(\Gamma)}).$$

Remark 2. It takes some skill to set up the adjoint equation correctly. It may be done using the variational formulation of the linearized equation, i.e. Eq. (20). The rule of thumb (which does not always work) is the following: Set up the variational formulation of the linearized system; replace the right-hand side with the variation of the criteria (excluding the higher-order terms). In this identity the test function w is replaced by the adjoint p, and the variation of the state $\delta\Psi$ is replaced by a test function w.

Schematically, $\delta E = (f, \delta\Psi) + (h, \delta v)$ and

$$(A\delta\Psi, w) = (g, \delta w) \qquad \forall w \in H,\ \delta\Psi \in I, \tag{24}$$

yield the adjoint-state equation

$$(Aw, p) = (f, w) \qquad \forall\, w \in I,\ p \in H. \tag{25}$$

This is called the adjoint equation because

$$(Aw, p) = (A^* p, w). \tag{26}$$

Corollary. If $V = H^{-\frac{1}{2}}(\Gamma_2)$, then the solution v^* satisfies

$$p|_{\Gamma_2} = 0. \tag{27}$$

5.2.3 Discretization

The finite element method is easily adapted to produce optimal control of PDEs because we simply have to replace all the respective spaces with their finite-dimensional approximations.

Indeed, let H_h be a finite element approximation of H^1_{01} and V_h an approximation of $H^{-\frac{1}{2}}(\Gamma_2)$. For example,

$$H_h = \{w_h \text{ continuous}: w_h|_T \text{ affine } \quad \forall T \in T_h, w_h|_{\Gamma_1} = 0\}, \tag{28}$$

$$V_h = \{v_h|_{\{0,x_1\}}: v_h|_\Gamma \text{ constant } \forall T \in T_h\}, \tag{29}$$

where T_h is a triangulation of Ω. Then (5) to (7) are approximated by

$$\min_{v \in V_h} E(v) = \int_a^b |(\Psi(v) - \Psi_d|^2 \, dx_1, \tag{30}$$

$$\int_\Omega \nabla\Psi \cdot \nabla w \, dx = \int_a^b vw \, dx_1 \qquad \forall w \in H_h; \Psi - u_\infty x_2 \in H_h \tag{31}$$

Notice that the controls, or variables of optimization, are

$$\{v_h|_{T_k \cap [a,b]}\}_{T_k \in T_h}.$$

To compute the derivatives of E with respect to these quantities, let us review briefly the previous calculation.

$$\delta E = \int_a^b 2(\Psi - \Psi_d)\delta\Psi \, dx_1 + o(\delta v). \tag{32}$$

$$\int_\Omega \nabla\delta\Psi \cdot \nabla w \, dx = \int_a^b \delta v w \, dx_1 \qquad \forall w \in H_h; \delta\Psi \in H_h. \tag{33}$$

Define p by

$$\int_\Omega \nabla w \cdot \nabla p \, dx = 2\int_a^b (\Psi - \Psi_d) w \, dx \qquad \forall w \in H_h; p \in H_h, \tag{34}$$

then

$$\delta E = \int_a^b p\delta v \, dx_1 = \sum_{T_k \in T_h} \delta v_k \int_{]a,b[\, \cap T_k} p \, dx_1 + o(\|\delta v\|). \tag{35}$$

Therefore, the gradient method with optimal step size is as follows.

Algorithm 1. [Solves (30) and (31)] (36)

[0. Choose $v^0 \in V_h$ (i.e., choose v_k, $\forall k$ such that $]a,b[\, \cap T_k \neq \varnothing$; choose M, ε.

For $m = 0, \ldots, M$ do

[1. Compute $\Psi^m \in H_h$ by solving the linear system (31).
[2. Compute $p^m \in H_h$ by solving the linear system (34), where Ψ is Ψ^m.

3. Set

$$u_k = -\int_{]a,b[\,\cap\, T_k} p^m dx_1, \qquad v(\rho)|_{T_k} = v_k^m + \rho u_k. \tag{37}$$

4. Compute an approximation ρ^m of

$$\min_{\rho > 0} E(v(\rho)) \tag{38}$$

(see Algorithm 2 of Chapter 4), and set

$$v^{m+1} = v(\rho^m). \tag{39}$$

If $\sum u_k^2 < \varepsilon$, stop.

5.3 Optimization of an Almost Straight Nozzle

5.3.1 Problem statement (see Fig. 5.2)

To illustrate the technique with Dirichlet conditions, let us formulate the problem in terms of the potential Φ of the flow:

$$\min_{v \in V} E(v) = \int_D |\nabla\Phi(v) - \mathbf{u}_d|^2 \, dx, \tag{40}$$

where $\Phi(v)$ is the solution of

$$\Delta\Phi = 0 \quad \text{in } \Omega, \qquad \Phi|_{\Gamma_1} = \Phi_\Gamma, \qquad \Phi|_{\Gamma_2} = v. \tag{41}$$

The problem is to find, if possible, a v on Γ_2 such that the velocity of the flow $\nabla\Phi$ equals a prescribed velocity v_d in a domain D; let Φ_Γ be the potential prescribed at the entrance and the exit of the nozzle. Once v is found, the boundary ∂S is computed from

$$0 = \frac{\partial\Phi}{\partial\mathbf{n}}\bigg|_{\partial S} \simeq \left(\frac{\partial\Phi}{\partial x_1} tg\beta - \frac{\partial\Phi}{\partial x_2}\right)\bigg|_{\Gamma_2} = \left(\frac{dv}{dx_1} tg\beta - \frac{\partial\Phi}{\partial x_2}\right)\bigg|_{\Gamma_2}, \tag{42}$$

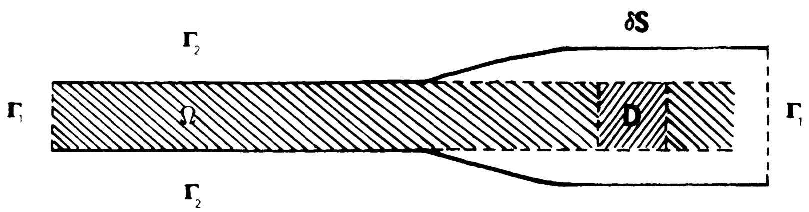


Fig. 5.2 Optimization of a nearly straight nozzle such that the velocity of the flow has a prescribed property in D.

that is

$$tg\beta = \frac{\partial\Phi/\partial x_2}{dv/dx_1}. \tag{43}$$

The set V should be chosen such that ∂S is close to Γ_2 and such that the integral in (40) exists. Therefore,

$$V \subset H^{\frac{1}{2}}(\Gamma_2). \tag{44}$$

5.3.2 Optimality conditions

To compute δE in terms of δv, we proceed as before:

$$\delta E = E(v + \delta v) - E(v) = 2\int_D (\nabla\Phi - \mathbf{u}_d)\cdot\nabla\delta\Phi\,dx + \int_D |\nabla\delta\Phi|^2\,dx, \tag{45}$$

$$\Delta\delta\Phi = 0 \quad \text{in } \Omega, \qquad \delta\Phi|_{\Gamma_1} = 0, \qquad \delta\Phi|_{\Gamma_2} = \delta v. \tag{46}$$

From (46), we know that the last integral in (45) is a $o(\|\delta v\|_{H^{\frac{1}{2}}})$. To get rid of $\delta\Phi$, we need to introduce an adjoint state variable p. Following the rule of thumb introduced in Section 5.2 (Remark 2), we write (46) in variational form

$$\begin{aligned} &\int_\Omega \nabla\delta\Phi\cdot\nabla w\,dx = 0 \qquad \forall w \in H_0^1(\Omega), \\ &\delta\Phi \in H^1(\Omega), \qquad \delta\Phi|_{\Gamma_1} = 0, \qquad \delta\Phi|_{\Gamma_2} = \delta v, \end{aligned} \tag{47}$$

and define p by

$$\int_\Omega \nabla w\cdot\nabla p\,dx = 2\int_D (\nabla\Phi - \mathbf{u}_d)\nabla w\,dx \qquad \forall w \in H_0^1(\Omega),\ p \in H_0^1(\Omega) \tag{48}$$

the boundary conditions for p are ambiguous, the rule of thumb is to set $p = \delta v$ on Γ_2, but this is forbidden since p may not depend on δv.

Some additional substitutions have to be done to replace w by $\delta\Phi$ in (48). Green's formula and (48) yield

$$\int_\Omega \nabla w\cdot\nabla p\,dx = 2\int_D (\nabla\Phi - \mathbf{u}_d)\cdot\nabla w\,dx + \int_\Gamma \frac{\partial p}{\partial n} w\,d\Gamma \qquad \forall w \in H^1(\Omega) \tag{49}$$

The easiest way to prove (49) is to define w^0 to be zero, except within a strip B near Γ_2 such that $B \cap D = \varnothing$, and in such a way that $w^0 = w$ on Γ. Then from (48), we have $\Delta p = 0$ in B; thus

$$\int_\Omega \nabla w^0\cdot\nabla p\,dx = \int_\Gamma \frac{\partial p}{\partial n} w\,d\Gamma. \tag{50}$$

Therefore, if (48) is used with w replaced by $w - w^0$, $w \in H^1(\Omega)$, (49) is derived. Let w in (47) be replaced by p and let w in (49) be replaced by $\delta\Phi$, and we obtain

$$2\int_D (\nabla\Phi - \mathbf{u}_d)\cdot\nabla\delta\Phi\,dx = \int_{\Gamma_2} \frac{\partial p}{\partial n}\delta v\,d\Gamma. \tag{51}$$

We summarize this result in the following proposition.

Proposition 2. *Let p be the solution of (48); then*

$$E(v+\delta v)-E(v)=\int_{\Gamma_2}\frac{\partial p}{\partial n}\delta v\,d\Gamma+o(\|\delta v\|_{H^{\frac{1}{2}}(\Gamma_2)})\qquad \forall\, v,\delta v\in H^{\frac{1}{2}}(\Gamma_2). \quad (52)$$

5.3.3 Discretization by finite differences

The finite element method could also be applied here, but for variety let us approximate the problem using the finite difference method:

$$\min_{\mathbf{v}} E(\mathbf{v})=\sum_{q^{i,j}\in D}|(\nabla_{2h}\Phi)_{ij}-\mathbf{u}_{d_{ij}}|^2h^2, \quad (53)$$

where $q^{i,j}=\{ih,jh\}$, $\mathbf{v}=\{v_1,\dots,v_{N-1}\}$,

$$(\nabla_{2h}\Phi)_{ij}=\left\{\frac{\Phi_{i,j+1}-\Phi_{i,j-1}}{2h},\frac{\Phi_{i+1,j}-\Phi_{i-1,j}}{2h}\right\}, \quad (54)$$

and Φ satisfies

$$\frac{\Phi_{i,j+1}+\Phi_{i,j-1}+\Phi_{i-1,j}+\Phi_{i+1,j}-4\Phi_{ij}}{h^2}=0,\qquad i,j=1,\dots,N-1, \quad (55)$$

$$\Phi_{i,0}=\Phi_{\Gamma_i},\qquad \Phi_{i,N}=\Phi_{\Gamma_i},\qquad \Phi_{0,j}=\Phi_{N,j}=v_j,$$
$$i=0,\dots,N, j=1,\dots,N-1. \quad (56)$$

Thus by the same argument

$$\delta E=2\sum_{q^{i,j}\in D}[(\nabla_{2h}\Phi)_{ij}-\mathbf{u}_{d_{ij}}](\nabla_{2h}\delta\Phi)_{ij}h^2+o(|\delta v|) \quad (57)$$

$$\frac{\delta\Phi_{i,j+1}+\delta\Phi_{i,j-1}+\delta\Phi_{i-1,j}+\delta\Phi_{i+1,j}-4\delta\Phi_{ij}}{h^2}=0\qquad i,j=1,\dots,N-1 \quad (58)$$

$$\delta\Phi_{i,0}=\delta\Phi_{i,N}=0,\ \delta\Phi_{0,j}=\delta\Phi_{N,j}=\delta v_j\qquad i=0,\dots,N; j=1,\dots,N-1. \quad (59)$$

From (54) we can group the terms with $\delta\Phi_{ij}$ in (57):

$$\begin{aligned}\delta E=&\,2\sum_{q^{i,j-1}\in D}[(\nabla_{2h}\Phi)_{i,j-1}-\mathbf{u}_{d_{i,j-1}}]_1\,\delta\Phi_{ij}\frac{h}{2}\\&-2\sum_{q^{i,j+1}\in D}[(\nabla_{2h}\Phi)_{i,j+1}-\mathbf{u}_{d_{i,j+1}}]_1\,\delta\Phi_{ij}\frac{h}{2}\\&+2\sum_{q^{i-1,j}\in D}[(\nabla_{2h}\Phi)_{i-1,j}-\mathbf{u}_{d_{i-1,j}}]_2\,\delta\Phi_{ij}\frac{h}{2}\\&-2\sum_{q^{i+1,j}\in D}[(\nabla_{2h}\Phi)_{i+1,j}-\mathbf{u}_{d_{i+1,j}}]_2\,\delta\Phi_{ij}\frac{h}{2}+o(|\delta v|). \end{aligned}\quad (60)$$

The subscript on the bracket indicates the coordinate component. Thus, the adjoint state is introduced as follows:

$$\frac{p_{i,j+1} + p_{i,j-1} + p_{i-1,j} + p_{i+1,j} - 4p_{i,j}}{h^2} =$$
$$\frac{1}{h}[\chi_D(\nabla_{2h}\Phi - \mathbf{u}_d)_1]_{i,j-1} - [\chi_D(\nabla_{2h}\Phi - \mathbf{u}_d)_1]_{i,j+1} +$$
$$\frac{1}{h}[\chi_D(\nabla_{2h}\Phi - \mathbf{u}_d)_2]_{i-1,j} - [\chi_D(\nabla_{2h}\Phi - \mathbf{u}_d)_2]_{i+1,j}$$
$$i,j = 1,\ldots,N-1, \quad (61)$$

$$p_{i,0} = p_{i,N} = p_{0,j} = p_{N,j} = 0 \qquad i,j = 0,\ldots,N. \quad (62)$$

Then a discrete Green's formula has to be worked out; it is done by multiplying (61) by $\delta\Phi_{ij}h^2$ and summing over i, j:
By restating (61) from (60), we find

$$\sum_{q^{i,j}\in D} [(\nabla_{2h}\Phi)_{ij} - u_{d_{ij}}](\nabla_{2h}\delta\Phi)_{ij}h^2$$
$$= \sum_{i,j=1,\ldots,N-1} (p_{i,j+1} + p_{i,j-1} + p_{i+1,j} + p_{i-1,j} - 4p_{ij})\,\delta\Phi_{ij}$$
$$= \sum_{\substack{i=1,\ldots,N-1\\ j=2,\ldots,N}} p_{i,j}\,\delta\Phi_{ij-1} + \sum_{\substack{i=1,\ldots,N-1\\ j=0,\ldots,N-2}} p_{ij}\,\delta\Phi_{ij+1}$$
$$+ \sum_{\substack{i=2,\ldots,N\\ j=1,\ldots,N-1}} p_{ij}\,\delta\Phi_{i-1,j} + \sum_{\substack{i=0,\ldots,N-2\\ j=1,\ldots,N-1}} p_{ij}\,\delta\Phi_{i+1,j}$$
$$-4 \sum_{i,j=1,\ldots,N-1} p_{ij}\,\delta\Phi_{ij}. \quad (63)$$

The second equality is a simple rearrangement of the indices. Now we use (58) so that all the terms with $\{i,j\} \in [1, N-1]^2$ disappear, provided we subtract out the missing terms; thus (63) becomes equal to

$$\sum_{i=1,\ldots,N-1} p_{i,N}\,\delta\Phi_{i,N-1} + \sum_{i=1,\ldots,N-1} p_{i,0}\,\delta\Phi_{i,1} + \sum_{j=1,\ldots,N-1} p_{N,j}\,\delta\Phi_{N-1,j}$$
$$+ \sum_{j=1,\ldots,N-1} p_{0,j}\,\delta\Phi_{1,j} - \sum_{i=1,\ldots,N-1} p_{i,1}\,\delta\Phi_{i,0} - \sum_{i=1,\ldots,N-1} p_{i,N-1}\,\delta\Phi_{i,N}$$
$$- \sum_{j=1,\ldots,N-1} p_{1,j}\,\delta\Phi_{0,j} - \sum_{j=1,\ldots,N-1} p_{N-1,j}\,\delta\Phi_{N,j} \quad (64)$$

Finally, we use (62) and (59) to find that

$$\delta E = -2 \sum_{j=1,\ldots,N-1} (p_{1,j} + p_{N-1,j})\,\delta v_j + o(|\delta\mathbf{v}|). \quad (65)$$

Let us summarize this result.

Proposition 3.

$$\frac{\partial E}{\partial v_j} = -2(p_{1,j} + p_{N-1,j}) \tag{66}$$

where p is the solution of (61) and (62).

Remark. Experience shows that we cannot find the discrete equation for p by using a simple finite difference approximation of (48); if it is not exactly (61), then the numerical error on the derivatives of E (order h in this case) rapidly dominates the gradient algorithms, and the step size $\rho > 0$ no longer exists.

Hint: Programming (66) may become a lengthly progress. However, there is a simple method to validate if the programming is correct: check, for instance, that

$$E(\mathbf{v} + \{0, \ldots, \tfrac{1}{100}, 0, \ldots, 0\}) \simeq E(\mathbf{v}) + \frac{\partial E/\partial v_j}{100}; \tag{67}$$

usually the two terms agree at least to the third decimal place.

The development of a gradient algorithm based on (66) to solve (40) and (41) is left to the reader.

5.4 Thickness Optimization Problem

5.4.1 Problem statement

Let Ω be a domain of $\mathbb{R}^2$, and let us consider the problem

$$\min_{v \in V} E(v) = \int_\Omega v|\nabla\Phi(v)|^2\,dx \tag{68}$$

with $\Phi(v)$ the solution of

$$-\nabla \cdot (v\nabla\Phi) = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = 0 \tag{69}$$

and

$$V = \left\{ v : m \le v(x) \le M \qquad \forall x \in \Omega;\ \int_\Omega v(x)\,dx = a \right\}. \tag{70}$$

This problem simulates the optimization of the energy associated with the thickness v of a membrane attached to Γ and with the vertical deformation $\Phi(x)$ due to the pressure f (see [17]). Maximum and minimum thicknesses are prescribed, as is the volume of the membrane (see Figure 5.3).

Many problems of this type arise in structural engineering (shells, in particular) that can be formulated as an optimal control problem with the control v being described by coefficients of the PDE (see, in particular, [6], [7], [29], [9]).

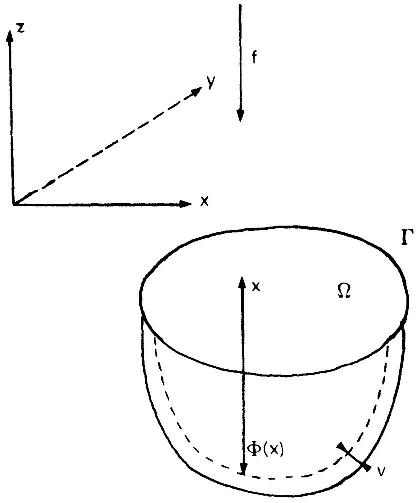


Fig. 5.3 Thickness optimization of a membrane whose vertical deformation under pressure at x is $\Phi(x)$.

5.4.2 Optimality conditions

As before, let δE and $\delta\Phi$ be the variations of E and Φ, respectively, under the change δv. Then, we have

$$\delta E = \int_\Omega \delta v|\nabla\Phi|^2\,dx + 2\int_\Omega v\nabla\Phi\cdot\nabla\delta\Phi\,dx + o(\|\delta v\|_\infty + \|\delta\Phi\|_1), \tag{71}$$

$$-\nabla\cdot(v\nabla\delta\Phi) = \nabla\cdot(\delta v\nabla\Phi) + \nabla\cdot(\delta v\nabla\delta\Phi) \quad \text{in } \Omega, \qquad \delta\Phi|_\Gamma = 0. \tag{72}$$

From (70) and (72), we find that

$$\|\delta\Phi\|_1 \le \frac{1}{m}\|\delta v\|_\infty\|\nabla\Phi\|_1. \tag{73}$$

To compute the second integral in (71) in terms of δv, we write (72) in variational form:

$$\int_\Omega v\nabla\delta\Phi\cdot\nabla w\,dx = -\int_\Omega \delta v\nabla\Phi\cdot\nabla w\,dx - \int_\Omega \delta v\nabla\delta\Phi\cdot\nabla w\,dx$$
$$\forall\, w\in H_0^1(\Omega),\ \delta\Phi\in H_0^1(\Omega). \tag{74}$$

Notice that the last integral is $o(\|\delta v\|_\infty)$, from (73); therefore, the adjoint state p is set to be the solution of

$$\int_\Omega v\nabla w\cdot\nabla p\,dx = 2\int_\Omega v\nabla\Phi\cdot\nabla w\,dx \qquad \forall\, w\in H_0^1(\Omega),\ p\in H_0^1(\Omega). \tag{75}$$

As before, set $w = \delta\Phi$ in (75) and $w = p$ in (74) and this yields

$$2\int_\Omega v\nabla\Phi\cdot\nabla\delta\Phi\,dx = -\int_\Omega \delta v\,\nabla\Phi\cdot\nabla p\,dx + o(\|\delta v\|_\infty). \tag{76}$$

However, (75) has an obvious solution $p = 2\Phi$; therefore,

$$\delta E = -2 \int_\Omega \delta v |\nabla \Phi|^2 \, dx + o(\|\delta v\|_\infty). \tag{77}$$

Proposition 3. *The solution v^* of (68) must satisfy*

$$|\nabla \Phi(v^*)(x)|^2 \begin{cases} = \lambda & \forall x \text{ such that } m < v^*(x) < M \\ \leq \lambda & \forall x \text{ such that } v^*(x) = m \\ \geq \lambda & \forall x \text{ such that } v^*(x) = M \end{cases} \tag{78}$$

for some constant λ.

PROOF. In fact, (78) is the Kuhn–Tucker optimality condition of (68); however, in this case, it is easy to prove directly. Let v be small and zero everywhere except in a small neighborhood of x' and in a small neighborhood of x''. If $v^*(x')$, $v^*(x'') \in]m, M[$, then (70) imposes on δv

$$\int_\Omega \delta v \, dx = 0, \quad \text{i.e.,} \quad \delta v(x') \simeq -\delta v(x''). \tag{79}$$

Since v^* is a solution only if $\delta E \geq 0$, we find from (77) that

$$-|\nabla \Phi(x')|^2 \, \delta v(x') - |\nabla \Phi(x'')|^2 \, \delta v(x'') \geq 0 \qquad \forall \, \delta v \text{ with (79)} \tag{80}$$

implies

$$|\nabla \Phi(x')|^2 = |\nabla \Phi(x'')|^2 \qquad \forall \, x', x'' \text{ such that } m < v^*(x'), v(x'') < M. \tag{81}$$

If $v^*(x') = m$, for instance, then in addition to (79), we must have

$$\delta v(x') \geq 0. \tag{82}$$

So (80) only yields

$$|\nabla \Phi(x')|^2 \leq |\nabla \Phi(x'')|^2. \tag{83}$$

□

Algorithm 2. [Solves (68).]
The reduced and projected gradient method is stated below.
[0. Choose N and choose $v^0 \in V$.

For $n = 0, \ldots, N$ do
1. Compute $\Phi^n = \Phi(v^n)$ by (69).
2. Set

$$I(\lambda) = \{x : v^n(x) > m \text{ or } |\nabla \Phi^n(x)|^2 > \lambda\} \cup \{x : v^n(x) < M \text{ or } |\nabla \Phi^n(x)|^2 < \lambda\} \tag{84}$$

and compute an approximation of λ such that

$$\int_{I(\lambda)} |\nabla \Phi^n|^2 \, dx = \lambda. \tag{85}$$

3. Set

$$v(\rho)(x) = \begin{cases} v^n(x) + \rho(|\nabla\Phi^n|^2 - \lambda) & \text{if } x \in I(\lambda) \\ v^n(x) & \text{if } x \notin I(\lambda) \end{cases} \tag{86}$$

and compute an approximation of

$$\rho^n = \arg\min_{\rho > 0} E(v(\rho)). \tag{87}$$

4. Set $u^{n+1} = v(\rho^n)$

Comments. This algorithm is the reduced gradient method with respect to the constraint on the volume because by construction

$$\int_\Omega [|\nabla\Phi^n|^2 - \lambda]\chi_{I(\lambda)}\, dx = 0.$$

Thus if $v^0 \in V$, all other v^n yield the same volume a. It is referred to as the projected gradient with respect to the box constraints m, M. Obviously, we ought to make the PDE and the functions Φ and v discrete and also incorporate some margin, say ε, into the constraints of $I(\lambda)$, as explained in Chapter 4.

CHAPTER 6

Optimality Conditions

6.1 Introduction

In Chapter 4 it was shown how optimality conditions of optimization problems are related to their respective gradients and are chosen so that algorithms may be developed to find feasible numerical solutions. Although it is sufficient to know how to derive such conditions on discrete problems only, it is useful to begin with the study of the continuous case since it is simpler and it may give a valuable interpretation to the solution.

Therefore, we examine a number of typical cases individually beginning with the simplest, the method of normal variations ([53], [54], [55]). The method of mappings [49] is described for mathematical justification when a weaker hypothesis is introduced in Chapter 8. The method of characteristic functions [18], [63] and the penalty method [34] are also given in Chapter 8 as alternative approaches.

For still other methods, the reader may consult [14], [15], [25].

6.2 Distributed Observations on a Fixed Domain

We begin with problems having criteria of the type

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_D f(\Phi(\Omega))\, dx.$$

For example,

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_D |\nabla \Phi(\Omega) - \mathbf{u}_d|^2\, dx, \tag{1}$$

where D is a given open set of Ω, $\mathbf{u}_d$ is a given vector-valued function of $L^2(D)^n$, and $\mathcal{O}$ is a subset of the set of open sets of $\mathbb{R}^n$ that satisfy

$$D \subset \Omega \subset C \tag{2}$$

for some given bounded set C.

Definition. Let Ω be a bounded open set of $\mathbb{R}^n$ with boundary Γ, and let $n(x)$ be the outer normal of Γ at $x \in \Gamma$. Assume that Ω is sufficiently regular so that for any $\alpha \in C^2(\Gamma)$, there exists $\lambda(\alpha)$ such that (see Figure 6.1)

$$\Gamma_{\lambda\alpha} = \{x + \lambda\alpha(x)n(x) : x \in \Gamma\} \tag{3}$$

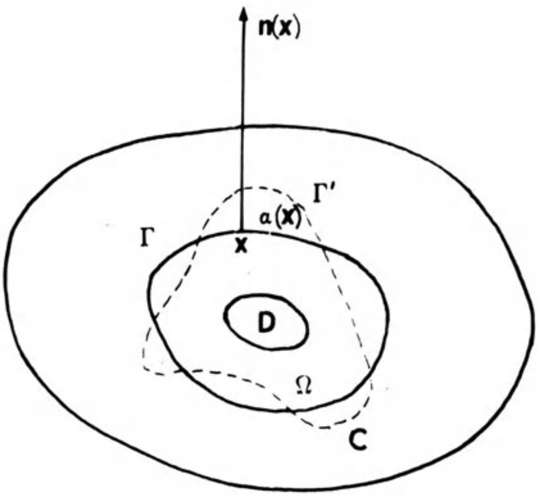


Fig. 6.1 Variations of Ω are constructed by moving the boundary Γ into Γ' a distance $\alpha(x)$ along the outernormal $\mathbf{n}(x)$; C is the security set ($\Omega \subset C$).

is the boundary of an open set $\Omega_{\lambda\alpha}$ close to Ω, for all $\lambda \in [0, \lambda(\alpha)]$. Then $F: \mathcal{O} \to \mathbb{R}^m$ is said to be *Γ-differentiable* if there exists an F' independent of α, such that

$$F(\Omega_\alpha) - F(\Omega) = \int_\Gamma F' \cdot \alpha \, d\Gamma + o(\|\alpha\|_{C^2}). \tag{4}$$

Remark 1. This definition is a somewhat informal Frechet differentiability of F; we make no attempt to relax the assumptions on Ω and α at this stage.

Remark 2. The Gateau derivative of F, F'_α, satisfies

$$F'_\alpha = \frac{d}{d\lambda} F(\Omega_{\lambda\alpha})\bigg|_{\lambda=0} = \int_\Gamma F' \cdot \alpha \, d\Gamma. \tag{5}$$

It is usually much easier to prove (5) than to prove (4). We may deduce (4) from (5), if it is possible to show that

i. F'_α is linear continuous with respect to α.

ii. $\displaystyle \lim_{\|\alpha\| \to 0} \frac{(F(\Omega_\alpha) - F(\Omega) - \|\alpha\| F'_{\alpha/\|\alpha\|})}{\|\alpha\|} = 0.$

In most cases we prove Γ-differentiability by this method: first prove (5), then observe that condition i holds, and then prove condition ii. This makes it advantageous to postpone proving condition ii until the end of the proof (the reader may skip that technical discussion).

Lemma 1. *If $\Phi'_\alpha(\Omega)$ exists, then*

$$\frac{d}{d\lambda} E(\Omega_{\lambda\alpha})\bigg|_{\lambda=0} = 2 \int_D \nabla\Phi'_\alpha \cdot (\nabla\Phi(\Omega) - \mathbf{u}_d) \, dx \tag{6}$$

with

$$\Phi'_\alpha = \frac{d}{d\lambda}\,\Phi(\Omega_{\lambda\alpha})\bigg|_{\lambda=0}. \tag{7}$$

PROOF.

$$E(\Omega_{\lambda\alpha}) - E(\Omega) = \int_D \left(|\nabla\Phi(\Omega_{\lambda\alpha}) - \mathbf{u}_d|^2 - |\nabla\Phi(\Omega) - \mathbf{u}_d|^2\right) dx$$
$$= 2\int_D \nabla\delta\Phi\cdot\left(\nabla\Phi(\Omega) - \mathbf{u}_d\right) dx + \int_D |\nabla\delta\Phi|^2\,dx$$

with

$$\delta\Phi = \Phi(\Omega_{\lambda\alpha}) - \Phi(\Omega).$$ □

6.2.1 Homogeneous Neumann conditions

Let $\Phi(\Omega)$ be the solution of

$$\Phi - \Delta\Phi = f \quad \text{in } \Omega, \qquad \frac{\partial\Phi}{\partial n}\bigg|_\Gamma = 0. \tag{8}$$

As usual Γ is the boundary of Ω. In variational form, (8) becomes

$$\int_\Omega (\Phi w + \nabla\Phi\cdot\nabla w - fw)\,dx = 0 \qquad \forall\, w \in H^1(\Omega),\ \Phi \in H^1(\Omega), \tag{9}$$

but if $\sim$ denotes any extension in C, (9) is also

$$\int_\Omega (\tilde\Phi\tilde w + \nabla\tilde\Phi\cdot\nabla\tilde w - f\tilde w)\,dx = 0 \qquad \forall\,\tilde w \in H^1(C),\ \tilde\Phi \in H^1(C).$$

Proposition 1. *If $\Phi(\Omega)$ is the solution of (9) and if Φ'_α is defined by (7), then*

$$\int_\Omega (\Phi'_\alpha w + \nabla\Phi'_\alpha\cdot\nabla w)\,dx = \int_\Gamma \alpha(fw - \Phi w - \nabla\Phi\cdot\nabla w)\,d\Gamma + o(\|\alpha\|_{C^2(\Gamma)})$$
$$\forall\, w \in C^1(\bar\Omega),\ \Phi'_\alpha \in H^1(\Omega), \tag{10}$$

provided that $\Gamma \in C^3, f \in C^0(\Omega)$.

PROOF. Let

$$\delta\Omega = \delta\Omega^+ \cup \delta\Omega^-, \tag{11}$$

$$\delta\Omega^+ = \Omega_\alpha - \overline{\Omega_\alpha \cap \Omega}, \tag{12}$$

$$\delta\Omega^- = \Omega - \overline{\Omega_\alpha \cap \Omega}. \tag{13}$$

Notice that from (3), we also have

$$\delta\Omega^+ = \{x + \beta n(x): x \in \Gamma; 0 < \beta < \max\{0, \alpha(x)\}\}, \tag{14}$$

$$\delta\Omega^- = \{x + \beta n(x): x \in \Gamma; \min\{0, \alpha(x)\} < \beta < 0\}. \tag{15}$$

Now from (9) with $\delta\phi = \phi(\Omega_\alpha) - \phi(\Omega)$

$$\begin{aligned} 0 &= \int_{\Omega_\alpha} (\Phi(\Omega_\alpha)\tilde{w} + \nabla\Phi(\Omega_\alpha)\cdot\nabla\tilde{w} - f\tilde{w})\,dx - \int_\Omega (\Phi(\Omega)\tilde{w} + \nabla\Phi(\Omega)\cdot\nabla\tilde{w} - f\tilde{w})\,dx \\ &= \int_{\Omega_\alpha\cap\Omega} (\delta\Phi\tilde{w} + \nabla\delta\Phi\cdot\nabla\tilde{w})\,dx + \int_{\delta\Omega^+} (\Phi(\Omega_\alpha)\tilde{w} + \nabla\Phi(\Omega_\alpha)\cdot\nabla w - f\tilde{w})\,dx \\ &\quad - \int_{\delta\Omega^-} (\Phi(\Omega)\tilde{w} + \nabla\Phi(\Omega)\cdot\nabla\tilde{w} - f\tilde{w})\,dx. \end{aligned} \tag{16}$$

If the integrands of the last two integrals are continuous and if $\alpha \in C^1$, we can use the mean value theorem for integrals and approximate the element of volume dx by $\alpha\,d\Gamma$; thus

$$\begin{aligned} 0 &= \int_{\Omega_\alpha\cap\Omega} (\delta\Phi\tilde{w} + \nabla\delta\Phi\cdot\nabla\tilde{w})\,dx + \int_{\Gamma\cap(\alpha>0)} (\Phi(\Omega_\alpha)\tilde{w} + \nabla\Phi(\Omega_\alpha)\cdot\nabla\tilde{w} - f\tilde{w})\alpha\,d\Gamma \\ &\quad - \int_{\Gamma\cap(\alpha<0)} (\Phi(\Omega)\tilde{w} + \nabla\Phi(\Omega)\cdot\nabla\tilde{w} - f\tilde{w})|\alpha|\,d\Gamma \\ &\quad + o(\|\alpha\|_{C^1}(\|\Phi\|_{C^1} + \|f\|_{C^0} + \|w\|_{C^1})). \end{aligned} \tag{17}$$

The hypothesis are sufficient for $\Phi(\Omega_\alpha) \to \Phi(\Omega)$ strongly in H^1 when $\lambda \to 0$ because the ε-cone property is implied by $\Gamma, \alpha \in C^1$ (Theorem 3 in Chapter 2). From Theorem 4 in Chapter 1, $\Gamma_{\lambda\alpha} \in C^2$ implies $\Phi(\Omega_{\lambda\alpha}) \in C^2$. Now $\Gamma \in C^3$, $\alpha \in C^2$ implies $\Gamma_{\lambda\alpha} \in C^2$; therefore,

$$\int_\Omega \delta\Phi w + \nabla\delta\Phi\cdot\nabla w\,dx = \int_\Gamma (\Phi w + \nabla\Phi\cdot\nabla w - fw)\alpha\,d\Gamma + o(\|\alpha\|_{C^2}), \tag{18}$$

and the result is in the form of (10). □

Remark. By Theorem 4 in Chapter 1 we have

$$\Gamma \in C^{2,\beta},\ f \in C^{0,\beta} \Rightarrow \Phi \in C^{2,\beta}. \tag{19}$$

The assumptions $\Gamma \in C^3$, $\alpha \in C^2$ are required only to ensure that $\Gamma_{\lambda\alpha} \in C^{2,\beta}\ \forall\,\lambda$. It is easy to extend the results to $\Gamma \in C^2$ only; it suffices to define $\Omega_{\lambda\alpha}$ by $x + \alpha(x)\mathbf{d}(x)$ instead of $x + \alpha(x)\mathbf{n}(x)$, where $\mathbf{d}$ is a regular direction. The method of mappings [49] can be utilized also to obtain (10) directly under a different set of hypotheses, as we shall see in Chapter 8.

Theorem 1. *Let $p \in H^1(\Omega)$ be the solution of*

$$\int_\Omega (pw + \nabla p \cdot \nabla w)\,dx = 2\int_D \nabla w \cdot (\nabla \Phi(\Omega) - \mathbf{u}_d)\,dx \qquad \forall\, w \in H^1(\Omega). \tag{20}$$

Assume $\Gamma \in C^3$, $f \in C^0(\Omega)$, then

$$E(\Omega_\alpha) - E(\Omega) = \int_\Gamma \alpha(fp - \Phi(\Omega)p - \nabla\Phi(\Omega)\cdot\nabla p)\,d\Gamma + o(\|\alpha\|_{C^2}). \tag{21}$$

PROOF. By replacing w by Φ'_α in (20) and w by p in (10), we get

$$2\int_D \nabla\Phi'_\lambda \cdot (\nabla\Phi(\Omega) - \mathbf{u}_d)\,dx = \int_\Gamma \alpha(fp - \Phi(\Omega)p - \nabla\Phi(\Omega)\cdot\nabla p)\,d\Gamma. \tag{22}$$

Therefore, (6) becomes (21). □

Corollary 1. *Assume that $\mathcal{O}$ is the set of Ω's containing D and contained in C. If Γ is C^3, Ω is a solution of (1) to (3), and the relations $D \subset \Omega \subset C$ are strictly contained, then*

$$\Phi - \Delta\Phi = f \quad in\ \Omega, \qquad \left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = 0, \tag{23}$$

$$p - \Delta p = -2\nabla\cdot[\chi_D(\nabla\Phi - \mathbf{u}_d)] \quad in\ \Omega, \qquad \left.\frac{\partial p}{\partial n}\right|_\Gamma = 0, \tag{24}$$

$$(\Phi p + \nabla\Phi\cdot\nabla p)|_\Gamma = fp|_\Gamma. \tag{25}$$

If the relations are not strictly contained, then (25) must be replaced by

$$\Phi p + \nabla\Phi\cdot\nabla p \quad \begin{array}{ll} \geq fp & on\ \Gamma\cap\partial C \\ \leq fp & on\ \Gamma\cap\partial D \\ = fp & elsewhere\ on\ \Gamma. \end{array} \tag{26}$$

PROOF. The interpretation of (20) becomes (24). If Ω is a solution, then

$$E(\Omega_\alpha) > E(\Omega) \qquad \forall\,\alpha \in C^2(\Gamma),\ \Omega_\alpha \in \mathcal{O}. \tag{27}$$

If the relation are strictly contained, then (21) and (27) imply (25) because α can have any sign as long as it is small. If the relations are not strictly contained, then α is positive on $\Gamma \cap \partial D$ and negative only on $\Gamma \cap \partial C$. □

6.2.2 Dirichlet conditions

Now let $\Phi(\Omega)$ be the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = 0. \tag{28}$$

Proposition 2. *If $\Phi(\Omega)$ is defined by (28) and*

$$\Phi'_\alpha = \frac{d}{d\lambda}\Phi(\Omega_{\lambda\alpha})|_{\lambda=0}, \tag{29}$$

where

$$\Gamma_{\lambda\alpha} = \{x + \lambda\alpha(x)n(x): x \in \Gamma\}, \tag{30}$$

then

$$-\Delta\Phi'_\alpha = 0 \quad in\ \Omega, \qquad \Phi'_\alpha|_\Gamma = -\alpha\frac{\partial\Phi}{\partial n}\bigg|_\Gamma, \tag{31}$$

provided that $\alpha \in C^2$, $\Gamma \in C^3$.

Proof. We have from (28)

$$-\Delta[\Phi(\Omega_\alpha) - \Phi(\Omega)] = 0 \quad \text{in } \Omega_\alpha \cap \Omega. \tag{32}$$

Also, for some $\theta(x) \in]0, \alpha(x)[$ by (28),

$$0 = \Phi(\Omega_\alpha)|_{x+\alpha n} = \Phi(\Omega_\alpha)|_x + \alpha\frac{\partial\Phi}{\partial n}(\Omega_\alpha)\bigg|_{x+\theta n}, \tag{33}$$

where the last member is a Taylor expansion of second order; this is permissable only if $\Phi(\Omega_\alpha) \in C^1$.

$$\begin{aligned}[\Phi(\Omega_\alpha) - \Phi(\Omega)]|_{x\in\Gamma\cap\bar\Omega_\alpha} &= \Phi(\Omega_\alpha)\bigg|_{x+\alpha n} - \alpha\frac{\partial\Phi}{\partial n}(\Omega_\alpha)\bigg|_{x+\theta n} - 0\\ &= -\alpha\frac{\partial\Phi}{\partial n}(\Omega_\alpha)\bigg|_{x+\theta n};\end{aligned} \tag{34}$$

$$[\Phi(\Omega_\alpha) - \Phi(\Omega)]|_{x\in\Gamma_\alpha\cap\bar\Omega} = 0 - \Phi(\Omega)|_{x+\alpha n} = -\alpha\frac{\partial\Phi}{\partial n}(\Omega)\bigg|_{x+\theta' n}. \tag{35}$$

Hence, the result follows since $\nabla\Phi(\Omega_\alpha) \in C^0(\Omega)$ by hypothesis and

$$\frac{\partial\Phi}{\partial n}(\Omega_\alpha) \to \frac{\partial\Phi}{\partial n}(\Omega) \quad \text{in } C^0, \tag{36}$$

by Theorem 6 of Chapter 1. □

Remark. The above proof is not very rigorous, in fact, since to establish (36) we use the trace theorem on a moving boundary. It can be justified; however, we need to work in a more detailed fashion, and the argument thus becomes very tedious. Later we study the method of mappings and this study shows that Proposition 2 is valid under even weaker assumptions about Γ (see Theorem 2 in Chapter 8).

Theorem 2. *Let $p \in H_0^1(\Omega)$ be the solution of*

$$-\Delta p = -2\nabla \cdot [\chi_D(\nabla\Phi(\Omega) - \mathbf{u}_d)] \quad in\ \Omega, \qquad p|_\Gamma = 0. \tag{37}$$

Then, if $\Gamma \in C^3$, $f \in C^0(\Omega)$ for the problems given in (1) and (28), we have

$$E(\Omega_\alpha) - E(\Omega) = \int_\Gamma \alpha \frac{\partial\Phi}{\partial n}(\Omega)\frac{\partial p}{\partial n}\,d\Gamma + o(\|\alpha\|_{C^2}). \tag{38}$$

Proof. The argument proposed here is similar to the one used in Theorem 1. From (37) and Green's formula, we find that

$$\int_\Omega \nabla p \cdot \nabla\Phi'_\alpha\,dx - \int_\Gamma \frac{\partial p}{\partial n}\Phi'_\alpha\,d\Gamma = 2\int_D (\nabla\Phi - \mathbf{u}_d)\nabla\Phi'_\alpha\,dx = \frac{d}{d\lambda}E(\Omega_{\lambda\alpha})\bigg|_{\lambda=0}, \tag{39}$$

and from (31), we have

$$\int_\Omega \nabla\Phi'_\alpha \cdot \nabla p\,dx = 0 \quad \text{and} \quad \Phi'_\alpha\bigg|_\Gamma = -\alpha\frac{\partial\Phi}{\partial n}\bigg|_\Gamma. \tag{40}$$

□

Corollary. *If Ω is the solution of (1) and (28), it must satisfy*

$$\frac{\partial\Phi}{\partial n}(\Omega)\frac{\partial p}{\partial n}\begin{cases} \leq 0 & on\ \Gamma \cap \partial C & (41)\\ \geq 0 & on\ \Gamma \cap \partial D & (42)\\ = 0 & on\ \Gamma - \Gamma \cap \partial C - \Gamma \cap \partial D & (43)\end{cases}$$

6.2.3 Homogeneous Frechet boundary conditions

Consider the case where $\Phi(\Omega)$ is the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega, \qquad \left(\Phi + \frac{\partial\Phi}{\partial n}\right)\bigg|_\Gamma = 0. \tag{44}$$

The variational formulation of this problem is

$$\int_\Omega \nabla\Phi \cdot \nabla w\,dx + \int_\Gamma \Phi w\,d\Gamma = \int_\Omega fw\,dx \qquad \forall w \in H^1(\Omega),\ \Phi \in H^1(\Omega). \tag{45}$$

Lemma 2. *Let Γ be the boundary of $\Omega \subset \mathbb{R}^n$, and let $\Gamma \in C^2$ and*

$$\Gamma_\alpha = \{x + \alpha(x)n(x) : x \in \Gamma\}; \tag{46}$$

then for $n = 2$ or 3,

$$\frac{d}{d\lambda}\int_{\Gamma_{\lambda\alpha}} g\,d\Gamma|_{\lambda=0} = \int_\Gamma \alpha\left(\frac{\partial g}{\partial n} - \frac{g}{R}\right)d\Gamma \qquad \forall\alpha \in C^1(\Gamma),$$

where R denotes the radius of curvature if $n = 2$ and the mean radius of curvature if $n = 3$ (see (52) where it states that $d\mathbf{n}/dl = -\mathbf{s}/R$ in $\mathbb{R}^3$).

PROOF. *Case 1* ($n = 2$): Let l_α, l, $\mathbf{s}_\alpha$, $\mathbf{s}$, and R denote the curvilinear abscissas of Γ_α and Γ, the tangent vectors, and the radius of curvature of Γ. From (46), we have

$$\frac{d\mathbf{x}_\alpha}{dl} = \frac{d\mathbf{x}}{dl} + \frac{d\alpha}{dl}\mathbf{n} + \alpha\frac{d\mathbf{n}}{dl} = \mathbf{s} + \dot{\alpha}\mathbf{n} - \alpha\frac{\mathbf{s}}{R}; \tag{47}$$

therefore,

$$dl_\alpha = \left[\left(1 - \frac{\alpha}{R}\right)^2 + \dot{\alpha}^2\right]^{\frac{1}{2}} dl = \left(1 - \frac{\alpha}{R}\right) dl + o(\|\alpha\|_{C^1}). \tag{48}$$

Thus, we can perform the following calculation:

$$\begin{aligned}\int_{\Gamma_\alpha} g\, d\Gamma &= \int_\Gamma g(x + \alpha n)\left(1 - \frac{\alpha}{R}\right) dl + o(\|\alpha\|)\\ &= \int_\Gamma g\, d\Gamma + \int_\Gamma \alpha\left(\frac{\partial g}{\partial n} - \frac{1}{R}g\right) d\Gamma + o(\|\alpha\|).\end{aligned} \tag{49}$$

Case 2 ($n = 3$): With the same notation and T for torsion, we have

$$\frac{d\mathbf{x}_\alpha}{dl} = \frac{d\mathbf{x}}{dl} + \frac{d\alpha}{dl}\mathbf{n} + \alpha\frac{d\mathbf{n}}{dl} = \mathbf{s} + \dot{\alpha}\mathbf{n} - \alpha\frac{\mathbf{s}}{R} - \alpha\frac{\mathbf{b}}{T}; \tag{50}$$

Thus

$$dl_\alpha = \left(1 - \frac{\alpha}{R}\right) dl + o(\|\alpha\|_{C^1}), \tag{51}$$

and if l_1, l_2 are two elements of length corresponding to orthogonals s_1 and s_2, we have

$$dl_{\alpha_1}\, dl_{\alpha_2} = \left[1 - \alpha\left(\frac{1}{R_1} + \frac{1}{R_2}\right)\right] dl_1\, dl_2 \tag{52}$$

The rest of the proof is identical to case 1.

Proposition 3. *Let $\Phi(\Omega)$ be the solution of (45); then*

$$\Phi'_\alpha = \frac{d}{d\lambda}\Phi(\Omega_{\lambda\alpha})|_{\lambda=0} \tag{53}$$

satisfies

$$\int_\Omega \nabla\Phi'_\alpha \cdot \nabla w\, dx + \int_\Gamma \Phi'_\alpha w\, d\Gamma = -\int_\Gamma \alpha\left(\nabla\Phi \cdot \nabla w + \frac{\partial}{\partial n}(\Phi w) - \frac{\Phi w}{R} - fw\right) d\Gamma. \tag{54}$$

PROOF. The proof is exactly the same as that of Theorem 1 except we must also account here for the variation of the integral on Γ by Φw. That may be done with the help of Lemma 2. □

Remark. Due to $\partial\Phi w/\partial n$, the adjoint state p must be regular for (54) to make sense when w is replaced by p.

6.2.4 Nonhomogeneous Neumann boundary conditions

Let $\Phi(\Omega)$ be the solution of

$$\Phi - \Delta\Phi = f \quad \text{in } \Omega, \qquad \left.\frac{\partial\Phi}{\partial n}\right|_\Gamma = g. \tag{55}$$

Proposition 4. *With the previous notation, Φ'_α satisfies*

$$\int_\Omega (\Phi'_\alpha w + \nabla\Phi'_\alpha \cdot \nabla w)\,dx = -\int_\Gamma \alpha\left(\Phi w + \nabla\Phi \cdot \nabla w - f - \frac{\partial}{\partial n}(gw) + \frac{gw}{R}\right)d\Gamma$$
$$\forall\, w \in C^1(\Omega). \tag{56}$$

Proof. We write (55) in variational form:

$$\int_\Omega (\Phi w + \nabla\Phi \cdot \nabla w - fw)\,dx = \int_\Gamma gw\,d\Gamma \qquad \forall\, w \in H^1(\Omega). \tag{57}$$

Then we repeat the proof of Theorem 1. By differentiation,

$$\int_\Omega (\delta\Phi w + \nabla\delta\Phi \cdot \nabla w)\,dx + \int_{\delta\Omega} (\Phi w + \nabla\Phi \cdot \nabla w - fw)\,dx = \delta\left[\int_\Gamma gw\,d\Gamma\right]. \tag{58}$$

The second integral is evaluated as before, and the last one by the use of Lemma 2. □

6.2.5 Nonhomogeneous Dirichlet conditions

Let $\Phi(\Omega)$ be the solution of

$$-\Delta\Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = g|_\Gamma. \tag{59}$$

Proposition 5. *Following the previous notation, Φ'_α satisfies*

$$-\Delta\Phi'_\alpha = 0 \quad \text{in } \Omega, \qquad \Phi'_\alpha|_\Gamma = -\alpha\left(\frac{\partial\Phi}{\partial n} - \frac{\partial g}{\partial n}\right). \tag{60}$$

Proof. The Taylor expansion of (34) becomes

$$\Phi(\Omega_\alpha)|_{x+\alpha n} - \Phi(\Omega)|_{x+\alpha n} = g(x + \alpha n) - g(x) - \alpha\frac{\partial\Phi}{\partial n} + o(\|\alpha\|) \tag{61}$$

$$= \alpha\frac{\partial g}{\partial n} - \alpha\frac{\partial\Phi}{\partial n} + o(\|\alpha\|).$$ □

Corollary. *For problem* (*1*) and (*59*), we must have

$$E(\Omega_\alpha) - E(\Omega) = -\int_\Gamma \alpha\left(\frac{\partial \Phi}{\partial n} - \frac{\partial g}{\partial n}\right)\frac{\partial p}{\partial n}\,d\Gamma + o(\|\alpha\|_{C^2}), \tag{62}$$

where p is the solution of (*37*).

6.3 Other Cases with Linear PDE

6.3.1 Criteria depending on the domain

Example 1. Consider the case

$$E(\Omega) = \int_\Omega |\nabla\Phi(\Omega) - \mathbf{u}_d|^2\,dx, \tag{63}$$

where $\Phi(\Omega)$ is a solution of any of the partial differential equations, studied in Section 6.2. Then by combining the technique of Lemma 1 and Proposition 1, we write formally:

$$\begin{aligned}\delta E &= \int_{\delta\Omega} |\nabla\Phi(\Omega) - \mathbf{u}_d|^2\,dx + 2\int_\Omega \nabla\delta\Phi\cdot(\nabla\Phi(\Omega) - \mathbf{u}_d)\,dx + o(\|\alpha\|)\\ &= \int_\Gamma \alpha|\nabla\Phi(\Omega) - \mathbf{u}_d|^2\,d\Gamma + 2\int_\Omega \nabla\delta\Phi\cdot(\nabla\Phi(\Omega) - \mathbf{u}_d)\,dx + o(\|\alpha\|)\end{aligned} \tag{64}$$

[see (11) for the definition of $\delta\Omega$]. So

$$\frac{dE}{d\lambda}(\Omega_{\lambda\alpha})|_{\lambda=0} = \int_\Gamma \alpha|\nabla\phi(\Omega) - \mathbf{u}_d|^2\,d\Gamma + 2\int_\Omega \nabla\Phi'_\alpha\cdot(\nabla\phi(\Omega) - \mathbf{u}_d)\,dx. \tag{65}$$

Example 2

$$E(\Omega) = \int_\Gamma |\phi(\Omega) - \phi_d|^2\,d\Gamma + \int_\Gamma |\nabla\phi(\Omega) - \mathbf{u}_d|^2\,d\Gamma. \tag{66}$$

For this case, we must use Lemma 2. Then

$$\begin{aligned}\delta E &= 2\int_\Gamma [\delta\phi(\phi(\Omega) - \phi_d) + \nabla\delta\phi\cdot(\nabla\phi(\Omega) - \mathbf{u}_d)]\,d\Gamma\\ &\quad + \int_\Gamma \alpha\left[\frac{\partial}{\partial n}[|\phi(\Omega) - \phi_d|^2 + |\nabla\phi(\Omega) - \mathbf{u}_d|^2]\right.\\ &\quad \left. - \frac{1}{R}[|\phi(\Omega) - \phi_d|^2 + |\nabla\phi(\Omega) - \mathbf{u}_d|^2]\right]d\Gamma.\end{aligned} \tag{67}$$

Thus

$$\frac{d}{d\lambda}E(\Omega_{\lambda\alpha})\bigg|_{\lambda=0} = 2\int_{\Gamma}[\phi'_\alpha(\phi(\Omega)-\phi_d)+\nabla\phi'_\alpha\cdot(\nabla\phi(\Omega)-\mathbf{u}_d)]\,d\Gamma$$
$$+\int_{\Gamma}\alpha\left[\frac{\partial}{\partial n}(|\phi(\Omega)-\phi_d|^2+|\nabla\phi(\Omega)-\mathbf{u}_d|^2)\right. \tag{68}$$
$$\left.-\frac{1}{R}(|\phi(\Omega)-\phi_d|^2+|\nabla\phi(\Omega)-\mathbf{u}_d|^2)\right]d\Gamma.$$

The applications of these formulae to the derivation of optimality conditions is left as an exercise.

6.3.2 General linear scalar elliptic operator

Consider the problem

$$\min_{\Omega\in\mathcal{O}} E(\Omega) = \int_{\Omega}|\nabla\phi(\Omega)-\mathbf{u}_d|^2\,dx, \tag{69}$$

where $\phi(\Omega)$ is the solution of

$$-\nabla\cdot\mathbf{A}\nabla\phi + a_0\phi = f \quad \text{in } \Omega, \qquad \phi|_\Gamma = g|_\Gamma \tag{70}$$

with $\Omega\subset\mathbb{R}^n$, $\mathbf{A}$ is an $n\times n$ matrix-valued function on Ω, and a_0, f, g are scalar functions. For (70) to be well-defined we assume ellipticity: $\gamma>0$ and

$$z^t\mathbf{A}(x)z \ge \gamma|z|^2, \qquad a_0(x)\ge 0 \qquad \forall x\in\Omega, \forall z\in\mathbb{R}^n. \tag{71}$$

Theorem 3. *For smooth data, the solution Ω of (69) and (70), if smooth, must satisfy*

$$\frac{d}{d\lambda}E(\Omega_{\alpha\lambda})\bigg|_{\lambda=0} = -\int_{\Gamma}\alpha\left(\frac{\partial\phi}{\partial n}-\frac{\partial g}{\partial n}\right)(2(\nabla\phi-\mathbf{u}_d)-\mathbf{A}^t\nabla p)\cdot\mathbf{n}\,d\Gamma$$
$$+\int_{\Gamma}\alpha|\nabla\phi-\mathbf{u}_d|^2\,d\Gamma\ge 0 \qquad \forall\,\alpha \textit{ compatible with } \mathcal{O}, \tag{72}$$

where p is the solution of

$$-\nabla\cdot\mathbf{A}^t\nabla p + a_0 p = -2\nabla\cdot(\nabla\phi-\mathbf{u}_d) \quad \text{in } \Omega, \qquad p|_\Gamma = 0. \tag{73}$$

PROOF. From (69) and following our usual notation, we have

$$\delta E = \int_{\delta\Omega}|\nabla\Phi-\mathbf{u}_d|^2\,dx + 2\int_{\Omega}\nabla\delta\phi\cdot(\nabla\phi-\mathbf{u}_d)\,dx + o(\|\alpha\|_{C^2}) \tag{74}$$

and when the integrand is continuous, the first integral becomes

$$\int_{\Gamma}\alpha|\nabla\phi-\mathbf{u}_d|^2\,d\Gamma + o(\|\alpha\|_{C^1}). \tag{75}$$

The second integral may be expressed in terms of p by use of Green's formula on (73):

$$2\int_\Omega \nabla\delta\phi(\nabla\phi - \mathbf{u}_d)\,dx = \int_\Omega [(\mathbf{A}^t\nabla p)\cdot\nabla\delta\phi + a_0 p\delta\phi]\,dx$$
$$+\int_\Gamma (2(\nabla\phi - \mathbf{u}_d)\cdot\mathbf{n} - \mathbf{A}^t\nabla p\cdot\mathbf{n})\delta\phi\,d\Gamma \tag{76}$$

provided that $\delta\phi \in H^1(\Omega)$. Now by a derivation similar to that of Proposition 2, we find from (70) that if $\phi|_\Gamma \in C^1$,

$$-\nabla\cdot\mathbf{A}\nabla\delta\phi + a_0\delta\phi = 0 \quad \text{in } \Omega, \qquad \delta\phi|_\Gamma = -\alpha\left(\frac{\partial\phi}{\partial n} - \frac{\partial g}{\partial n}\right)\bigg|_\Gamma + o(\|\alpha\|). \tag{77}$$

By applying Green's formula again, (77) multiplied by p yields

$$\int_\Omega [(\mathbf{A}\nabla\delta\Phi)\cdot\nabla p + a_0\delta\phi p]\,dx = 0 \text{ because } p|_\Gamma = 0. \tag{78}$$

Thus by (78) and (74), (76) becomes

$$2\int_\Omega \nabla\delta\phi\cdot\nabla(\phi - \mathbf{u}_d)\,dx = -\int_\Gamma \alpha(2(\nabla\phi - \mathbf{u}_d) - \mathbf{A}^t\nabla p)\cdot\mathbf{n}$$
$$\times\left(\frac{\partial\phi}{\partial n} - \frac{\partial g}{\partial n}\right)d\Gamma + o(\|\alpha\|); \tag{79}$$

so (75) and (79), substituted in (74), prove (72). □

Remark. When $\mathbf{A} = \mathbf{I}$, $a_0 = 0$, $\mathbf{u}_d = 0$, and $\Delta g = 0$, (73) has an obvious solution since

$$-\Delta p = 2f, \qquad p|_\Gamma = 0; \tag{80}$$

so $p = 2(\phi - g)$. Then (72) becomes

$$E'_\alpha = -\int_\Gamma \alpha\left[2\left(\frac{\partial\phi}{\partial n} - \frac{\partial g}{\partial n}\right)^2 - |\nabla\phi|^2\right]d\Gamma \geq 0 \qquad \forall\,\alpha \text{ admissible.} \tag{81}$$

To make the problem given in (69) and (70) nontrivial, let us take

$$\mathcal{O} = \left\{\Omega : \int_\Omega dx = 1\right\}. \tag{82}$$

Then (81) leads to the free boundary problem

$$-\Delta\phi = f \quad \text{in } \Omega, \qquad \phi|_\Gamma = g|_\Gamma \tag{83}$$
$$\frac{\partial\phi}{\partial n} = 2\frac{\partial g}{\partial n} \pm \sqrt{K + \left(\frac{\partial g}{\partial s}\right)^2 + 3\left(\frac{\partial g}{\partial n}\right)^2} \quad \text{on } \Gamma,$$

where K is a constant determined by (82) (see the proof of Proposition 3 of Chapter 5).

6.3.3 Biharmonic equation

As an example of optimum design on fourth-order systems, consider the problem

$$\min_{\Omega\in\mathcal{O}} E(\Omega) = \int_D |\phi(\Omega) - \phi_d|^2 \, dx,$$

where $\phi(\Omega)$ is the solution of

$$\Delta^2\phi = f \quad \text{in } \Omega, \qquad \phi|_\Gamma = 0, \qquad \left.\frac{\partial\phi}{\partial n}\right|_\Gamma = 0. \tag{84}$$

As usual, the data are assumed to be smooth enough to imply continuity of integrands and functions as needed. Calling $\delta\phi$ the variation of ϕ due to the variation of Ω, we have, by (84),

$$\Delta^2\delta\phi = 0 \quad \text{in } \Omega, \qquad \delta\phi|_\Gamma = -\alpha\left.\frac{\partial\phi}{\partial n}\right|_\Gamma = 0. \tag{85}$$

The additional condition needed is obtained in a similar way. Since (84) also implies that $\nabla\phi = 0$ on Γ, we have

$$\begin{aligned}[\nabla\phi(\Omega_\alpha) - \nabla\phi(\Omega)]|_{x+\alpha n} &= -\nabla\phi(\Omega)(x+\alpha n)\\ &= -\nabla\phi(\Omega)(x) - \alpha\frac{\partial}{\partial n}\nabla\phi(\Omega)(x) + o(\|\alpha\|);\end{aligned} \tag{86}$$

Thus,

$$\left.\frac{\partial\delta\phi}{\partial n}\right|_\Gamma = -\alpha\frac{\partial^2\phi}{\partial n^2} + o(\|\alpha\|). \tag{87}$$

Then we proceed as before

$$\delta E = 2\int_D \delta\phi(\phi - \phi_d)\, dx + o(\|\alpha\|); \tag{88}$$

and we introduce $p \in H_0^2(\Omega)$ such that

$$\Delta^2 p = 2\chi_D(\phi - \phi_d) \quad \text{in } \Omega, \qquad p|_\Gamma = \left.\frac{\partial p}{\partial n}\right|_\Gamma = 0. \tag{89}$$

We find that

$$\begin{aligned}\delta E = \int_\Omega (\Delta^2 p)\delta\phi\, dx &= \int_\Omega \Delta p\, \Delta\delta\phi\, dx + \int_\Gamma \frac{\partial}{\partial n}(\Delta p)\delta\phi\, d\Gamma\\ &\quad - \int_\Gamma \Delta p \frac{\partial\delta\phi}{\partial n}\, d\Gamma + o(\|\alpha\|).\end{aligned} \tag{90}$$

Hence,

$$\frac{d}{d\lambda} E(\Omega_{\lambda\alpha})|_{\lambda=0} = -\int_\Gamma \alpha\left[\frac{\partial \Delta p}{\partial n}\frac{\partial \phi}{\partial n} - \Delta p \frac{\partial^2 \Phi}{\partial n^2}\right] d\Gamma. \tag{91}$$

6.3.4 Stokes problem

Consider the minimum drag problem described in Chapter 2:

$$\min_{\Omega\in\mathcal{O}} E(\Omega) = \int_\Omega |\nabla \mathbf{u} + \nabla \mathbf{u}^t|^2\, dx = \int_\Omega (u_{i,j} + u_{j,i})(u_{i,j} + u_{j,i})\, dx, \tag{92}$$

where $\mathbf{u}$ is the solution of

$$-\Delta \mathbf{u} + \nabla p = 0 \quad \text{in } \Omega, \qquad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega, \qquad \mathbf{u}|_{\Gamma_\infty} = \mathbf{u}_\infty, \qquad \mathbf{u}|_S = 0. \tag{93}$$

where $\Gamma = \Gamma_\infty \cup S$, $\Gamma_\infty = \partial C$, and

$$\mathcal{O} = \left\{\Omega \text{ open set of } \mathbb{R}^3 : \int_\Omega dx = a,\ \Omega = C - \overline{\mathring{S}}\right\}. \tag{94}$$

Theorem 4. *If the solution of (92) to (94) is smooth, and if $\mathbf{u}_\infty$ is constant, the solution satisfies*

$$\left|\frac{\partial \mathbf{u}}{\partial n}\right|\Bigg|_\Gamma = K \tag{95}$$

for some constant K because

$$\frac{d}{d\lambda} E(\Omega_{\lambda\alpha})\Bigg|_{\lambda=0} = -2\int_\Gamma \left|\frac{\partial \mathbf{u}}{\partial n}\right|^2 \alpha\, d\Gamma. \tag{96}$$

PROOF. As before, let $\delta E, \delta\mathbf{u}, \delta p, \delta\Omega$ be the variations of these variables when Ω is mapped into Ω_α [see (11) for definition of $\delta\Omega$]. From (92)

$$\delta E = \int_{\delta\Omega} |\nabla \mathbf{u} + \nabla \mathbf{u}^t|^2\, dx + 2\int_\Omega [\nabla \delta\mathbf{u}(\nabla \mathbf{u} + \nabla \mathbf{u}^t) + \nabla \delta \mathbf{u}^t \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^t)]\, dx$$
$$+ o(\|\delta \mathbf{u}\|_{H^1}) + o(\|\alpha\|); \tag{97}$$

when $\delta\Omega$ is smooth and $\nabla \mathbf{u}$ is continuous (see [38]), the first integral becomes

$$\int_\Gamma \alpha |\nabla \mathbf{u} + \nabla \mathbf{u}^t|^2\, d\Gamma + o(\|\alpha\|_{C^2}) = 2\int_\Gamma \alpha \left|\frac{\partial \mathbf{u}}{\partial n}\right|^2 d\Gamma + o(\|\alpha\|_{C^2}) \tag{98}$$

(because $\mathbf{u}|_\Gamma = 0$). From (93), we have

$$-\Delta \delta\mathbf{u} + \nabla \delta p = 0 \quad \text{in } \Omega, \qquad \nabla \cdot \delta \mathbf{u} = 0 \quad \text{in } \Omega, \qquad \delta\mathbf{u}|_{\Gamma_\infty} = 0,$$
$$\delta \mathbf{u}|_S = -\alpha \frac{\partial \mathbf{u}}{\partial n}\bigg|_S + o(\|\alpha\|). \tag{99}$$

We also have

$$\int_\Omega \nabla\delta\mathbf{u}\,\nabla\mathbf{u}^t\,dx = \int_\Omega \delta u_{i,j}u_{j,i}\,dx = -\int_\Omega \delta u_i u_{j,ij} + \int_\Gamma \delta u_i u_{j,i}\cos(n,x_j)\,d\Gamma$$
$$= \int_\Gamma \left(\delta u_n \frac{\partial u_n}{\partial n} + \delta u_s \frac{\partial u_n}{\partial s}\right) d\Gamma = 0 \tag{100}$$

and

$$\int_\Omega \nabla\delta\mathbf{u}\,\nabla\mathbf{u}\,dx = \int_\Omega -(\Delta\mathbf{u})\delta\mathbf{u}\,dx + \int_\Gamma \frac{\partial\mathbf{u}}{\partial n}\delta\mathbf{u}\,d\Gamma$$
$$= \int_\Omega p\nabla\cdot\delta\mathbf{u}\,dx - \int_\Gamma p\delta\mathbf{u}\cdot\mathbf{n}\,d\Gamma + \int_\Gamma \frac{\partial\mathbf{u}}{\partial n}\delta\mathbf{u}\,d\Gamma. \tag{101}$$

Therefore,

$$2\int_\Omega (\nabla\delta\mathbf{u} + \nabla\delta\mathbf{u}^t)(\nabla\mathbf{u} + \nabla\mathbf{u}^t)\,dx = 4\int_\Gamma \left(\frac{\partial\mathbf{u}}{\partial n} - p\mathbf{n}\right)\delta\mathbf{u}\,d\Gamma$$
$$= 4\int_\Gamma \alpha\left(\frac{\partial\mathbf{u}}{\partial n} - p\mathbf{n}\right)\frac{\partial\mathbf{u}}{\partial n}\,d\Gamma + o(\|\alpha\|), \tag{102}$$

which simplifies further since $\mathbf{n}\cdot\partial\mathbf{u}/\partial n = -\partial u_s/\partial s = 0$. Finally,

$$\delta E = -2\int_S \alpha\left|\frac{\partial\mathbf{u}}{\partial n}\right|^2 d\Gamma + o(\|\alpha\|). \tag{103}$$

This proves (96). To get (95), we write that δE is positive for all α such that

$$\int_\Gamma \alpha\,d\Gamma = o(\|\alpha\|). \tag{104}$$

This is the condition by which $\Omega \in \mathcal{O}$ implies $\Omega_\alpha \in \mathcal{O}$. □

Computation of S: Lighthill (in [53]) proved that (93) to (95) imply that a conical shape is obtained for the leading and trailing edges of the solution if the cone is symmetric to the axis and the angle of the cone must be 120°.

The ellipsoid of minimum drag E^* is known (see [33]); thus by using one iteration only of the method of steepest descent with a fixed step size and an initial optimal ellipsoid, we can obtain a very good approximation for the solution S^* (see Figure 6.2):

$$S^* = \{x + \alpha(x)n(x) : x \in E^*\} \tag{105}$$

$$\alpha(x) = \rho\left[\left|\frac{\partial\mathbf{u}}{\partial n}(E^*)(x)\right|^2 - \frac{\int_{E^*}\left|\frac{\partial\mathbf{u}}{\partial n}(E^*)\right|^2 d\Gamma}{\int_{E^*} d\Gamma}\right]. \tag{106}$$

This result has been confirmed by Bourot [10].

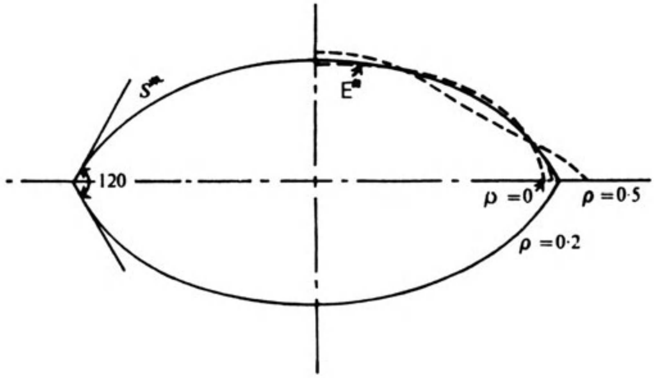


Fig. 6.2 Minimum drag profile in Stokes flow S^*. $E^*(\rho = 0)$ is the minimum drag ellipsoid revolution.

6.3.5 Navier–Stokes equation

As an example of a nonlinear system we may also examine the minimum drag problem when the fluid is described by the Navier–Stokes equation:

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_\Omega |\nabla \mathbf{u}(\Omega) + \nabla \mathbf{u}^t(\Omega)|^2 \, dx, \tag{107}$$

where $\mathbf{u}$ is the solution of

$$-\nu \, \Delta \mathbf{u} + \mathbf{u}\nabla \mathbf{u} + \nabla p = 0 \quad \text{in } \Omega, \qquad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega,$$
$$\mathbf{u}|_{\Gamma_\infty} = \mathbf{u}_\infty, \qquad \mathbf{u}|_S = 0. \tag{108}$$

It is not difficult to establish the problem statement that

$$\frac{d}{d\lambda} E(\Omega_{\lambda\alpha})\bigg|_{\lambda=0} = -\int_S \alpha \left[\left(\frac{\partial \mathbf{u}}{\partial n}\right)^2 - \frac{\partial \mathbf{u}}{\partial n}\frac{\partial \mathbf{P}}{\partial n}\right] d\Gamma, \tag{109}$$

where $\{\mathbf{P}, q\}$ is the solution of

$$-\nu\Delta P_i - \mathbf{u}\nabla P_i - \mathbf{u} \cdot \frac{\partial \mathbf{P}}{\partial x_i} + (\nabla q)_i = -\nu\Delta \mathbf{u}_i, \qquad \nabla \cdot \mathbf{P} = 0 \quad \text{in } \Omega, \qquad \mathbf{P}|_\Gamma = 0. \tag{110}$$

However, the mathematical justification becomes difficult for the following reasons:

- Equation (108) must have a unique solution that is continuously differentiable on Γ.
- Equation (110) must also have the same property.
- The solutions also must be shown to converge strongly in H^1 when $\lambda \to 0$.

The derivation of (109) is left as an exercise; its justification can be found in [55].

Computations of the optimal shape were attempted in [30] by use of the boundary layer properties of (108); the results are shown in Figure 6.3.

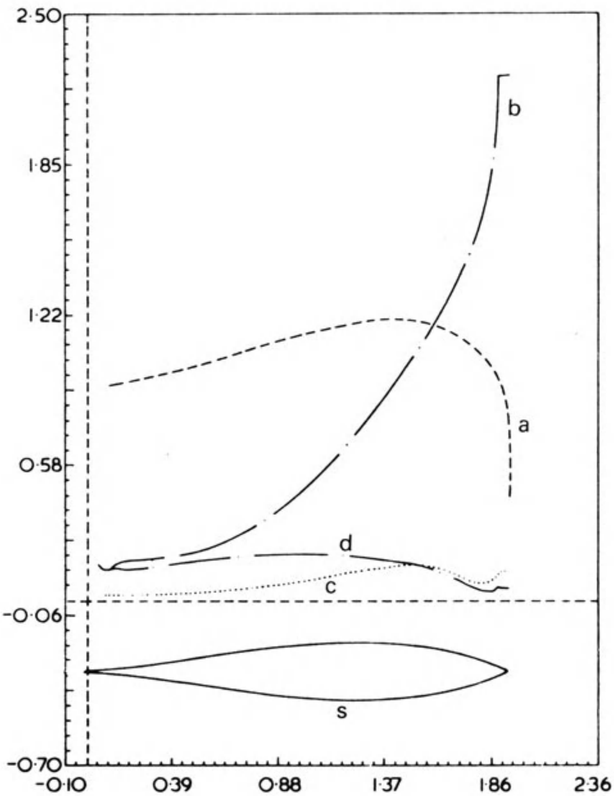


Fig. 6.3 Minimum drag profile (at given volume) in laminar flow S. The curves are (a) $\mathbf{U}_s$ at the top of the boundary layer, (b) $\partial \mathbf{u}_s/\partial \mathbf{n}$, (d) $\partial \mathbf{P}/\partial \mathbf{n} - \partial \mathbf{u}/\partial \mathbf{n}$, and (c) $(\partial \mathbf{u}/\partial \mathbf{n})(\partial \mathbf{P}/\partial \mathbf{n} - \partial \mathbf{u}/\partial \mathbf{n})$.

6.3.6 Shape design with eigenvalues in the criteria

Many problems of structure optimization involve a criteria that depends on the first or second eigenvalue (vibration modes, for example). Consider the problem model

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \lambda_2(\Omega), \tag{111}$$

where $\lambda_2(\Omega)$ is the second eigenvalue of the Dirichlet problem

$$-\Delta\phi = \lambda_2 \phi \quad \text{in } \Omega, \qquad \phi|_\Gamma = 0; \tag{112}$$

with the normalization

$$|\phi|_0^2 = 1, \qquad \phi \geq 0, \tag{113}$$

the eigenfunction ϕ is unique. (If it is the first eigenvalue, then there is a simpler method since $\lambda_1 = \min_{\phi \in H_0^1(\Omega)} \{|\nabla\phi|^2 : |\phi|_0^2 = 1\}$.

Proposition. *If $\Gamma \in C^3$, $\alpha \in C^2$, then λ, ϕ are Γ-differentiable, and letting $\lambda'_{2\alpha}, \phi'_\alpha$ denote, as usual, $d\phi(\Omega\rho\alpha)/d\rho$ and $d\lambda_2(\Omega\rho\alpha)/d\rho$ at $\rho = 0$, we have*

$$\lambda'_{2\alpha} = -\int_\Gamma \left(\frac{\partial\phi}{\partial n}\right)^2 d\Gamma,$$

$$-\Delta\phi'_\alpha = \lambda_2\phi'_\alpha + \lambda'_{2\alpha}\phi \quad \textit{in } \Omega, \qquad \phi'_\alpha|_\Gamma = -\alpha \frac{\partial\phi}{\partial n}\bigg|_\Gamma. \tag{114}$$

PROOF. As usual, Ω_α is the domain of the boundary

$$\Gamma_\alpha = \{x + \alpha(x)n(x) : x \in \Gamma\}, \tag{115}$$

and the hypothesis implies that $\phi(\Omega_\alpha)$ and $\phi(\Omega)$ are C^1; so as before (see Proposition 1),

$$\phi'_\alpha|_\Gamma = -\alpha \frac{\partial\phi}{\partial n}\bigg|_\Gamma. \tag{116}$$

Now by differentiating (112), we find that if the derivatives exist, they satisfy

$$-\Delta\phi'_\alpha = \lambda_2\phi'_\alpha + \lambda'_{2\alpha}\phi \quad \text{in } \Omega, \tag{117}$$

and from (113)

$$\int_\Omega \phi'_\alpha\phi \, dx = 0. \tag{118}$$

To compute $\lambda'_{2\alpha}$, we multiply (117) by ϕ and integrate:

$$\begin{aligned} \lambda'_{2\alpha} &= -\int_\Omega \Delta\phi'_\alpha\phi \, dx - \lambda_2 \int_\Omega \phi'_\alpha\phi \, dx = -\int_\Omega \Delta\phi'_\alpha\phi \, dx \\ &= -\int_\Omega \phi'_\alpha\Delta\phi \, dx + \int_\Gamma \phi'_\alpha \frac{\partial\phi}{\partial n} d\Gamma \end{aligned} \tag{119}$$

(the last equality is Green's formula). Thus from (112) and (116), we obtain (114). The Γ-differentiability is as usual. □

Corollary.

$$E(\Omega_\alpha) - E(\Omega) = -\int_\Gamma \alpha\left(\frac{\partial\phi}{\partial n}\right)^2 d\Gamma + o(\|\alpha\|_{C^2}). \tag{120}$$

For further details about the control of multiple eigenvalues the reader is referred to [49] and to [67].

CHAPTER 7

Discretization with Finite Elements

7.1 Introduction

Here we deal with the numerical solution of optimum design problems using computers. Of the three numerical methods for solving elliptic partial differential equations, the finite element method (FEM) is the obvious one to choose to use when the domains are the unknowns. We see that the FEM yields much simpler gradients than either the finite difference method or the boundary element method; these two methods are presented in Chapter 8. The FEM is presented first for a Neumann problem. Two other cases, a Dirichlet problem and a transmission problem, are treated.

7.2 Neumann Problem

7.2.1 Position of problem

The problem we use to illustrate the method is

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_D |\nabla\Phi - \mathbf{u}_d|^2 \, dx, \tag{1}$$

where Φ is the solution of

$$-\Delta\Phi + a\Phi = f \quad \text{in } \Omega, \qquad \left.\frac{\partial\Phi}{\partial\mathbf{n}}\right|_\Gamma = 0 \tag{2}$$

and

$$\mathcal{O} = \{\Omega \text{ open set of } \mathbb{R}^n : D \subset \Omega \subset C\}. \tag{3}$$

To establish the existence and uniqueness of Φ by (2), for all Ω we assume that $a \geq 0$ and

$$a > 0 \quad \text{or} \quad \left(\operatorname{supp} f \subset D \quad \text{and} \quad \int_D f \, dx = 0\right), \tag{4}$$

$$f \in L^2(\Omega),\ \mathbf{u}_d \in L^2(\Omega)^n,\ \mathbb{C} \text{ bounded.} \tag{5}$$

We recall that by Theorem 5 of Chapter 3, when $\mathcal{O}$ is replaced by

$$\mathcal{O}^\varepsilon = \{\Omega \in \mathcal{O} : \Omega \text{ has the } \varepsilon\text{-cone property}\}, \tag{6}$$

the problem in (1), (2), and (6) has a solution Ω^ε; whether Ω^ε tends to a solution of

(1) to (3) when $\varepsilon \to 0$ is known only in certain cases. From the numerical point of view (6) is not really a restriction; indeed, if it does not hold, the boundary Γ is too complicated to be approximated numerically.

7.2.2 Discretization

In variation form (2) becomes

$$\int_{\Omega} (\nabla\Phi \cdot \nabla w + a\Phi w - fw)\, dx = 0 \qquad \forall\, w \in H^1(\Omega), \qquad \Phi \in H^1(\Omega). \tag{7}$$

Let $\mathscr{T}_h = \{T_k\}_1^M$ be a triangulation of Ω such that

- T_k = triangle or tetrahedron, $\quad \cup\, T_k = \Omega_h \subset \Omega$. (8)
- Vertices of $\Gamma_h \in \Gamma$; corners of Γ = vertex of Γ_h. (9)
- $T_k \cap T_l = \varnothing$, a vertex, a full side (or face), or T_k. (10)

The parameter h is the size of the largest side or edge, and we assume that we have a family of triangulations $\mathscr{T}_h$ with properties (8) to (10) such that no angle tends to 0 or π when $h \to 0$. Let P^m be the space of polynomials of degree m on Ω, and let us denote by

$$H_h^m = \{w_h \in C^\circ(\Omega_h) : w_h|_{T_k} \in P^m \qquad \forall\, T_k \in \mathscr{T}_h\} \tag{11}$$

the space of continuous piecewise polynomial functions on Ω_h.

It is well-known (see [20], for example, and Chapter 1) that H_h^m is of finite dimension; so the problem

$$\int_{\Omega_h} (\nabla\Phi_h \cdot \nabla w_h + a\Phi_h w_h - f w_h)\, dx = 0 \qquad \forall\, w_h \in H_h^m,\ \Phi_h \in H_h^m, \tag{12}$$

reduces to the solution of a linear symmetric positive definite system plus the numerical computation of some integrals. More precisely, if $\{w^i\}_1^N$ is a basis for H_h^m, (12) is equivalent to

$$\mathbf{A}\Phi = F, \tag{13}$$

where

$$A_{ij} = \int_{\Omega_h} \nabla w^i \cdot \nabla w^j + a w^i w^j\, dx; \qquad F_i = \int_{\Omega_h} f w^i\, dx; \tag{14}$$

$$\Phi^h = \sum_1^N \Phi_i w^i \tag{15}$$

The $\{w^i\}$ are polynomials of degree $\leq m$ on T_k; so A_{ij} can be computed exactly. To approximate F_i, one possibility is to define

$$F_i = \int_{\Omega_h} f_h w^i\, dx, \tag{16}$$

where $f_h \in H_h^m$, $f_h \simeq f$. In the case $m = 1$ (conforming finite element method of degree 1), if $\{q^j\}_1^{N'}$ denote the vertices of $\mathscr{T}_h$, $\{w^i\}$ are uniquely determined by

$$w^i(q^j) = \delta_{ij} \qquad \forall\, i, j = 1, \dots N'; N = N'. \tag{17}$$

In the case $m = 2$, if $\{q^{jk}\}$ denote the middles of the sides of vertices $\{q^j, q^k\}$. w_i is uniquely determined by

$$w^i(q^j) = \delta_{\mathbf{ij}} \qquad \forall\, \mathbf{i}, \mathbf{j} = \{1, \dots, N'\} \cup (\{1, \dots, N'\} \times \{1, \dots, N'\}). \tag{18}$$

If $\{\lambda_i(x)\}_0^n$ are the barycentric coordinates of $x \in T_k$,

$$x \in T_k \Rightarrow x = \sum_{0, \dots, n} \lambda_i q^{k_i}, \qquad \lambda_i \geq 0, \sum_{0, \dots, n} \lambda_i = 1,$$

where $\{q^{k_i}\}_0^n$ are the vertices of T_k, then (17) gives

$$w^i(x) = \lambda_i(x) \qquad \forall\, x \in T_k, \tag{19}$$

whereas (18) gives

$$w^{\mathbf{i}}(x) = \begin{cases} -\lambda_i(x)(1 - 2\lambda_i(x)) & \text{if } \mathbf{i} = i \in 1, \dots, N', \quad (20) \\ 4\lambda_i(x)\lambda_j(x) & \text{if } \mathbf{i} = \{i, j\} \in \{1, \dots, N'\} \times \{1, \dots, N'\}. \quad (21) \end{cases}$$

Obviously, (1) may be approximated by

$$\min_{\Omega_h \in \mathcal{O}_h} E(\Omega_h) = \int_{D_h} |\nabla \Phi_h - \mathbf{u}_h|^2 \, dx, \tag{22}$$

where u_h is an approximation of $\mathbf{u}_d$ such that

$$\mathbf{u}_h|_{T_k} \in P^{m-1} \qquad \forall\, T_k \in \mathscr{T}_h \tag{23}$$

and

$$\mathcal{O}_h = \{\Omega_h = \cup T_k : D_h \subset \Omega_h \subset \mathbb{C}_h \qquad \forall\, \mathscr{T}_h\}, \tag{24}$$

where D_h and $\mathbb{C}_h$ are approximations of D and $\mathbb{C}$ created by the unions of the elements of $\mathscr{T}_h$.

Remark. Note that the real degrees of freedom for optimization are the coordinates of the vertices of $\mathscr{T}_h$. Even though only the boundary nodes are of interest, the interior nodes must also be moved to keep $\mathscr{T}_h$ regular.

Proposition 1. *If $\mathcal{O}_h \neq \varnothing$, the discrete problem in (12), (22), and (24) has a solution.*

PROOF. The criteria are continuous functions, bounded from below, of the coordinates of the vertices of $\mathscr{T}_h$: and $\mathcal{O}_h$ is closed. □

7.2.3 Computation of gradients: $\mathbf{P}^1$ element

Now consider the calculation of the derivatives of E with respect to the coordinates of the vertices $\{q^i\}_1^N$ of $\mathscr{T}_h$. For clarity, we begin with the case $m = 1$ in (11).

Proposition 2. *Let T'_j be the element obtained from $T_j \in \mathcal{T}_h$ by translating one of its vertices q^k into $q^k + \delta q^k$. Let $w^i(\cdot)$ be the basis function associated with the vertex $q^i \in T_j$ [see (17)]. Similarly, let $w'^i(\cdot)$ be the same basis function when q^k is replaced by $q^k + \delta q^k$.* Then

$$w'^i(x) - w^i(x) = -w^k(x)\nabla w^i(q^k)\cdot \delta q^k + o(|\delta q^k|) \qquad \forall x \in T_j \cap T'_j,$$
$$\forall q^i, q^k \text{ vertices of } T_j. \quad (25)$$

PROOF. Let $\{q^{r_l}\}_0^n$ be the vertices of T_j, and since $q^i, q^k \in T_j$, we assume that $r_0 = k, r_1 = i$. By (17), we have

$$w^i(q^{r_l}) = \delta_{r_l,i}, \qquad l = 0,\dots,n. \quad (26)$$

By differentiating,

$$\delta w^i(q^{r_l}) + \delta_{r_l k}\nabla w^i(q^k)\cdot \delta q^k = o(|\delta q^k|), \qquad l = 0,\dots,n, \quad (27)$$

which can be rewritten as

$$-\frac{1}{\nabla w^i(q^k)\cdot \delta q^k}\,\delta w^i(q^{r_l}) = \delta_{r_l,k} + o(|\delta q^k|), \qquad l = 0,\dots,n. \quad (28)$$

If we compare (28) with (26), we find that

$$-\frac{1}{\nabla w^i(q^k)\cdot \delta q^k}\,\delta w^i(\cdot) = w^k(\cdot) + o(|\delta q^k|) \quad \text{on } T_j \quad (29)$$

because (26) defines w^i uniquely on T_j. □

Proposition 3. *Let g be a continuously differentiable function on T_j. Let T'_j be obtained from T_j by translating q^k into $q^k + \delta q^k$. Then*

$$\int_{T'_j - T_j \cap T'_j} g\,dx - \int_{T_j - T'_j \cap T_j} g\,dx = \int_{T_j} \delta q^k \cdot \nabla(g w^k)\,dx + o(|\delta q^k|) \quad (30)$$

PROOF. Let $\delta q(\cdot)$ be the piecewise linear continuous vector-valued function that equals δq^k at q^k and 0 at all other vertices of $\mathcal{T}_h$. Then by the mean value theorem for integrals (see Figure 7.1)

$$\int_{T'_j - T_j \cap T'_j} g\,dx = \int_{(\partial T_j)\cap\{x:\delta q\cdot n>0\}} g(x)\,\delta q(x)\cdot n(x)\,d\Gamma(x) + o(|\delta q^k|), \quad (31)$$

$$\int_{T_j - T_j \cap T'_j} g\,dx = \int_{(\partial T_j)\cap\{x:\delta q\cdot n<0\}} g(x)|\delta q(x)\cdot n(x)|\,d\Gamma(x) + o(|\delta q^k|). \quad (32)$$

From the divergence theorem, we have

$$\int_{\partial T_j} g\,\delta q\cdot n\,d\Gamma = \int_{T_j} \nabla\cdot(g\delta q)\,dx, \quad (33)$$

and by definition of $\delta q(\cdot)$, we have

$$\delta q(x) = w^k(x)\,\delta q^k \qquad \forall x \in \Omega. \quad (34)$$

□

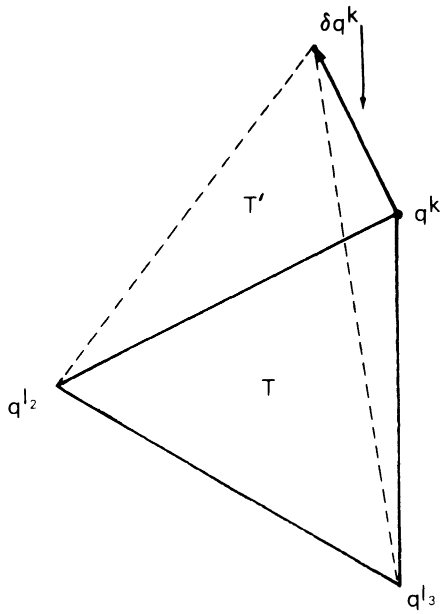


Fig. 7.1 Deformation of the triangle T into T' when q^k moves to $q^k + \delta q^k$.

Theorem 1. *Assume a, f continuous on Ω_h. Let Φ_h, Φ'_h be the solutions of (12) with $\mathscr{T}_h$ and $\mathscr{T}'_h$, respectively, where $\mathscr{T}'_h$ is obtained from $\mathscr{T}_h$ by moving vertex q^k to $q^k + \delta q^k$. Let $\delta\tilde{\Phi}_h \in H^1_h$ be the solution of*

$$\begin{aligned}\int_{\Omega_h} (\nabla\delta\tilde{\Phi}_h \cdot \nabla w_h + a\,\delta\tilde{\Phi}_h w_h)\,dx = &-\int_{\Omega_h} \{\delta q^k \cdot \nabla\big(w^k w_h(a\Phi_h - f)\big) \\ &+ \delta q^k \cdot \nabla w^k \nabla\Phi_h \cdot \nabla w_h\}\,dx \\ &+ \int_{\Omega_h} \{(\nabla w^k \nabla w_h + a w^k w_h)\nabla\Phi_h \cdot \delta q^k \\ &+ \big(\nabla\Phi_h \nabla w^k + (a\Phi_h - f)w^k\big)\nabla w_h \cdot \delta q^k\}\,dx \\ &\forall w \in H^1_h. \quad (35)\end{aligned}$$

Then

$$\|\Phi'_h - \Phi_h - \delta\tilde{\Phi}_h + w^k\nabla\Phi_h \cdot \delta q^k\|_{H^1} = o(|\delta q^k|) \tag{36}$$

(*the derivatives are evaluated to be pointwise* (*no Dirac masses*)).

PROOF. By (15) and (25)

$$\begin{aligned}\delta\Phi_h &= \sum \delta\Phi_i w^i + \Phi_i\,\delta w^i + \delta\Phi_i\,\delta w^i \\ &= \sum \delta\Phi_i w^i - w^k\nabla w^i \cdot \delta q^k \Phi_i + \delta\Phi_i\,\delta w^i + o(\delta q^k) \\ &= \delta\tilde{\Phi}_h - w^k\nabla\Phi_h\,\delta q^k + \delta\Phi_i\,\delta w^i + o(\delta q^k),\end{aligned} \tag{37}$$

where

$$\delta\tilde{\Phi}_h = \sum \delta\Phi_i w^i. \tag{38}$$

Note that $\delta\Phi_h \notin H_h^1$, but $\delta\tilde{\Phi}_h \in H_h^1$. Equation (12), which defines $\Phi_h \in H_h^1$, can also be written as

$$\sum_{T_j \in T_h} \int_{T_j} (\nabla\Phi_h \cdot \nabla w_h + a\Phi_h w_h - f w_h)\, dx = 0 \qquad \forall\, w_h \in H_h^1.$$

Similarly, the definition of $\Phi'_h \in H_h^{1\prime}$ (built with $\mathscr{T}'_h$) is

$$\sum_{T'_j \in \mathscr{T}_h} \int_{T'_j} (\nabla\Phi'_h \cdot \nabla w'_h + a\Phi'_h w'_h - f w'_h)\, dx = 0 \qquad \forall\, w'_h \in H_h^{1\prime} \tag{39}$$

By subtracting, we find

$$\begin{aligned}
&\sum_j \int_{T'_j \cap T_j} (\nabla\delta\Phi_h \cdot \nabla w_h + a\,\delta\Phi_h w_h + \nabla\Phi_h \cdot \nabla\delta w_h + (a\Phi_h - f)\,\delta w_h)\, dx \\
&\quad + \sum_j \int_{T'_j - T_j \cap T'_j} (\nabla\Phi'_h \cdot \nabla w'_h + a\Phi'_h w'_h - f w'_h)\, dx \\
&\quad - \sum_j \int_{T_j - T'_j T'_j} (\nabla\Phi_h \cdot \nabla w_h + a\Phi_h w_h - f w_h)\, dx = \text{higher-order terms,}
\end{aligned} \tag{40}$$

where $\delta\Phi_h$ is given by (37) and $\delta w_h = w'_h - w_h$. The higher-order terms are products of two of the terms on the left-hand side of (40). Now we use (30) to express the last two sums in terms of the δq^k and from (25), we have an expression for δw_h, namely,

$$\delta w_h = -w^k \nabla w_h \cdot \delta q^k + o(|\delta q^k|). \tag{41}$$

The difference between T_j and $T'_j \cap T_j$ is small; thus we obtain

$$\begin{aligned}
&\int_{\Omega_h} \nabla\delta\Phi_h \cdot \nabla w_h + a\,\delta\Phi_h w_h\, dx \\
&\quad - \int_{\Omega_h} \nabla\Phi_h \cdot \nabla(w^k \nabla w_h \cdot \delta q^k) + (a\Phi_h - f) w^k \nabla w_h \cdot \delta q^k\, dx \\
&\quad + \sum_j \int_{T_j} \delta q^k \cdot \nabla(w^k[\nabla\Phi_h \cdot \nabla w_h + a\Phi_h w_h - f w_h])\, dx = \text{higher-order terms.}
\end{aligned} \tag{42}$$

Now we make use of (37); after simplifying, (35) is obtained. The higher-order terms in (42) are, as usual, o in δq^k, or terms of order $\delta\Phi_h\, \delta q^k$. Thus taking (42) as a definition of $\delta\Phi_h$ yields

$$\|\delta\Phi_h\|_{H^1} \le C|\delta q^k|, \tag{43}$$

which, in turn, yields (36). □

Theorem 2. *If E is given by (22), (12), and (11) with $m = 1$, then*

$$\frac{\partial E}{\partial q_l^k} = -\int_{\Omega_h} \frac{\partial}{\partial x_l} \{w^k(\nabla\Phi_h \cdot \nabla p_h + (a\Phi_h - f)\, p_h)\}\, dx$$
$$+ \int_{\Omega_h} \Bigg[(\nabla w^k \cdot \nabla p_h + a w^k p_h) \frac{\partial \Phi_h}{\partial x_l}$$
$$+ \big(\nabla\Phi_h \cdot \nabla w^k + (a\Phi_h - f) w^k\big) \frac{\partial p_h}{\partial x_l} \Bigg] dx \qquad \forall\, q^k \notin D_h,\ l = 1, \ldots, n, \tag{44}$$

where p_h is the solution of

$$\int_{\Omega_h} (\nabla p_h \cdot \nabla w_h + a p_h w_h)\, dx = 2 \int_{D_h} (\nabla\Phi_h - u_h) \cdot \nabla w_h\, dx$$
$$\forall\, w_h \in H_h^1,\ p_h \in H_h^1. \tag{45}$$

Proof. From (22), we have

$$\frac{\partial E}{\partial q_l^k} = \int_{D_h} 2(\nabla\Phi_h - \mathbf{u}_h) \cdot \nabla\left(\frac{\partial \Phi_h}{\partial q_l^k}\right) dx. \tag{46}$$

From (35),

$$\int_\Omega \left(\nabla \frac{\partial\Phi_h}{\partial q_l^k} \cdot \nabla w_h + a \frac{\partial \Phi_h}{\partial q_l^k} w_h\right) dx$$
$$= -\int_{\Omega_h} \frac{\partial}{\partial x_l} w^k\{(\nabla\Phi_h \cdot \nabla w_h + w_h(a\Phi_h - f))\}\, dx$$
$$+ \int_{\Omega_h} (\nabla w^k \cdot \nabla w_h + a w^k w_h) \frac{\partial \Phi_h}{\partial x_l}\, dx$$
$$+ \int_{\Omega_h} \{\nabla\Phi_h \nabla w^k + (a\Phi_h - f) w^k\} \frac{\partial w_h}{\partial x_l}\, dx \qquad \forall\, w_h \in H_h^1. \tag{47}$$

Therefore, if p_h is the solution of (45), we have

$$\frac{\partial E}{\partial q_l^k} = \int_{\Omega_h} \left(\nabla p_h \cdot \nabla \frac{\partial \Phi_h}{\partial q_l^k} + a \frac{\partial \Phi_h}{\partial q_k^l} p_h\right) dx = -\int_{\Omega_h} p_h \frac{\partial}{\partial x_l} \big(w^k(a\Phi_h - f)\big)\, dx \tag{48}$$
$$+ \int_{\Omega_h} (\nabla w^k \cdot \nabla p_h + a w^k p_h) \frac{\partial \Phi_h}{\partial x_l}\, dx$$
$$+ \int_{\Omega_h} \left(\nabla\Phi_h \cdot \nabla w^k \frac{\partial p_h}{\partial x_l} - \nabla\Phi_h \cdot \nabla p_h \frac{\partial w^k}{\partial x_l}\right) dx. \qquad \square$$

Remark. Another way of writing (44) is

$$E(\Omega_h') - E(\Omega_h) = -\int_{\Omega_h} \{p_h \nabla \cdot [\delta q_h (a\Phi_h - f)] - (\nabla \delta q_h \cdot \nabla \Phi_h) \cdot \nabla p_h$$
$$+ \nabla \Phi_h \cdot \nabla p_h \nabla \cdot \delta q_h \tag{49}$$
$$- (\nabla \delta q_h \cdot \nabla p_h + a \delta q_h p_h) \cdot \nabla \Phi_h\}\, dx + o(\delta q_h),$$

where $\delta q_h \in (H_h^1)^n$,

$$\delta q_h(x) = \Sigma\, \delta q^k w^k(x), \tag{50}$$

and δq^k is zero if $q^k \in D_h$.

7.2.4. Computational algorithms

The solution is found by successive approximations starting from an initial guess Ω_h^o; the algorithm is then developed from the gradient methods described in Chapter 4. However, some precautions must be applied to prevent the triangles of $\mathscr{T}_h$ from becoming flat. There are two possibilities. The simplest, but not always the best, is to put no restrictions on the directions of δq^k but to limit its module (see Figure 7.2). Thus the gradient method becomes as stated below.

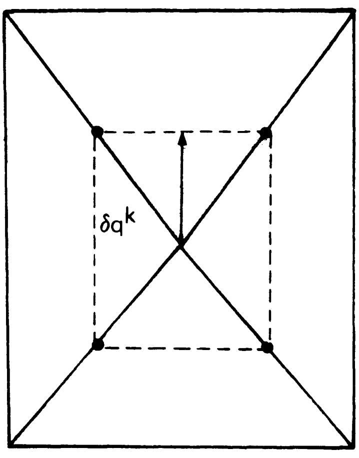


Fig. 7.2 To prevent the triangles from becoming flat, the displacement of the vertices may be limited to the region inside the broken line.

Algorithm 1

[0. Choose Ω_h^0, i.e., $\{q^{k,0}\}$. Choose M, ε

For $m' = 0, \ldots, M$ do

[1. Compute $\Phi_h^{m'}$ by (12) and (11) (with $m = 1$).
[2. Compute $p_h^{m'}$ by (45).

3. Set

$$g_l^k = \int_{\Omega_h} \left[p_h^{m'} \frac{\partial}{\partial x_l} w^k (a\Phi_h^{m'} - f) - (\nabla w^k \cdot \nabla p_h^{m'} + a w^k p_h^{m'}) \frac{\partial \Phi_h^{m'}}{\partial x_l} - \nabla \Phi_h^{m'} \cdot \nabla w^k \frac{\partial p_h^{m'}}{\partial x_l} + \nabla \Phi_h^{m'} \cdot \nabla p_h^{m'} \frac{\partial w^k}{\partial x_l} \right] dx, \qquad l = 1, \dots, n, \qquad \forall q^k \notin D_h; \tag{51}$$

$g_l^k = 0$ else.

4. Let $q^{k,m'}(\rho) = q^{k,m'} + \rho g^k$; compute $\rho_{\max}$ the maximum allowable ρ (see Figure 7.2); compute $\rho^{m'}$ an approximation of

$$\operatorname*{arg\,min}_{0 < \rho < \rho_{\max}} E(\{q^{k,m'}(\rho)\}), \tag{52}$$

where E is given by (22) and (12).

5. Set $q^{k,m'+1} = q^{k,m'}(\rho^{m'})$; if $\sum (g_l^k)^2 < \varepsilon$, stop. (53)

Convergence: As stated, Algorithm 1 could still generate triangulations with flat triangles in the limit case. One way out of this difficulty is to choose a minimum angle beyond which the triangles are not to be flattened. Equivalently, a $\rho_{\min}$, is chosen with $\rho_{\max} < \rho_{\min}$, one sets $g_l^k = 0$ on all k, l that tend to violate this condition. Then Algorithm 1 converges in the usual sense for the optimization algorithms; that is, all accumulations points, when $M \to +\infty$, satisfy the optimality conditions:

$$-\int_\Omega [p_h \nabla \cdot (\delta q_h (a\Phi_h - f)) - (\nabla p_h \cdot \nabla \delta q_h + a \delta q_h \cdot p_h) \nabla \Phi_h - (\nabla \delta q_h \cdot \nabla \Phi_h) \cdot \nabla p_h$$

$$\nabla p_h + \nabla \Phi_h \cdot \nabla p_h \nabla \cdot \delta q_h] \, dx \geq 0 \qquad \forall \delta q_h \text{ allowable.} \tag{54}$$

The difficulty with this method is that optimal triangulations in the sense of E minimized, Γ_h fixed, may be quite impossible from the engineering point of view, as shown in Figure 7.3.

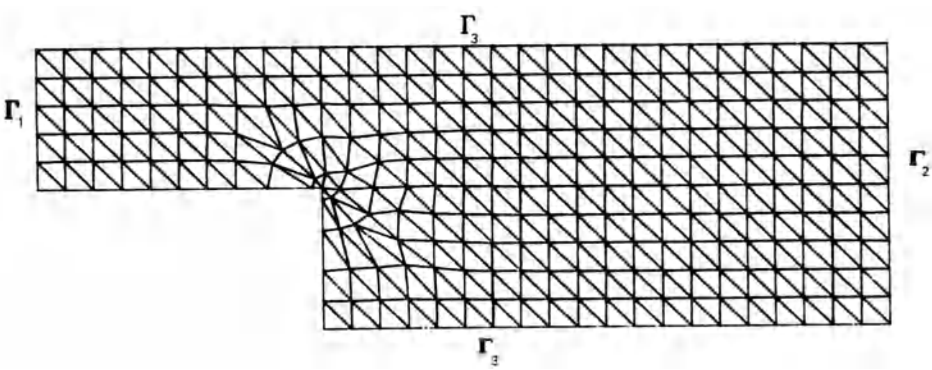


Fig. 7.3 An optimal triangulation in the sense that $|\nabla \Phi_h|_0$ is minimum (From R. Glowinski, Stanford report STAN-CS-79-720; computed by A. Marrocco).

$$\min_{T_h} \left\{ \int_{\Omega_h} |\nabla \Phi_h|^2 \, dx : \int_{\Omega_h} \nabla \Phi_h \cdot \nabla w_h \, dx = \int_{\Gamma_2} w_h \, d\Gamma \qquad \forall w_h \in H_h^1, w_h|_{\Gamma_1} = 0, \Phi_h|_{\Gamma_1} = 0 \right\}$$

Then the only solution is to link the motion of the interior nodes to that of the boundary nodes. To do this, let F be the set of indices of the boundary nodes:

$$\{q^k\}_{k\in F} = \text{boundary nodes}. \tag{55}$$

Let $F^c = \{1,\dots,N\} - F$ be the nodes of $\Omega_h - D_h$. Assume we know some function G^k that gives us the position of q^k, $k \in F^c$, when the boundary nodes are known, i.e.,

$$q^k = G^k(\{q^l\}_{l\in F}) \qquad \forall\, k \in F^c. \tag{56}$$

Then

$$\delta q_j^k = \sum_{l\in F}\sum_{i=1}^{n} \frac{\partial G_j^k}{\partial q_i^l}\delta q_i^l + o(|\delta q|) \qquad \forall\, k \in F^c, \forall\, j = 1,\dots,n, \tag{57}$$

and the new derivatives of E with respect to boundary nodes only are

$$\begin{aligned}\frac{\partial E}{\partial q_i^l} = \int_{\Omega_h} \Bigg[& p_h \frac{\partial}{\partial x_i}(w^l(a\Phi_h - f)) + (\nabla w^l \cdot \nabla p_h + a w^l p_h)\frac{\partial \Phi_h}{\partial x_i} - \nabla\Phi_h \cdot \nabla w^l \frac{\partial p_h}{\partial x_i} \\ & + \nabla\Phi_h \cdot \nabla p_h \frac{\partial w^l}{\partial x_i} + \sum_{\substack{k\in F^c\\ j=1,\dots,n}} \frac{\partial G_i^k}{\partial q_j^l}\Bigg\{ p_h \frac{\partial}{\partial x_j}(w^k(a\Phi_h - f)) \\ & + (\nabla w^k \cdot \nabla p_h + a w^k) p_h \frac{\partial \Phi_h}{\partial x_j} - \nabla\Phi_h \cdot \nabla w^k \frac{\partial p_h}{\partial x_j} + \nabla\Phi_h \cdot \nabla p_h \frac{\partial w^k}{\partial x_j}\Bigg\}\Bigg]\,dx \\ & \forall\, l \in F, \forall\, i = 1,\dots,n. \end{aligned} \tag{58}$$

Thus the same gradient method becomes the following:

Algorithm 2

[0. Choose Ω_h^0, i.e., $\{q^{k,0}\}_{k\in F}$. Choose M, ε

For $m' = 0,\dots,M$ do

1. Compute $\Phi_h^{m'}$ by (12) and (11) (with $m = 1$).
2. Compute $p_h^{m'}$ by (45).
3. Set

$$g_i^l = -\frac{\partial E}{\partial q_i^l} \quad \text{given by (58)}, \qquad l \in F, i = 1,\dots,n.$$

4. Compute an approximation $\rho^{m'}$ of

$$\arg\min_{\rho>0} E(\{q^{l,m'} + \rho g^l\}_{l\in F}). \tag{59}$$

5. Compute $\Omega_h^{m'+1}$ by setting

$$q^{l,m'+1} = q^{l,m'} + \rho^{m'} g^l, \qquad l \in F; \qquad q^{k,m'+1} = G^k(\{q^l\}); \tag{60}$$

if $\sum (g_i^l)^2 < \varepsilon$, stop.

The convergence of this algorithm is implied by Theorem 3 of Chapter 4. If faster convergence is required, the conjugate gradient can be used in this framework (that is not the case with Algorithm 1).

Remark. The mappings G^k defined by (56) may be known implicitly only (a subroutine of triangulation that the optimizer does not necessarily understand, for example). Then $\nabla_q G^k$ is computed by finite differences; for example,

$$\frac{\partial G^k}{\partial q_j^l} \simeq \left(G^k\left(q_j^l + \frac{1}{1000}\right) - G^k(q_j^l)\right) \times 1000. \tag{61}$$

However, this requires n number of N calls of G, which may be quite expensive. This is the drawback of Algorithm 2: when (61) is too expensive, the programming of the functions G^k are usually time-consuming.

7.2.5 Application example

A simple problem to consider is the optimization of nozzles, stated by

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_D |\nabla\Phi(\Omega) - \mathbf{u}_d|^2 \, dx, \tag{62}$$

where $\Phi(\Omega)$ is the solution of

$$\Delta\Phi = 0 \quad \text{in } \Omega, \qquad \left.\frac{\partial\Phi}{\partial n}\right|_{\Gamma_2 \cup \Gamma_4} = 0, \; \Phi|_{\Gamma_1 \cup \Gamma_3} = \Phi_\Gamma \tag{63}$$

with $\partial\Omega = \bigcup_{1,\dots,4} \Gamma_i$ and (see Figure 7.4)

$$\mathcal{O} = \{\Omega : \Gamma_1, \Gamma_2, \Gamma_3 \text{ fixed}, \Gamma_4 = \text{any curve } x_2 = g(x_1) \text{ which intersect } \Gamma_1, \Gamma_3\}.$$

This problem is made discrete with triangular finite elements of degree 1, for example, 140 triangles and 90 vertices as in the case of Figure 7.4. The internal

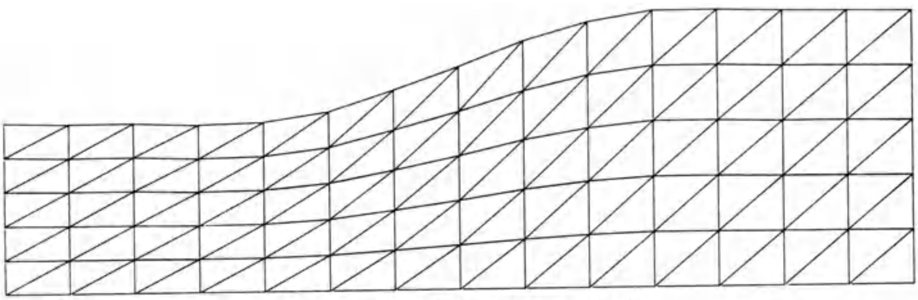


Fig. 7.4 Initial triangulation of the half nozzle Ω_o (from Angrand [4]).

vertices q^l on a vertical line are linked to the upper boundary vertex q^k by a linear map:

$$\delta q_2^l = q_2^l \frac{\delta q_2^k}{q_2^k}. \tag{64}$$

Figure 7.4 shows Ω^0, Figure 7.5 shows a few $\Omega^{m'}$, and Figure 7.6 shows Ω^M for $M = 30$. The criterion has been reduced by a factor 500:

$$E(\Omega^0) = 0.0437, \qquad E(\Omega^{30}) = 0.797 \times 10^{-4}.$$

The linear systems are solved by Choleski factorizations (the total central-processing-unit (CPU) time is 30 seconds on an IBM 3033).

For another application, see also [64].

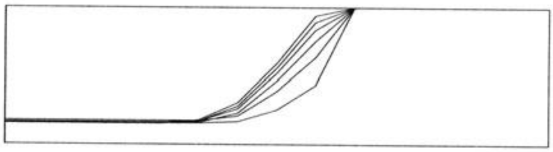


Fig. 7.5 An intermediate nozzle (from Angrand [4]).

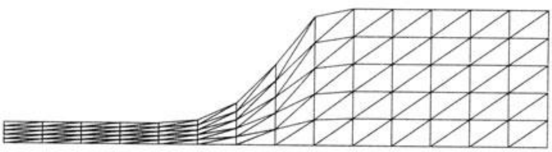


Fig. 7.6 The computed optimum profile after 30 iterations (from Angrand [4]).

7.2.6 Higher-order and non-conforming isoparametric elements

The above analysis applies to the case where $m > 1$ without any difficulty. With higher-order elements, however, the nodes are not necessarily vertices; so if they are moved independently, the triangles do not remain triangles. For this purpose we recall a definition of isoparametric elements: If $\{q^i\}$ is a set of nodes for which $\{w^k\}$ defined by

$$w^k(q^i) = \delta_{ki} \qquad \forall\, i; \qquad w^k|_{T_j} \in \mathrm{P}^m \qquad \forall\, j \tag{65}$$

forms a basis of H_h^m, then we define

$$H_h'^m = \{w_h : w_h \text{ is continuous at } \{q^i\}, w_h|_{T_j} \in P^m \qquad \forall\, T_j \in \mathscr{T}_h\}. \tag{66}$$

If $\{q^i\}$ are translated to $\{q^i + \delta q^i\}$, the triangles become curved, so that H_h^m is no longer suitable. However, (65) and (66) define a good approximation space if $\{\delta q^i\}$ are not too large. With this modification Propositions 2 and 3 apply with the same proof.

Proposition 4. *Let q^i, q^k be two nodes of triangle T_j, and let $w^i(\cdot)$ be the basis function associated with q^i, i.e.,*

$$w^i(q^l) = \delta_{il} \qquad \forall\, l; \qquad w^i|_{T_j} \in P^m \qquad \forall j. \tag{67}$$

If q^k translates to $q^k + \delta q^k$, then w^i changes to $w^i + \delta w^i \in H_h'^m$, and

$$\delta w^i(x) = -w^k(x)\nabla w^i(q^k)|_{T_j} \cdot \delta q^k + o(|\delta q^k|) \qquad \forall\, x \in T_j \cap T_j', \tag{68}$$

where T_j' is the transformed element obtained from T_j.

Proposition 5. *With the notation of Proposition 4, let $g \in C^1(T_j)$. Then*

$$\int_{T_j' - T_j \cap T_j'} g\,dx - \int_{T_j - T_j' \cap T_j} g\,dx = \int_{T_j} \delta q^k \cdot \nabla(gw^k)\,dx + o(|\delta q^k|). \tag{69}$$

Theorem 3. *Let $\mathscr{T}'_h$ be the transform of $\mathscr{T}_h$ where one node q^k translates into $q^k + \delta q^k$. Assume a and f are continuous, and let Φ_h be the solution of*

$$\int_{\Omega_h} (\nabla\Phi_h \nabla w_h + (a\Phi_h - f)w_h)\,dx = 0 \qquad \forall\, w_h \in H_h^m\,(\text{or } H_h'^m),\ \Phi_h \in H_h^m\ (\text{or } H_h'^m) \tag{70}$$

when $\mathscr{T}_h$ is changed to $\mathscr{T}'_h$, Φ_h becomes Φ'_h, and if $\delta\tilde{\Phi}_h \in H_h^m$ (or $H_h'^m$) is the solution of

$$\begin{aligned}\int_{\Omega_h} (\nabla\delta\tilde{\Phi}_h \nabla w_h + a\delta\tilde{\Phi}_h w_h)\,dx = &-\int_{\Omega_h} \delta q^k \nabla\big(w^k(\nabla\Phi_h \cdot \nabla w_h + (a\Phi_h - f)w_h\big)\,dx \\ &+ \int_{\Omega_h} \{(\nabla w^k \cdot \nabla w_h + aw^k w_h)\nabla\Phi_h(q^k) \cdot \delta q^k \\ &+ [\nabla\Phi_h \cdot \nabla w^k + (a\Phi_h - f)w^k]\nabla w_h(q^k) \cdot \delta q^k\}\,dx\end{aligned} \tag{71}$$

(the derivatives are evaluated pointwise). Then

$$\|\Phi'_h - \Phi_h - \delta\tilde{\Phi}_h + w^k\nabla\Phi_h(q^k) \cdot \delta q^k\|_{H^1} = o(|\delta q^k|).$$

Proof. Same as for Theorem 1 except for the simplifications at the end because the gradients are evaluated at q^k in some terms. □

Theorem 4. *Theorem 2 also holds for $m > 1$ and for isoparametric elements:*

$$\begin{aligned}\frac{\partial E}{\partial q_l^k} = -\int_{\Omega_h} \Big\{&\frac{\partial}{\partial x_l}\big(w^k(\nabla\Phi_h \cdot \nabla p_h + (a\Phi_h - f)p_h\big) - (\nabla p^k \cdot \nabla w_h + aw^k \cdot p_h)\frac{\partial\Phi_h}{\partial x_l}(q^k) \\ &- (\nabla\Phi_h \cdot \nabla w^k + (a\Phi_h - f)w^k)\frac{\partial p_h}{\partial x_l}(q^k)\Big\}\,dx.\end{aligned} \tag{72}$$

Remark. Isoparametric elements must in principle be close in shape to triangles. Therefore, it is best to keep the nonvertex nodes linked to the vertices as long as possible in the optimization alogrithm. A similar analysis can also be done for the usual conforming elements.

7.2.7 Quadrilateral elements

Another approximation of $H^1(\Omega)$ in (7) is built from quadrangulations $\mathcal{Q}_h$ of $\Omega_h\{\Omega_h = uQ_j : Q_j \in \mathcal{Q}_h\}$. For clarity, we assume $m = 1$ or 2. Let Q^m be the space of polynomials in $x \in \Omega_h$ of degree $\leq m$ in *each variable* x_i, $i = 1, \ldots, n$. Let $\{q^i\}$ be the nodes, i.e., the vertices of the elements if $m = 1$ and the vertices plus the midpoints plus the center points if $m = 2$. Let w^i be defined by

$$w^i(q^k) = \delta_{ik} \qquad \forall\, k, \qquad w^i|_{Q_j} \in Q^m \qquad \forall j, \tag{73}$$

where one axis is normal to an edge (face) of Q_j, and let

$$\tilde{H}_h^m = \{w_h : w_h \text{ continuous at the nodes, } w_h|_{Q_j} \in Q^m \qquad \forall j\}. \tag{74}$$

Again $\{w^i\}$ is a basis for $\tilde{H}_h^m$, and $\tilde{H}_h^m$ "converges" to $H^1(\Omega)$ when the size h of the sides tends to zero [with some restrictions placed on the shape of the quadrangles; in particular, their shape should not be too different from either rectangles or bricks, see [20], for example].

The problem given in (1) and (2) is also approximated by (12) and (22) with $\tilde{H}_h^m$. By inspection, we can check that propositions 4 and 5 also hold since the definition of $\{w^i\}$ is the same [compare (67) and (73)]. Therefore, Theorems 1 and 2 also hold for isoparametric quadrilateral elements with w_i^k defined by (73).

7.3 Dirichlet Conditions

7.3.1 Problem statement

Consider the function

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_\Omega |\Phi(\Omega) - \Phi_d|^2\, dx, \tag{75}$$

where $\Phi(\Omega)$ is solution of

$$-\nabla \cdot \rho \nabla \Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = \Phi_\Gamma; \tag{76}$$

the data $\Phi_d, \rho, f, \Phi_\Gamma$ are assumed to be smooth and

$$\rho(x) \geq \rho_0 > 0 \qquad \forall\, x \in \mathbb{R}^n. \tag{77}$$

This problem may arise with $\rho = 1$ in electrostatic units with an electrostatic potential Φ, which is desired to be equal to Φ_d, and where f is the distribution of charges.

If $\mathcal{O}$ is a set of bounded open sets with uniformly Lipchitz boundaries, or the cone property exists, then the above problem has at least one solution.

7.3.2 Discretization

To illustrate the method, let (76) be made discrete by quadrilateral elements of degree 1; however, this is just to fix the ideas because the same arguments apply to any Lagrangian element, as outlined in the previous paragraph. Thus we consider

$$\min E(\Omega_h) = \int_{\Omega_h} |\Phi_h - \Phi_d|^2\, dx, \tag{78}$$

$$\begin{aligned}&\int_{\Omega_h} \rho_h \nabla\Phi_h \nabla w_h\, dx = \int_{\Omega_h} f w_h\, dx \qquad \forall\, w_h \in \tilde{H}_h^1,\ w_h|_{\Gamma_h} = 0;\\ &\Phi_h \in \tilde{H}_h^1, \qquad \Phi_h(q^j) = \Phi_\Gamma(q^j) \qquad \forall\, q^j \in \Gamma_h,\end{aligned} \tag{79}$$

where ρ_h is piecewise constant on $\mathcal{Q}_h$, and for simplicity we assume that the value ρ_j is attached to the element Q_j, i.e.,

$$\rho_h(x) = \rho_j \qquad \forall\, x \in Q_j. \tag{80}$$

This relation is kept when Q_j is moved and transformed.

For another case, see Chapter 9.

Theorem 5. *If Φ_h is the solution of (79) and $\{q^k\}$ are the vertices of $\mathcal{Q}_h$, and if $\Phi'_{h,kl}$ is the solution of*

$$\begin{aligned}\int_{\Omega_h} \rho_h \nabla\Phi'_{h,kl} \cdot \nabla w_h\, dx = &\int_{\Omega_h} -\frac{\partial}{\partial x_l}[(\rho_h \nabla\Phi_h \cdot \nabla w_h - f w_h) w^k]\, dx\\ &+ \int_{\Omega_h} \{\rho_h \nabla w^k \cdot \nabla w_h \frac{\partial \Phi_h}{\partial x_l}(q^k)\\ &+ (\rho_h \nabla\Phi_h \cdot \nabla w^k - f w^k)\frac{\partial w_h}{\partial x_l}(q^k)\}\, dx\\ &\qquad \forall w_h \in \tilde{H}_h^1,\ w_h|_{\Gamma_h} = 0\end{aligned} \tag{81}$$

$$\Phi'_{h,kl} \in \tilde{H}_h^1, \qquad \Phi'_{h,kl}(q^j) = -\delta_{jk}\frac{\partial \Phi_\Gamma}{\partial x_l}(q^j) \qquad \forall\, q^j \in \partial\Omega_h,$$

then

$$\frac{\partial \Phi_h}{\partial q_l^k} = \Phi'_{h,kl} - w^k \frac{\partial \Phi_h}{\partial x_l}(q^k).$$

Proof. First we prove that we can differentiate (79) and write

$$\int_{\delta\Omega_h} (\rho_h \nabla\Phi_h \cdot \nabla w_h - f w_h)\, dx + \int_{\Omega_h} (\rho_h \nabla\delta\Phi_h \cdot \nabla w_h + \rho_h \nabla\Phi_h \cdot \nabla\delta w_h - f\delta w_h)\, dx = o(|\delta q|), \tag{82}$$

where Q'_j is Q_j transformed by moving the vertices and

$$\int_{\delta\Omega_h} g\,dx = \sum_j \int_{Q'_j - Q'_j \cap Q_j} g\,dx - \int_{Q_j - Q'_j \cap Q_j} g\,dx. \tag{83}$$

Indeed (82) may be obtained by substituting in (79) Q_h and Q'_h as follows:

$$\sum_j \int_{Q_j \cap Q'_j} (\rho_j \nabla\Phi_h \cdot \nabla w_h - f w_h)\,dx + \int_{Q_j - Q_j \cap Q'_j} (\rho_j \nabla\Phi_h \cdot \nabla w_h - f w_h)\,dx = 0 \tag{84}$$

$$\sum_j \int_{Q_j \cap Q'_j} (\rho_j \nabla\Phi'_h \cdot \nabla w'_h - f w'_h)\,dx + \int_{Q'_j - Q_j \cap Q'_j} (\rho_j \nabla\Phi'_h \nabla w'_h - f w'_h)\,dx = 0. \tag{85}$$

Then (84) is subtracted from (85), and in the domain $Q'_j \cap Q_j$, Φ'_j and w'_h are replaced by $\Phi_h + \delta\Phi_h$ and $w_h + \delta w_h$ (note that when ρ_h is not defined by (80), there may be an additional term).

Now that (82) is valid, we use Proposition 4 to compute δw_h, if the nodes q^k are translated by δq^k by linearity

$$w_h(x) = \sum w_i w^i(x); \tag{86}$$

Thus

$$\delta w_h = -w^k \nabla w_h(q^k) \cdot \delta q^k + o(\delta q^k). \tag{87}$$

To compute the first integral in (82) [see (83)], we use Proposition 5

$$\int_{\delta\Omega_h} (\rho_h \nabla\Phi_h \nabla w_h - f w_h)\,dx = \sum_j \int_{Q_j} \delta q^k \cdot \nabla(w^k(\rho_h \nabla\Phi_h \cdot \nabla w_h - f w_h))\,dx + o(\delta q^k); \tag{88}$$

Thus (82) becomes

$$\begin{aligned}
\int_{\Omega_h} \rho_h \nabla\delta\Phi_h \cdot \nabla w_h\,dx &= -\sum_j \int_{Q_j} \delta q^k \cdot \nabla[w^k(\rho_h \nabla\Phi_h \cdot \nabla w_h - f w_h)]\,dx \\
&\quad + \int_{\Omega_h} [\rho_h \nabla\Phi_h \cdot \nabla w^k \nabla w_h(q^k) \cdot \delta q^k \\
&\quad - f w^k \nabla w_h(q^k) \cdot \delta q^k]\,dx + o(\delta q^k) \\
&= \int_{\Omega_h} [\rho_h(\nabla\Phi_h \cdot \nabla w^k \nabla w_h(q^k) \cdot \delta q^k - \nabla\Phi_h \cdot \nabla w_h \nabla w^k \cdot \delta q^k) \\
&\quad + \delta q^k \cdot \nabla(f w_h w^k) - f w^k \nabla w_h(q^k) \cdot \delta q^k]\,dx + o(\delta q^k).
\end{aligned} \tag{89}$$

Now we examine the boundary conditions. If $\{q^i\}_{i\in F}$ denote the boundary nodes, we have by (79),

$$\Phi_h = \sum_{i\notin F} \Phi_i w^i + \sum_{i\in F} \Phi_\Gamma(q^i) w^i. \tag{90}$$

Therefore,

$$\begin{aligned}
\delta\Phi_h &= \sum_{i\notin F} (\delta\Phi_i w^i + \Phi_i \delta w^i) \\
&\quad + \sum_{i\in F} \Phi_\Gamma(q^i)\,\delta w^i + \nabla\Phi_\Gamma(q^k)\cdot\delta q^k w^k + o(\delta q^k) \\
&= \sum_{i\notin F} \left(\delta\Phi_i w^i - \Phi_i w^k \nabla w^i(q^k)\cdot\delta q^k\right) + \sum_{i\in F} \Phi_\Gamma(q^i) w^k \nabla w^i(q^k)\cdot\delta q^k \\
&\quad + \nabla\Phi_\Gamma(q^k)\cdot\delta q^k w^k.
\end{aligned} \tag{91}$$

The part belonging to $\tilde{H}_h^m$, we call $\delta\tilde{\Phi}_h$ and we get

$$\delta\tilde{\Phi}_h = \sum_{i\notin F} \delta\Phi_i w^i + \nabla\Phi_\Gamma(q^k)\cdot\delta q^k w^k = \sum_i \Phi'_{h,kl}\,\delta q_l^k.$$

Thus, if $j \in F$,

$$\delta\tilde{\Phi}_h(q^j) = \sum \Phi_{h,kl}\,\delta q_l^k\,\delta_{jk} = -\nabla\Phi_\Gamma(q^k)\,\delta q^k\,\delta_{jk}. \tag{92}$$

Theorem 6.

$$\begin{aligned}
\frac{\partial}{\partial q_l^k} E(\Omega_h) &= \int_{\Omega_h} \left[\frac{\partial}{\partial x_l}((\Phi_h - \Phi_d)^2 w^k) - 2(\Phi_h - \Phi_d) w^k \frac{\partial \Phi_h}{\partial x_l}(q^k)\right] dx \\
&\quad + \int_{\Omega h} \rho_h \left[\nabla\Phi_h \cdot \nabla w^k \frac{\partial p_h}{\partial x_l}(q^k) + \nabla w^k \cdot \nabla p_h \frac{\partial \Phi_h}{\partial x_l}(q^k)\right] dx \\
&\quad + \int_{\Omega_h} \left(2\chi_h(\Phi_h - \Phi_d) - \rho_h \nabla p_h \cdot \nabla\chi_h\right) dx \\
&\quad + \int_{\Omega_h} \left[\frac{\partial}{\partial x_l}(w^k f p_h) - f w^k \frac{\partial p_h}{\partial x_l}(q^k)\right] dx,
\end{aligned} \tag{93}$$

where p_h is the solution of

$$\int_{\Omega_h} \rho_h \nabla p_h \nabla w_h\, dx = 2\int_{\Omega_h} (\Phi_h - \Phi_d) w_h\, dx$$
$$\forall\, w_h \in \tilde{H}_h^1,\ w_h|_{\Gamma_h} = 0; \quad p_h \in \tilde{H}_h^1,\ p_h|_{\Gamma_h} = 0, \tag{94}$$

and χ_h is 0 if q^k is not a boundary point and

$$\chi_h = -\frac{\partial}{\partial x_l}(\phi_\Gamma(q^k)) w^k \quad \text{if } q^k \in \Gamma_h. \tag{95}$$

PROOF. By (78) and (83) and the fact that $\delta\Phi_h = \delta\tilde{\Phi}_h - w^k \nabla\Phi_h \cdot \delta q^k$, we have

$$\delta E(\Omega_h) = \int_{\delta\Omega_h} |\Phi_h - \Phi_d|^2\,dx + 2\int_{\Omega_h} \delta\tilde{\Phi}_h(\Phi_h - \Phi_d)\,dx$$
$$- 2\int_{\Omega_h} w^k(\Phi_h - \Phi_d)\nabla\Phi_h\,\delta q^k\,dx$$

By (94), with $w_h = \delta\tilde{\Phi}_h - \delta\tilde{\Phi}_{h|\Gamma_h}$,

$$2\int_{\Omega_h} \delta\tilde{\Phi}_h(\Phi_h - \Phi_d)\,dx = 2\int_{\Omega_h} \delta\tilde{\Phi}_h|_{\Gamma_h}(\Phi_h - \Phi_d)\,dx$$
$$+ \int_{\Omega_h} \rho_h\nabla p_h\nabla\delta\tilde{\Phi}_h\,dx - \int_{\Omega_h} \rho_h\nabla\rho_h\nabla\delta\tilde{\Phi}_{h|\Gamma_h}\,dx, \tag{96}$$

where

$$\delta\tilde{\Phi}_{h|\Gamma_h} = \sum_{i\in F} \delta\tilde{\Phi}_h(q^i)w^i = -\nabla\Phi_\Gamma(q^k)\,\delta q^k w^k\,\delta(k \in F). \tag{97}$$

To obtain (94), we use (81) with the substitution $w_h = p_h$ to express the second integral in (96).

Theorem 7. *The results of Theorems 5 and 6 are also valid with any other lagrangian isoparametric element.*

7.4 Other Problems

7.4.1 Boundary integrals

Consider the case

$$E(\Omega_h) = \int_{\Gamma_h} |\Phi_h - \Phi_d|^2\,d\Gamma, \tag{98}$$

where Φ_h is solution of a Neumann problem. Then

$$\delta E = \int_{\Gamma_h} 2(\Phi_h - \Phi_d)\,\delta\Phi_h\,d\Gamma + \int_{\delta\Gamma_h} |\Phi_h - \Phi_d|^2\,d\Gamma + o(\delta q). \tag{99}$$

The first integral is evaluated as before by means of an adjoint equation with a nonzero righthand-side equal to

$$2\int_{\Gamma_h} (\Phi_h - \Phi_d)w_h\,d\Gamma.$$

The second integral means (see Figure 7.7) that

$$\int_{\delta\Gamma_h} |\Phi_h - \Phi_d|^2 \, d\Gamma = \sum_{l \in F} \int_{\{q'^l, q'^{l+1}\}} [\Phi_h(q(s)) - \Phi_d(q(s))]^2 \, ds - \int_{\{q^l, q^{l+1}\}} [\Phi_h(q(s)) - \Phi_d(q(s))]^2 \, ds. \tag{100}$$

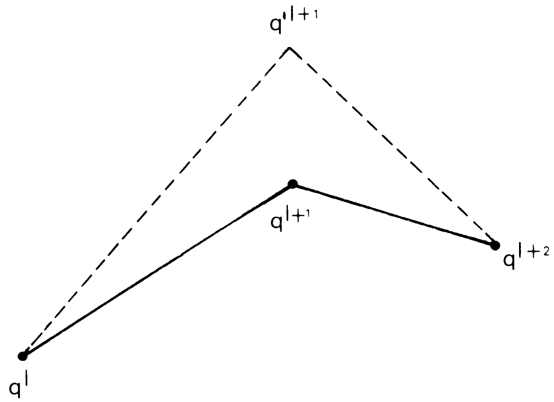


Fig. 7.7 Modification of Γ_h when q^{l+1} moves to q'^{l+1}.

Thus if q^k only varies and if $\{q^{k-1}, q^k\}$ and $\{q^k, q^{k+1}\}$ are straight segments, it is equal to 0 if $q^k \notin \Gamma_h$; otherwise, it is equal to

$$\int_{\{q^{k-1}, q^k\}} |\Phi_h - \Phi_d|^2 \, \delta q^k \cdot \frac{q^k - q^{k-1}}{|q^{k-1} - q^k|^2} \, d\Gamma + \int_{\{q^k, q^{k+1}\}} |\Phi_h - \Phi_d|^2 \, \delta q^k \cdot \frac{q^k - q^{k+1}}{|q^{k+1} - q^k|^2} \, d\Gamma + \int_{\{q^{k-1}, q^k\} \cup \{q^k, q^{k+1}\}} \nabla |\Phi_h - \Phi_d|^2 \cdot \delta q^k w^k \, d\Gamma, \tag{101}$$

where w^k is the P^1 basis function attached to vertex q^k. This formula can be generalized to isoparametric elements, and it takes a simpler form if the following substitution is used:

$$\int_{\Gamma_h} |\Phi_h - \Phi_d|^2 \, d\Gamma = \int_{\Omega_h} \nabla \cdot (\tilde{n}_h |\Phi_h - \Phi_d|^2) \, dx, \tag{102}$$

where $\tilde{n}_h$ is any extension of n_h such that

$$\tilde{n}_h \in \tilde{H}_h^m, \; \tilde{n}_h \cdot n_{T_k} = -\tilde{n}_h \cdot n_{Tl} \text{ on } T_k \cap T_l \qquad \forall k, l \tag{103}$$

where n_{T_k} is the outer normal to T_k.

Proposition 6. *Let g_h be a continuous piecewise polynomial of degree $\leq m$* on Γ_h. *Then*

$$\frac{\partial}{\partial q_l^k}\int_{\Gamma_h} g_h\,d\Gamma = \int_{\Gamma_h}\frac{\partial g_h}{\partial q_l^k}\,d\Gamma + \int_{\Omega_h}\frac{\partial}{\partial x_l}(w^k \nabla\cdot(\tilde{n}_h g_h))\,dx + \int_{\Gamma_h} g_h\frac{\partial \tilde{n}_h}{\partial q_l^k}\cdot n\,d\Gamma$$
$$-\int_{\Gamma_h} w^k g_h \frac{\partial \tilde{n}_h}{\partial x_l} n\,d\Gamma, \qquad \forall\, q^k \in \Gamma_h,\ l = 1,\ldots,n, \quad (104)$$

where $\tilde{n}_h$ is defined by (103).

Proof. We use (102), and we write

$$\delta\int_{\Gamma_h} g_h\,d\Gamma = \delta\int_{\Omega_h}\nabla\cdot(\tilde{n}_h g_h)\,dx$$
$$\simeq \int_{\Omega_h}\nabla\cdot(\tilde{n}_h\,\delta g_h)\,dx + \int_{\delta\Omega_h}\cdot(\tilde{n}_h g_h)\,dx + \int_{\Omega_h}\nabla\cdot(\delta\tilde{n}_h g_h)\,dx. \quad (105)$$

The first integral on the right-handside gives the first integral on the right-hand side of (104). The second integral is evaluated by means of Proposition 5. Then in the last integral, we use

$$\int_{\Omega_h}\nabla\cdot\delta n_h g_h\,dp = \int_{\Gamma} g_h\,\delta\tilde{n}_h\cdot n\,d\Gamma \quad (106)$$

Finally, the terms containing $\nabla\cdot$ of a continuous term are reintegrated by parts; this causes the term $\nabla\cdot(w^i\,\delta n g_h)$ to disappear:

$$\sum_{q^i\in\Gamma_h}\int_{\Omega_h}\nabla\cdot(w^i\,\delta n g_h)\,dx = \int_{\Gamma_h}\sum_{q^i\in\Gamma_h} w^i\,\delta n g_h \mathbf{n}\,d\Gamma = \tfrac{1}{2}\int_{\Gamma_h} g_h\,\delta|n|^2\,d\Gamma = 0.$$

□

7.4.2 Nonhomogeneous Neumann problem

Suppose Φ_h is the solution of

$$\int_{\Omega_h}(\nabla\Phi_h\cdot\nabla w_h + a\Phi_h w_h - f w_h)\,dx = \int_{\Gamma_h} g_h w_h\,d\Gamma \qquad \forall\, w_h\in H_h^m,\ \Phi_h\in H_h^m. \quad (107)$$

Then Proposition 6 enables us to compute the variation $\delta\Phi_h$ with respect to δq^k:

$$\int_{\Omega_h}(\nabla\delta\Phi_h\cdot\nabla w_h + a\delta\Phi_h w_h)\,dx = -\int_{\delta\Omega_h}(\nabla\Phi_h\cdot\nabla w_h + a\Phi_h w_h - f w_h)\,dx$$
$$-\int_{\Omega_h}\big(\nabla\Phi_h\cdot\nabla\delta w_h + (a\Phi_h - f)\,\delta w_h\big)\,dx$$
$$+\,\delta\int_{\Gamma_h} g_h w_h\,d\Gamma; \quad (108)$$

$$\delta \int_{\Gamma_h} g_h w_h \, d\Gamma = \int_{\Gamma_h} g_h \, \delta w_h \, d\Gamma + \int_{\Omega_h} \delta q^k \nabla\big(w^k \nabla \cdot (\tilde{n}_h g_h w_h)\big) \, dx$$
$$- \int_{\Gamma_h} w^k g_h w_h (\nabla \tilde{n}_h \cdot \delta q^k) \cdot n \, d\Gamma + \int_{\Gamma_h} g_h w_h \, \delta \tilde{n}_h \cdot n \, d\Gamma \tag{109}$$

So from Propositions 4 and 5, we find

$$\int_{\Omega_h} (\nabla \delta \tilde{\Phi}_h \cdot \nabla w_h + a \, \delta \tilde{\Phi}_h w_h) \, dx = -\int_{\Omega_h} \delta q^k \cdot \nabla\big(w^k(\nabla \Phi_h \cdot \nabla w_h + a\Phi_h w_h - f w_h)\big) \, dx$$
$$+ \int_{\Omega_h} (\nabla w^k \cdot \nabla w_h + a w^k w_h) \nabla \Phi_h(q^k) \cdot \delta q^k \, dx$$
$$+ \int_{\Omega_h} (\nabla \Phi_h \cdot \nabla w^k + a\Phi_h w^k - f w^k) \nabla w_h(q^k) \cdot \delta q^k \, dx$$
$$+ \int_{\Gamma_h} \{ g_h w^k [\nabla w_h(q^k) \cdot \delta q^k + w_h (\nabla n_h \cdot \delta q^k) \cdot n]$$
$$- \delta q^k \cdot n w^k \nabla \cdot (\tilde{n} g w_h) \} \, d\Gamma + \int_{\Gamma_h} g_h w_h \, \delta \tilde{n}_h \cdot n \, d\Gamma \tag{110}$$

$$\delta \Phi_h \simeq \delta \tilde{\Phi}_h - w^k \nabla \Phi_h(q^k) \cdot \delta q^k.$$

7.4.3 Other problems

1. If g_h is not continuous, then Proposition 6 does not hold. This is the case if the criteria are an approximation of $|\partial \Phi / \partial \mathbf{n} - g|$ on Γ. In this case, we use (104) on each triangle near the boundary or we approximate directly the boundary integral by a volume integral such as

$$\int_\Gamma |\nabla \Phi - u_d|^2 \, d\Gamma \simeq \frac{1}{h} \int_{D_h} |\nabla \Phi_h - u_d|^2 \, dx, \tag{111}$$

   where D_h is the set of elements that have sides on Γ_h.
2. Problems with Frechet conditions may be treated similarily to the nonhomogeneous Neumann problems.
3. A transmission problem is treated in Chapter 9.

7.5 Convergence

The convergence of the discretized problem to the continuous problem is straightforward. For example, with problems (1), (2), (6) and (22), (12), with

$$\mathcal{O}_h^\varepsilon = \{\Omega_h \in \mathcal{O}_h : \Omega_h \text{ has the } \varepsilon\text{-cone property}\}, \tag{112}$$

we have the following result.

Theorem 8 (E. Cara)
As $h \to 0$ there exists a subsequence $\{\Omega_h\}$ solution of (22), (12), (112), which converges (Hausdorff) to Ω solution (1), (2), (6) and $\{\phi_h\}$ converges strongly in H^1 to ϕ.

PROOF

Taking $w_h = \phi_h$ in (12) yields

$$\|\phi_h\|_{1,\Omega_h} \leq \|f\|_0/\min\{a, 1\} \qquad \forall h \tag{113}$$

From the results of Chapter 3, the ε-cone property and the boundedness of Ω_h, for some subsequence and some Ω in $\mathcal{O}^\varepsilon$ we have

$$\Omega_h \to \Omega \qquad \text{Hausdorff, } \chi_{\Omega_h} \to \chi_\Omega \text{ in } L^\infty. \tag{114}$$

This and (113) allows to let $h \to 0$ in (12) and find (2). Now taking again $w_h = \phi_h$ in (12) and letting $h \to 0$ yields:

$$\|\phi_h\|_{1,\Omega_h} \to \|\phi\|_{1,\Omega} \tag{115}$$

Therefore, the convergence is strong in $H^1(\Omega)$ and

$$E(\Omega_h) \leq E(\Omega_h') \qquad \forall \Omega_h' \in \mathcal{O}_h^\varepsilon \tag{116}$$

will give when $h \to 0$

$$E(\Omega) \leq E(\Omega') \qquad \forall \Omega' \in \mathcal{O}^\varepsilon \tag{117}$$

□

Other Methods

8.1 Introduction

In this chapter two different methods are presented for the computation of optimality conditions with respect to the domain: the method of mappings [50], [61] and the method of characteristic functions [18], [63]. These methods lead naturally to numerical algorithms using the finite difference method. Thus, finite difference solutions of shape design problems as studied in [18], [48], [35] are also presented here. Finally, we also analyze the feasibility of the boundary element method.

8.2 Method of Mappings

8.2.1 Problem statement

For simplicity, let us consider a simple problem, for example,

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_{\Omega} |\phi(\Omega) - \phi_d|^2 \, dx, \tag{1}$$

where $\phi(\Omega)$ is the solution of

$$-\Delta\phi + a_0\phi = f \quad \text{in } \Omega, \qquad \phi_{|\Gamma} = 0, \tag{2}$$

or stated in variational form,

$$\int_{\Omega} (\nabla\phi \cdot \nabla w + a_0\phi w - fw) \, dx = 0 \qquad \forall\, w \in H_0^1(\Omega),\ \phi \in H_0^1(\Omega). \tag{3}$$

Recall that when Ω is the image of a domain of reference C by a bijection T, then T itself becomes the variable of optimization. More precisely, following Murat–Simon [49], we introduce

$$\mathcal{T}^{k,\infty} = \{T\colon \mathbb{R}^n \to \mathbb{R}^n\colon T \text{ bijective};\ T, (I + T)^{-1} \in W^{k,\infty}(\mathbb{R}^n)^n\}. \tag{4}$$

Let $k \geq 1$ and assume that $\mathcal{O}$ is included in

$$\mathcal{O}^{k,\infty} = \{T(C)\colon T \in \mathcal{T}^{k,\infty}\}. \tag{5}$$

Then by a change of variable $X = T^{-1}(x)$, everything can be expressed on C:

$$E(\Omega) = E(T) = \int_C |(\phi - \phi_d) \circ T|^2 \det(\nabla T) \, dx \tag{6}$$

and $\hat{\phi} = \phi \circ T$ is the solution of

$$\int_C (\nabla\hat{\phi} \cdot \nabla T^{-t} \nabla T^{-1} \nabla\hat{w} + a_0 \hat{\phi}\hat{w} - \hat{f}\hat{w}) \det(\nabla T)\, dx = 0$$
$$\forall\, \hat{w} \in H_0^1(C),\ \hat{\phi} \in H_0^1(C). \quad (7)$$

8.2.2 Solution existence

Since all domains are now fixed, T becomes the unknown. A theorem of the existence of a solution can be obtained within this framework. To do this, we introduce the following expression

$$d_{k,\infty}(\Omega_1,\Omega_2) = \inf_{\substack{T \in \mathcal{T}^{k,\infty} \\ T(\Omega_1) = \Omega_2}} \{\|T - I\|_{k,\infty} + \|T^{-1} - I\|_{k,\infty}\}, \quad (8)$$

where

$$\|T\|_{k,\infty} = \operatorname{ess\,sup}_{x \in \mathbb{R}^n} \left(\sum_{0 \le m \le k} |D^m T|^2_{\mathbb{R}^n} \right)^{\frac{1}{2}}. \quad (9)$$

Lemma 1. *There exists μ_k such that $\delta_{k,\infty} = \inf\{\sqrt{\ \ } d_{k,\infty}, \mu_k\}$ defines a distance function on $\mathcal{O}^{k,\infty}$. Furthermore, $\mathcal{O}^{k,\infty}$ is complete for this distance, and when $k \ge 2$ and C is bounded, all bounded sequences $\{\Omega^m\}$, $d_k(\Omega_1, \Omega^m) \le$ constant, have an $\mathcal{O}^{k-1,\infty}$ accumulation point that belongs to $\mathcal{O}^{k,\infty}$.*

PROOF. See [50] □

Theorem 1. *Suppose C is bounded and suppose its boundary is $W^{2,\infty}$. If $\mathcal{O}$ is bounded and closed in $\mathcal{O}^{2,\infty}$ (with respect to $\delta_{k,\infty}$), then E has a minimum on $\mathcal{O}$.*

PROOF. If $\{T^m\}$ is a minimizing sequence for E and $\Omega^m = T^m(C)$, then we can extract a convergent subsequence with respect to the distance $\delta_{1,\infty}$. Thus, $\{\nabla T^{m-1}\}$ converges, and it is possible to reach the limit, $m \to +\infty$, in (7). □

8.2.3 Optimality conditions

Our purpose here is to compute

$$\lim_{T' \to T} \frac{E(T') - E(T)}{\|T' - T\|_{k,\infty}}. \quad (10)$$

It is much easier to do this when $T = I$, the identity, and $C = \Omega$ in (6) and (7). Let $\tau \in W^{k,\infty}$ and let T' be

$$T(\lambda) = (I + \lambda\tau)^{-1}; \quad (11)$$

when λ is small, $T(\lambda) \in \mathcal{T}^{k,\infty}$. Also, we have

$$\nabla T(\lambda)^{-1} = I + \lambda\nabla\tau; \qquad \det \nabla T(\lambda) = 1 - \lambda\nabla \cdot \tau + o(\lambda). \quad (12)$$

From (6), if the derivative in λ exists,

$$\lim_{\lambda \to 0} \frac{1}{\lambda}\,[E(T(\lambda)) - E(\Omega)] = \int_\Omega \left[\frac{d}{d\lambda}\left((\phi(\lambda) - \phi_d) \circ T(\lambda) \right)^2 \Big|_{\lambda=0} + |\phi - \phi_d|^2 \nabla \cdot \tau \right] dx. \tag{13}$$

Therefore, to find (10), we prove that the derivative in (13) exists and is linear in τ.

Lemma 2

$$\int_\Omega \left| \frac{d}{d\lambda}[g \circ (I + \lambda\tau)^{-1}] \Big|_{\lambda=0} + \nabla g \cdot \tau \right|^2 dx = 0 \qquad \forall g \in H^1(\Omega), \tag{14}$$

and if $\lambda \to \Phi(\lambda)$ is differentiable in $L^2(\Omega)$,

$$\int_\Omega \frac{d}{d\lambda}(\phi(\lambda) - \phi_d)^2 \circ T(\lambda)\, dx \Big|_{\lambda=0} = \int_\Omega \left(2 \frac{d\phi}{d\lambda}\Big|_{\lambda=0} (\phi - \phi_d) - \nabla[(\phi - \phi_d)]^2 \cdot \tau \right) dx \tag{15}$$

for $\tau \in W^{1,\infty}$.

Proof. (See [61]). From the formula for derivatives of composite functions, we have

$$\begin{aligned} \frac{d}{d\lambda} g \circ (I + \lambda\tau)^{-1} &= \frac{\partial g}{\partial x_i} \frac{d}{d\lambda}(x_i + \lambda\tau_i(\lambda))^{-1} \\ &= -\frac{\partial g}{\partial x_i}\tau_i \qquad \text{at } \lambda = 0. \end{aligned} \tag{16}$$

□

Proposition 1. *Let $\hat{\Phi}(\lambda) \in H_0^1(\Omega)$ be the solution of (7) with $C = \Omega$ and $T = (I + \lambda\tau)^{-1}$. If $\tau \in W^{1,\infty}$ and $f \in L^2(\Omega)$,* then the derivative *$\hat{\Phi}'_\tau$ of $\hat{\Phi}$ in λ at $\lambda = 0$ exists and is the solution of*

$$-\Delta\hat{\Phi}'_\tau + a_0\hat{\Phi}'_\tau = \nabla \cdot \big((\nabla\tau + \nabla\tau^t - I\nabla \cdot \tau)\nabla\Phi\big) - \nabla f \cdot \tau - \Phi - f \quad \text{in } \Omega,$$
$$\Phi'_{\tau|\Gamma} = 0. \tag{17}$$

Proof. With these results, (7) is

$$\int_\Omega \big(\nabla\hat{\Phi} \cdot (I + \lambda\nabla\tau)(I + \lambda\nabla\tau^t)\nabla\hat{w} + a_0\hat{\Phi}\hat{w} - \hat{f}\hat{w}\big) \det(I + \lambda\nabla\tau)^{-1}\, dx = 0. \tag{18}$$

By differentiating with respect to λ, we find that $\hat{\Phi}'_\tau$ exists because

$$\int_\Omega (\nabla\hat{\Phi}'_\tau \cdot \nabla w + a_0\hat{\Phi}'_\tau w)\,dx = -\int_\Omega [\nabla\Phi \cdot (\nabla\tau + \nabla\tau^t)\nabla w - \nabla f \tau w$$
$$- (\nabla\Phi \cdot \nabla w + a_0\Phi\hat{w} - fw)\nabla \cdot \tau]\,dx$$
$$\forall \hat{w} \in H_0^1(\Omega) \quad (19)$$

has a unique solution. □

Notice that $\hat{w}$ can be assumed to be independent of λ in this calculation, but $\hat{f}$ cannot. Notice also that $\hat{\Phi}'_\tau$ is not $d\Phi(\Omega_{\lambda\tau})/d\lambda$ at $\lambda = 0$.

Theorem 2. *Assume* $\tau \in W^{1,\infty}$, $\Phi_d \in H^1(\Omega)$, *and* $f \in L^2(\Omega)$. *Let* $\Omega_\tau = (I + \tau)^{-1}(\Omega)$; *then*

$$E(\Omega_\tau) - E(\Omega) = -\int_\Gamma \left(\Phi_d^2 + \frac{\partial\Phi}{\partial n}\frac{\partial p}{\partial n}\right)\tau \cdot n\,d\Gamma + o(\|\tau\|_{1,\infty}), \quad (20)$$

where p is the solution of

$$-\Delta p + a_0 p = 2(\Phi - \Phi_d) \quad \text{in } \Omega; \qquad p|_\Gamma = 0. \quad (21)$$

PROOF. From (13) and (15) we have

$$\frac{d}{d\lambda}E(\Omega_{\lambda\tau})\bigg|_{\lambda=0} = \int_\Omega [2\Phi'_\tau(\Phi - \Phi_d) - \nabla(\Phi - \Phi_d)^2 \cdot \tau - (\Phi - \Phi_d)^2\nabla \cdot \tau]\,dx$$
$$= \int_\Omega 2\Phi'_\tau(\Phi - \Phi_d)\,dx - \int_\Gamma \Phi_d^2\tau \cdot n\,d\Gamma. \quad (22)$$

If p is defined by (21), then multiplying by Φ'_τ and integrating yields

$$\int_\Omega (\nabla p \cdot \nabla\hat{\Phi}'_\tau + a_0 w\hat{\Phi}'_\tau)\,dx = 2\int_\Omega \Phi'_\tau(\Phi - \Phi_d)\,dx, \quad (23)$$

and from (19) we obtain (24)

$$E(\Omega_\tau) - E(\Omega) = -\int_\Gamma \Phi_d^2\tau \cdot n\,d\Gamma - \int_\Omega \{\nabla\Phi \cdot (\nabla\tau + \nabla\tau^t)\nabla p - \nabla f p\tau$$
$$-(\nabla\Phi \cdot \nabla p + a_0\Phi p - fp)\nabla \cdot \tau\}\,dx. \quad (24)$$

From (24) after integration by parts,

$$E(\Omega_\tau) - E(\Omega) = -\int_\Gamma \left(\Phi_d^2 + \frac{\partial\Phi}{\partial n}\frac{\partial p}{\partial n}\right)\tau \cdot n\,d\Gamma$$
$$+ \int_\Omega [+\nabla f p - \nabla(a_0\Phi p - fp) \quad (25)$$
$$+ \nabla\phi\,\Delta p + \nabla p\,\Delta\phi]\tau\,dx + o(\|\tau\|).$$

It is left as an exercise for the reader to show that the second integrand vanishes.

Now let us check that E is not only Gateau differentiable but also Frechet differentiable. If we wish to write (22) for $E(\Omega_\tau) - E(\Omega)$, we must add, to the right-hand side, a term bounded by [see (13)]

$$\int_\Omega \Phi_\tau'^2 \, dx + \|\Phi - \Phi_d\|_{H^2}^2 \|\tau\|_\infty^2 + \|\Phi - \Phi_d\|_0^2 \|\tau\|_{1,\infty}^2. \tag{26}$$

From (19) we see that $\|\Phi_\tau'\|_1$ is bounded by $C\|\tau\|_{1,\infty}(\|\Phi\|_1 + \|f\|_0)$; therefore (20) holds.

Next, we show that we can recover the usual optimality conditions by this method.

Corollary. *Assume that Ω is a solution of (1) and (2) and that its boundary Γ is C^1. Assume that $\Phi_d \in H^1$ and $f \in L^2(\Omega)$; then*

$$n \cdot \tau \left(\frac{\partial \phi}{\partial n} \frac{\partial p}{\partial n} \bigg|_\Gamma + \Phi_d^2|_\Gamma \right) \leq 0 \qquad \forall \tau \text{ allowable.} \tag{27}$$

8.3 Finite Difference Discretization

8.3.1 Explicit mappings

Let us consider the simple case of Figure 8.1 where Ω is the image of the unit square by a x_2-affine transformation T:

$$x_1 = T_1(x_1, x_2) = x_1; \qquad x_2 = T_2(x_1, x_2) = g(x_1)x_2. \tag{28}$$

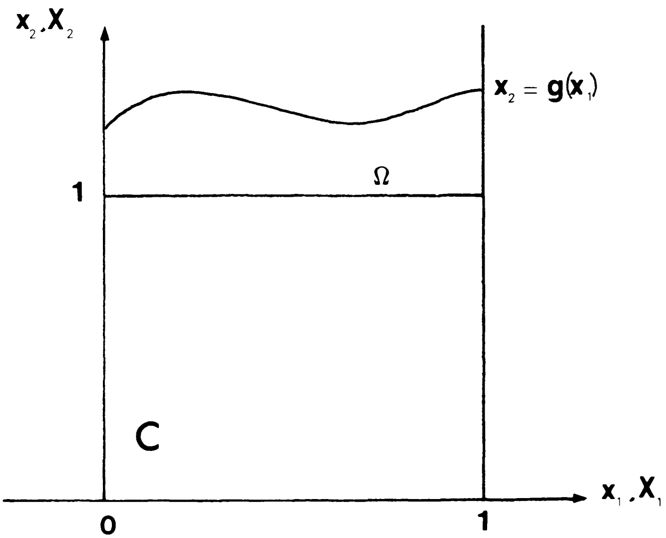


Fig. 8.1 Ω is limited by the curve g, it is easily mapped from the unit square by an affine x_2 map.

To solve (1), we use (6) and (7) and make (7) discrete by the finite difference method.

Let h be the mesh size; let $\hat{\phi}_{i,j}$ denote the value of $\phi \circ T$ at $X = \{(i-1)h, (j-1)h\}$, $1 \le i, j \le N \simeq 1/h$. As (7) is equivalent to

$$-\nabla \cdot (\nabla T^{-t} \nabla T^{-1} \nabla \hat{\phi} \det(\nabla T)) + (a_0 \hat{\phi} - \hat{f}) \det(\nabla T) = 0 \quad \text{in } C,$$
$$\hat{\phi}|_{\partial C} = 0, \quad (29)$$

we approximate it by Eq. (47) of Chapter 1 with Φ replaced by $\hat{\Phi}$,

$$A = \nabla T^{-t} \nabla T^{-1} \det(\nabla T), \qquad a = a_0 \det(\nabla T), \tag{30}$$

and $f_{i,j}$ replaced by $f[T((i-1)h, (j-1)h)] \det(\nabla T)$. The boundary conditions are

$$\hat{\phi}_{i,N} = \hat{\phi}_{i,1} = \hat{\phi}_{j,N} = \hat{\phi}_{j,1} = 0, \qquad i, j = 1, \ldots, N. \tag{31}$$

From (28), we see that the unknowns are $u = \{u_i\}_1^N$, $u_i = g((i-1)h)$; so the problem becomes

$$\min_{u \in \mathscr{U}} E_h(u) = \sum_{i,j=1}^{N} |\hat{\Phi}_{ij} - \Phi_d((i-1)h, (j-1)hu_i)|^2 h^2 u_i \tag{32}$$

with, for example

$$\mathscr{U} = \{u = \{u_1, \ldots, u_N\} : \mu \le u_i \le M\}. \tag{33}$$

The control u appears in the coefficient of the finite difference equation by $f((i-1)h, (j-1)hu_i)$ and

$$\nabla T_{ij}^{-1} = \begin{bmatrix} 1 & \dfrac{-g' X_2}{g} \\ 0 & \dfrac{1}{g} \end{bmatrix}_{i,j} \simeq \begin{bmatrix} 1 & \dfrac{(u_{i+1} - u_{i-1})(j-1)}{2u_i} \\ 0 & \dfrac{1}{u_i} \end{bmatrix}. \tag{34}$$

In order to compute $\partial E_h / \partial u_k$, let us introduce the finite difference operator ∇_h,

$$(\nabla_h g)(x) = \left\{ \frac{1}{h}\left(g\left(x_1 + \frac{h}{2}, x_2\right) - g\left(x_1 - \frac{h}{2}, x_2\right)\right), \frac{1}{h}\left(g\left(x_1, x_2 + \frac{h}{2}\right) \right.\right.$$
$$\left.\left. - g\left(x_1, x_2 - \frac{h}{2}\right)\right)\right\}, \tag{35}$$

and the divergence $\nabla_h \cdot$ is written similarly. Then (1.47) applied to (29) simplified to

$$[-\nabla_h \cdot (\nabla_h T^{-t} \nabla_h T^{-1} \nabla_h \hat{\Phi} \det(\nabla_h T))]_{ij}$$
$$+ (a_0 \Phi_{ij} - f((i-1)h, (j-1)hu_i)) \det(\nabla_h T)_{ij} = 0, \qquad i, j = 2, \ldots, N-1. \tag{36}$$

Theorem 3.

$$\frac{\partial E}{\partial u_k} = \sum_{j=1}^{N} [|\hat{\Phi} - \tilde{\Phi}_d|_{kj}^2 h^2] - \sum_{j=1}^{N} \left[2(\hat{\Phi} - \tilde{\Phi}_d) \frac{\partial \tilde{\Phi}_d}{\partial x_2} + p\left(\frac{\partial \tilde{f}}{\partial x_2} - a_0 \Phi + \tilde{f}\right)\right]_{kj} (j-1)h^3 + \sum_{i,j=1}^{N} h^2 p_{ij} \chi_{ij}, \tag{37}$$

where $\sim$ means evaluation at $(k-1)h$, $(j-1)hu_k$ *and where* $\{p_{kj}\}$ *is the solution of*

$$\begin{aligned} &[-\nabla_h \cdot A \nabla_h p + a_0 pu]_{ij} = 2(\hat{\Phi} - \tilde{\Phi}_d)_{ij} \qquad i, j = 2, \ldots, N \\ &p_{iN} = p_{ii} = p_{ij} = p_{Nj} = 0 \end{aligned} \tag{38}$$

with A *given by (41) and* χ_{ij} *given by (48) to (52).*

Proof. The proof is not difficult; it follows the same pattern. From (32), we have

$$\frac{\partial E_h}{\partial u_k} = \sum_{i,j=1}^{N} 2h^2 [\hat{\Phi}_{ij} - \Phi_d((i-1)h, (j-1)hu_i)] \left(\frac{\partial \hat{\Phi}_{ij}}{\partial u_k} - \left(\frac{\partial \tilde{\Phi}_d}{\partial x_2}\right)_{ij} \delta_{jk}(j-1)h\right) + \sum_{j=1}^{N} [|\hat{\Phi}_{k,j} - \tilde{\Phi}_{dk,j}| h^2], \tag{40}$$

where $\sim$ means that the function is evaluated at $\{(i-1)h, (j-1)hu_i\}$. To compute $\partial\hat{\Phi}/\partial u_k$, let us differentiate (36). Letting

$$\mathbf{A} = \nabla_h T^{-t} \nabla_h T^{-1} \det(\nabla_h T), \tag{41}$$

we get

$$\begin{aligned} [-\nabla_h \cdot (\mathbf{A} \nabla_h \delta\Phi) + a_0\, \delta\Phi u]_{ij} = &\left[\left(\nabla_h \cdot (\delta \mathbf{A} \nabla_h \Phi) + \delta u_k \frac{\partial \tilde{f}}{\partial x_2} \delta_{ik}(j-1)h\right) \det(\nabla_h T)\right]_{i,j} \\ &- (a_0 \Phi_{i,j} - \tilde{f}_{i,j})\delta_{i,k}\, \delta u_k + o(\delta u_k) \end{aligned} \tag{42}$$

since, from (34),

$$\det(\nabla T)_{i,j} = u_i. \tag{43}$$

Let us introduce the $\{p_{i,j}\}$ solution of (38). The reader should verify the discrete Green's formula:

$$\sum_{i,j=1}^{N} (\nabla_h \mathbf{A} \nabla_h \delta\Phi)_{i,j} p_{i,j} = \sum_{ij}^{N} (\nabla_h \mathbf{A} \nabla_h p)_{i,j}\, \delta\Phi_{i,j}. \tag{44}$$

Therefore, (38) and (42) imply that

$$\sum_{i,j=1}^{N} 2h^2(\Phi_{i,j} - \tilde{\Phi}_{di,j})\,\delta\Phi_{i,j} = \sum h^2[\nabla_h \cdot (\delta \mathbf{A} \nabla_h \Phi)]_{i,j} p_{i,j} + \delta u_k \sum_{j=1}^{N} \left[\left(\frac{\partial \tilde{f}}{\partial x_2}\right)_{k,j} - a_0 \Phi_{k,j} + \tilde{f}_{k,j}\right] \times p_{k,j}(j-1)h^3 + o(\delta u_k). \tag{45}$$

Finally, we must examine $[\nabla_h \cdot (\delta \mathbf{A} \nabla_h \Phi)]_{i,j} = \chi_{i,j}\,\delta u_k$.

From (41),

$$\mathbf{A} = \begin{bmatrix} g & -g'X_2 \\ -g'X_2 & \dfrac{g'^2 X_2^2}{g} + \dfrac{1}{g} \end{bmatrix}; \tag{46}$$

Thus

$$\delta \mathbf{A} = \begin{bmatrix} \delta g & -\delta g' X_2 \\ -\delta g' x_2 & \dfrac{2g'X_2^2\delta g'}{g} - \dfrac{\delta g(1 + g'^2 X_2^2)}{g^2} \end{bmatrix}. \tag{47}$$

Therefore, recalling that $g_{i\pm\frac{1}{2}} = (g_{i+1} + g_i)/2$, we get

$$\frac{\partial}{\partial u_k} A_{11}^{i\pm\frac{1}{2},j} = \frac{\delta_{i\pm 1,k} + \delta_{i,k}}{2} \qquad (\delta = \text{Kronecker symbol}), \tag{48}$$

$$\frac{\partial}{\partial u_k} A_{22}^{i,j\pm\frac{1}{2}} = -\frac{\delta_{ik}\left(1 + (u_{i+1} - u_{i-1})^2 (j \pm \frac{1}{2} - 1)^2\right)}{u_k^2} + \frac{(u_{i+1} - u_{i-1})(\delta_{i+1,k} - \delta_{i-1,k})(j \pm \frac{1}{2} - 1)^2}{2u_i}, \tag{49}$$

$$\frac{\partial}{\partial u_k} A_{12}^{i,j\pm\frac{1}{2}} = -\frac{(\delta_{i+1,k} - \delta_{i-1,k})(j \pm \frac{1}{2} - 1)}{2}, \tag{50}$$

$$\frac{\partial}{\partial u_k} A_{12}^{i\pm\frac{1}{2},j} = -\frac{[(\delta_{i+1,k} - \delta_{i-1,k}) + (\delta_{i+1\pm 1,k} - \delta_{i-1\pm 1,k})](j-1)}{4}, \tag{51}$$

and

$$\begin{aligned} \chi_{ij} = \frac{1}{h^2}\Bigg[&\frac{\partial A_{11}^{i+\frac{1}{2},j}}{\partial u_k}(\hat{\Phi}_{i+1,j} - \hat{\Phi}_{ij}) - \frac{\partial A_{11}^{i-\frac{1}{2},j}}{\partial u_k}(\hat{\Phi}_{i,j} - \hat{\Phi}_{i-1,j}) \\ &+ \frac{\partial A_{22}^{i,j+\frac{1}{2}}}{\partial u_k}(\hat{\Phi}_{i,j+1} - \hat{\Phi}_{i,j}) - \frac{\partial A_{22}^{i,j-\frac{1}{2}}}{\partial u_k}(\hat{\Phi}_{i,j} - \hat{\Phi}_{i,j-1}) \\ &+ \frac{\partial A_{12}^{i+\frac{1}{2},j}}{\partial u_k}(\hat{\Phi}_{i+\frac{1}{2},j+\frac{1}{2}} - \hat{\Phi}_{i+\frac{1}{2},j-\frac{1}{2}}) - \frac{\partial A_{12}^{i-\frac{1}{2},j}}{\partial u_k}(\hat{\Phi}_{i-\frac{1}{2},j+\frac{1}{2}} - \hat{\Phi}_{i-\frac{1}{2},j-\frac{1}{2}}) \\ &+ \frac{\partial A_{12}^{i,j+\frac{1}{2}}}{\partial u_k}(\Phi_{i+\frac{1}{2},j+\frac{1}{2}} - \Phi_{i-\frac{1}{2},j+\frac{1}{2}}) - \frac{\partial A_{12}^{i,j-\frac{1}{2}}}{\partial u_k}(\Phi_{i+\frac{1}{2},j-\frac{1}{2}} - \Phi_{i-\frac{1}{2},j-\frac{1}{2}}) \Bigg]. \end{aligned} \tag{52}$$

□

Algorithm. To solve (32) and (36).

0. Set $u_i^1 = 1$; choose M.
   For $m = 1, \ldots, M$ do
1. Compute $E_h(u^m)$ by (36).
2. Compute $\partial E^m/\partial u_k$, $k = 1, \ldots, N$ by (37) and set

$$H_k^m = \begin{cases} 0 \text{ if } -\dfrac{\partial E^m}{\partial u_k} > 0 \text{ and } u_k = M \\ 0 \text{ or if } -\dfrac{\partial E^m}{\partial u_k} < 0 \text{ and } u_k = \mu, \\ -\dfrac{\partial E^m}{\partial u_k} \quad \text{else:} \end{cases} \tag{53}$$

3. Compute an approximation ρ^m of the solution of (see Chapter 4)

$$\min_{\rho > 0} E(u^m + \rho H^m). \tag{54}$$

   Set $u^{m+1} = u^m + \rho^m H^m$.

Theorem 4. *All accumulation points u^* of $\{u^m\}$ will satisfy $H = 0$ [see (53)].*

For the proof, see Chapter 4.

Application: Begis and Glowinski [8] have used this method from a somewhat different perspective by using the finite element method, however, applied to a regular mesh it can be shown that it is equivalent to the finite difference method.

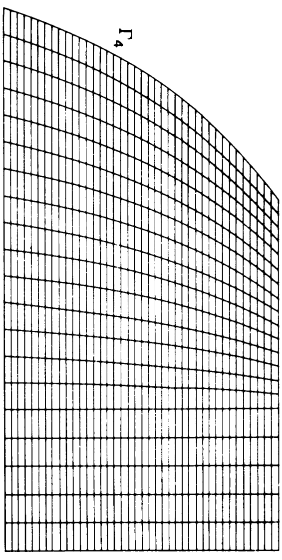


Fig. 8.2 Computation of a porous dyke. Γ_4 is the free surface below which the water seeps. The picture also shows the triangulation (from Begis and Glowinski [8]).

The problem is a slightly different one and is stated as

$$\min_g \left\{ \int_{\Gamma_4} |\Phi - g|^2 \, d\Gamma : \Delta\Phi = 0 \text{ in } \Omega, \right.$$
$$\Phi = 1 \text{ on } \Gamma_1, \Phi = x_2 \text{ on } \Gamma_2,$$
$$\left. \frac{\partial\Phi}{\partial n} = 0 \text{ on } \Gamma_3 \cup \Gamma_4 \right\} \tag{55}$$

where the control is Γ_4; the other parts of Γ are fixed. The numerical results are shown on Figure 8.2. This problem corresponds to the determination of Γ_4, the free surface of water in a porous dam.

8.3.2 Implicit mappings

It is not always possible to construct explicitly the mappings $T: C \to \Omega$. This is true if no prior information is known about the general shape of the solution. In that case, we may define T implicitly. For the sake of clarity we present the method in two dimensions where T is a conformal mapping.

If the equation of $\Gamma = \partial\Omega$ is

$$x_1 = g_1(s), \qquad x_2 = g_2(s), \qquad s \in]0, 1[, \tag{56}$$

then T can be built by solving

$$\Delta T = 0 \quad \text{in } C, \tag{57}$$

$$T(X(s)) = g(s) \qquad \forall\, X(s) \in S = \partial C. \tag{58}$$

Note that the parameter s is still undetermined; thus many mappings T can be built in this manner.

We make use of the degree of freedom to select a T which has

$$\nabla T^{-t} \nabla T^{-1} = \text{diagonal matrix.} \tag{59}$$

Note that (57) implies that for some U,

$$\nabla T_i = \left\{ \frac{\partial U_i}{\partial x_2}, -\frac{\partial U_i}{\partial x_1} \right\}^t \qquad i = 1, 2. \tag{60}$$

Therefore,

$$\det(\nabla T)^2 \nabla T^{-t} \nabla T^{-1} = \begin{bmatrix} U_{2,1}^2 + U_{1,1}^2 & U_{2,1}U_{2,2} + U_{1,1}U_{1,2} \\ U_{2,1}U_{2,2} + U_{1,1}U_{1,2} & U_{1,2}^2 + U_{2,2}^2 \end{bmatrix}. \tag{61}$$

Following [48], we choose U such that

$$U_{1,2} = -U_{2,1}, \qquad U_{2,2} = U_{1,1}. \tag{62}$$

Since these relations are the Cauchy conditions for conjugates, this is possible when Γ is made of four pieces and (58) is replaced by [see (60) to (62)]

$$T_1|_{S_1} = u_1(x_2); \qquad \left.\frac{\partial T_1}{\partial \mathbf{n}}\right|_{S_2} = \dot{u}_2(x_1); \qquad T_1|_{S_3} = u_3(x_2);$$

$$\left.\frac{\partial T_1}{\partial \mathbf{n}}\right|_{S_4} = \dot{u}_4(x_1); \tag{63}$$

$$\left.\frac{\partial T_2}{\partial \mathbf{n}}\right|_{S_2} = \dot{u}_1(x_2); \qquad T_2|_{S_2} = u_2(x_1); \qquad \left.\frac{\partial T_2}{\partial \mathbf{n}}\right|_{S_3} = -\dot{u}_3(x_2);$$

$$T_2|_{S_4} = u_4(x_1), \tag{64}$$

where $S_1, \ldots, S_4$ are the four sides of the square C (Figure 8.3), and the μ_i are related to the equations of the boundaries Γ_i. For example,

$$\Gamma_1 = \{u_1(x_2), T_2(0, x_2) : x_2 \in]0, 1[\}. \tag{65}$$

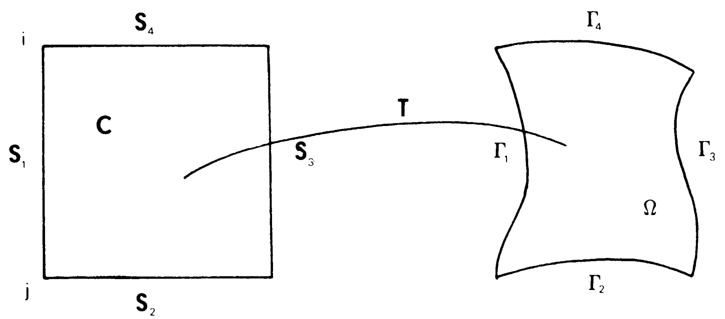


Fig. 8.3 Implicit mapping. Ω is found as $T(C)$ when it is topologically isomorphic to the unit square. Here T is also conforming.

There is also a compatibility condition between (63) and (64) because $\nabla \cdot T = 0$:

$$\int_0^1 (u_4 + u_2)\, dx_1 + \int_0^1 (u_3 + u_1)\, dx_2 = 0 \tag{66}$$

Now the problem given in (6) and (7) reduces to

$$\min_u E(u) = \int_C (\hat{\Phi} - \Phi_d \circ T)\, dX, \tag{67}$$

where $\{\hat{\Phi}, T\}$ is the solution of

$$-\left(\frac{\partial^2 \hat{\Phi}}{\partial x_1^2} + \frac{\partial^2 \hat{\Phi}}{\partial x_2^2}\right) \frac{1}{T_{1,1} T_{2,2} - T_{1,2} T_{2,1}} + a_0 \hat{\Phi} = f \circ T \text{ in } C, \tag{68}$$

$$\Phi|_S = 0, \tag{69}$$

$$\Delta T = 0 + \text{boundary conditions (63) and (64).} \tag{70}$$

Thus, the problem is again transformed into a classical optimal control problem with an augmented state $\{\Phi, T\}$.

Discretizations and computations of $\partial E/\partial u$ present no particular difficulty—the formulas are perhaps even less complicated than in the last case treated. From the strictly numerical point of view, this method is more expensive to simulate on a computer because of (70), however, its advantage is that the corresponding meshes in the variable domains are always smooth and "orthogonal." Figure 8.4 shows the result of this method for the same problem as treated in (55) and for the case where Γ_1, Γ_2, and Γ_3 are not parallel to the axis.

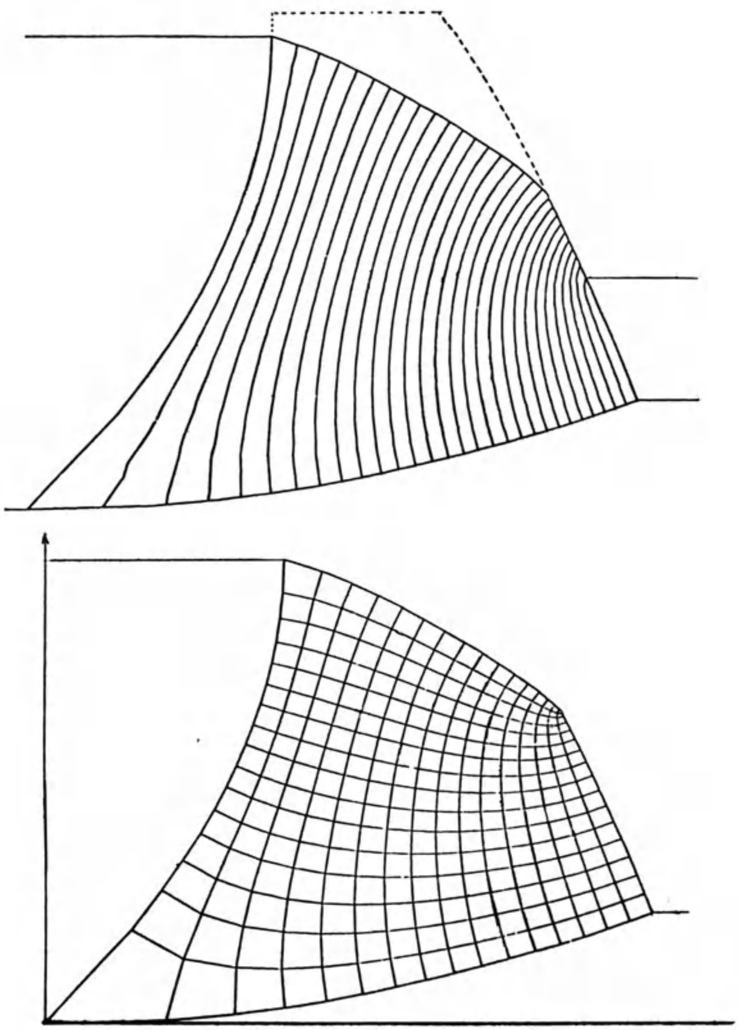


Fig. 8.4 Computation of a porous dyke (as in Figure 8.2). Here the sides of the dyke are not parallel (from Morice [48]).

8.4 Method of Characteristic Functions

8.4.1 Transmission problem

Now let us consider the following problem:

$$\min_{\Omega \subset \mathbb{C}} E(\Omega) = \int_D |\Phi(\Omega) - \Phi_d|^2 \, dx \tag{71}$$

with $\Phi(\Omega)$ the solutions, (for $a_i > 0$) of

$$\begin{aligned} &-a_1 \Delta\Phi_1 + a_0\Phi_1 = f \quad \text{in } \Omega, \\ &-a_2 \Delta\Phi_1 + a_0\Phi_1 = f \quad \text{in } \mathbb{C} - \Omega, \\ &a_1\frac{\partial\Phi_1}{\partial\mathbf{n}} = a_2\frac{\partial\Phi_2}{\partial\mathbf{n}} \quad \text{on } \partial\Omega - \partial\Omega \cap \partial\mathbb{C}, \qquad a_i\frac{\partial\Phi_i}{\partial\mathbf{n}} = 0 \quad \text{on } \partial\mathbb{C}. \end{aligned} \tag{72}$$

If we let χ denote the characteristic function of Ω, then this problem may be rewritten in terms of χ:

$$\min_{\chi \in X} E(\chi) = \int_D |\Phi(\chi) - \Phi_d|^2 \, dx \tag{73}$$

with $\Phi(\chi)$ the solution of

$$\int_{\mathbb{C}} [(a_1\chi - a_2(1-\gamma)]\nabla\Phi\nabla w + a_0\Phi w - fw)\,dx = 0 \quad \forall w \in H^1(\mathbb{C}) \tag{74}$$

and

$$X = \{\chi : \chi \leq \chi(\mathbb{C}); \chi(x) = 0 \text{ or } 1 \quad \forall x \text{ in } \mathbb{C}\}. \tag{75}$$

So again (73) to (75) become a problem of optimal control with the controls in the coefficients of the PDE, however, the constraints set X makes this problem particularly difficult to solve. The exact calculation of the optimality conditions is nevertheless interesting since it yields the following proposition, see [18], [63], and [16].

Proposition 2. *Suppose Ω is a smooth solution of (71) and p is the solution of*

$$-\nabla \cdot a\nabla p + a_0 p = 2(\Phi - \Phi_d)\chi(D) \quad \text{in } \mathbb{C}, \qquad \left.\frac{\partial p}{\partial n}\right|_\Gamma = 0, \tag{76}$$

where $a = a_1$ in Ω, a_2 in $\mathbb{C} - \Omega$. Then, we must have

$$(a_1 - a_2)\nabla\Phi\nabla p \begin{cases} \geq 0 & \forall x \in \Omega, \\ \leq 0 & \forall x \in C - \Omega. \end{cases} \tag{77}$$

Proof. Let $\delta\chi$ be an allowable ($\chi + \delta\chi \in X$) variation of χ; then from (73)

$$\delta E = E(\chi + \delta\chi) - E(\chi) = 2\int_D \delta\Phi(\Phi(\chi) - \Phi_d)\,dx + \int_D |\delta\Phi|^2\,dx.$$

Now from (74), for all w in $H^1(\mathbb{C})$, we have

$$\int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi \nabla\Phi \cdot \nabla w\, dx + \int_{\mathbb{C}} (a\nabla\,\delta\Phi\nabla w + a_0\,\delta\Phi w)\, dx$$
$$+ \int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi\nabla\,\delta\Phi\nabla w\, dx = 0. \quad (78)$$

As before, (76) in a weak form leads to

$$2\int_D \delta\Phi(\Phi - \Phi_d)\, dx = \int_{\mathbb{C}} a(\nabla p\nabla\,\delta\Phi + a_0 p)\, dx = -\int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi\nabla\Phi\nabla p\, dx$$
$$- \int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi\nabla\,\delta\Phi\nabla p\, dx. \quad (79)$$

Therefore,

$$\delta E = -\int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi\nabla\Phi\nabla p\, dx - \int_{\mathbb{C}} (a_1 - a_2)\,\delta\chi\nabla\,\delta\Phi\nabla p\, dx + \int_D |\delta\Phi|^2\, dx. \quad (80)$$

Letting $w = \delta\Phi$ in (78) yields

$$\|\delta\Phi\|_1 \le C_1\|\nabla\Phi\|_\infty \left(\int_{\mathbb{C}} |\delta\chi|\right)^{\frac{1}{2}}. \quad (81)$$

Therefore, the last two integrals in (80) are small compared with the first one.

The optimality condition is now easily obtained by taking $\delta\chi = 1, 0,$ or -1 in suitable sets. □

Comment. When $a_2 \to 0$, Proposition 2 should give the usual optimality condition for the Neumann problem, and indeed it does. However, it also gives a new condition:

$$\nabla\Phi\nabla p \ge 0 \quad \text{in } \Omega. \quad (82)$$

This nonboundary information is interesting. Suppose Ω is computed by an optimization method based on the optimality conditions of Chapter 6, and suppose it does not satisfy (82). Then the new condition means that a "hole" must be added (or subtracted) to Ω.

This information is used in [18] to develope an algorithm to solve (71) and (72). The domain $\mathbb{C}$ is divided into N subdomains C_i and

$$\Omega = \bigcup_{i \in I} C_i$$

If $(a_1 - a_2)\nabla\Phi\nabla p < 0$ in C_j, then j is removed from I, and conversely, if it is positive, j is not removed.

8.4.2 Dirichlet problem: penalization

Consider the problem model

$$\min_{D \subset \Omega \subset \mathbb{C}} E(\Omega) = \int_{\mathbb{D}} |\Phi - \Phi_d|^2 \, dx \tag{83}$$

with

$$-\Delta \Phi = f \quad \text{in } \Omega, \qquad \Phi|_\Gamma = 0. \tag{84}$$

Let $\chi(\Omega)$ be the characteristic function of Ω, and let Φ^ε be the solution of the following problem

$$-\Delta \Phi^\varepsilon + \frac{1}{\varepsilon}(1 - \chi(\Omega))\Phi^\varepsilon = f \quad \text{in } \Omega, \qquad \Phi^\varepsilon|_{\partial\mathbb{C}} = 0. \tag{85}$$

Lemma 1.

$\Phi^\varepsilon \to \Phi$ strongly in $L^2(\mathbb{C})$ when $\varepsilon \to 0$.

PROOF. Multiplying (85) by Φ^ε and integrating over $\mathbb{C}$ yields

$$\int_{\mathbb{C}} |\nabla \Phi^\varepsilon|^2 \, dx + \frac{1}{\varepsilon}\int_{\mathbb{C}-\Omega} \Phi^{\varepsilon^2} \, dx \le \|f\|_0 \|\Phi^\varepsilon\|_0. \tag{86}$$

So $\{\Phi^\varepsilon\}$ is bounded in $H^1(\mathbb{C})$, and $\{\Phi^\varepsilon/\sqrt{\varepsilon}\}$ is bounded in $L^2(\mathbb{C} - \Omega)$. Therefore, for some subsequence, we have

$$\Phi^\varepsilon \to 0 \quad \text{in } \mathbb{C} - \Omega,$$

$$\Phi^\varepsilon \to \Psi \quad \text{and} \quad \Delta \Psi = f \quad \text{in } \Omega.$$

Remark. Stronger convergences can be proved (see [34]).

Proposition 3. *Let Φ^ε be the solution of (85), and let*

$$E(\chi) = \int_D |\Phi^\varepsilon - \Phi_d|^2 \, dx. \tag{87}$$

Then

$$E(\chi') - E(\chi) = \int_{\mathbb{C}} \frac{1}{\varepsilon}(\chi' - \chi)\Phi^\varepsilon p^\varepsilon \, dx + o\left(\int_{\mathbb{C}} \frac{1}{\varepsilon}|\chi' - \chi| \, dx\right), \tag{88}$$

where p^ε is the solution of

$$-\Delta p^\varepsilon + \frac{1}{\varepsilon}(1 - \chi)p^\varepsilon = 2\chi(D)(\Phi - \Phi_d) \quad \text{in } \mathbb{C}, \qquad p^\varepsilon|_{\partial\mathbb{C}} = 0. \tag{89}$$

PROOF. The proof is not different from that of Proposition 2. From (85),

$$-\Delta \delta\Phi^\varepsilon + \frac{1}{\varepsilon}(1 - \chi - \delta\chi)\delta\Phi^\varepsilon = \frac{1}{\varepsilon}\delta\chi\Phi^\varepsilon \quad \text{in } \mathbb{C}, \qquad \delta\Phi^\varepsilon|_{\partial\mathbb{C}} = 0, \tag{90}$$

and from (87) and (89)

$$\delta E = 2\int_D \delta\Phi^\varepsilon(\Phi^\varepsilon - \Phi_d)\,dx + \int_D (\delta\Phi^\varepsilon)^2\,dx$$
$$= \int_{\mathbb{C}} \left(\nabla p^\varepsilon\,\nabla\delta\Phi^\varepsilon + \frac{1}{\varepsilon}(1-\chi)p^\varepsilon\delta\Phi^\varepsilon\right)dx + \int_D (\delta\Phi^\varepsilon)^2\,dx. \tag{91}$$

By (90), $\delta\chi\ \delta\Phi^\varepsilon$ and $\delta\Phi^{\varepsilon 2}$ are shown to be small, and (91) is transformed into

$$\delta E = \int_{\mathbb{C}} \frac{1}{\varepsilon}\delta\chi\Phi^\varepsilon p^\varepsilon\,dx + o\left(\int_{\mathbb{C}}\frac{1}{\varepsilon}|\delta\chi|\,dx\right). \tag{92}$$

8.4.3 Discretization by finite differences

Consider, for simplicity, the case where $\mathbb{C} =]0,1[\times]0,1[$ and we are given a uniform grid of mesh size h. Let Δ^h_{ij} be the five-point discrete Laplace operator at $\{ih, jh\}$:

$$\Delta^h_{ij}\Phi = \frac{\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 4\Phi_{i,j}}{h^2}. \tag{93}$$

Let χ^h_{ij} be an approximation of χ at $\{ih, jh\}$. Then (85) is approximated by

$$-\Delta^h_{ij}\Phi^\varepsilon + \frac{1}{\varepsilon}(1-\chi^h_{ij})\Phi^\varepsilon_{ij} = f_{ij}, \qquad i,j = 1,\ldots,N-1, \tag{94}$$

$$\Phi^\varepsilon_{i,0} = \Phi^\varepsilon_{i,N} = \Phi_{0,j} = \Phi_{N,j} = 0, \qquad i,j = 0,\ldots,N,\ N \simeq \frac{1}{h}, \tag{95}$$

and $E(\chi)$ is approximated by

$$E_h(\chi^h) = \sum_{\{ih,jh\}\in D} (\Phi^\varepsilon_{ij} - \Phi_{dij})^2 h^2. \tag{96}$$

Proposition 4.

$$E_h(\chi^h + \delta\chi^h) - E_h(\chi^h) = \sum_{i,j=0,\ldots,N} \frac{1}{\varepsilon}\delta\chi^h_{ij}\Phi^\varepsilon_{ij}p^\varepsilon_{ij}h^2 + o\left(\frac{1}{\varepsilon}\delta\chi^h_{ij}\right), \tag{97}$$

where p^ε is the solution of

$$-\Delta^h_{ij}p^\varepsilon + \frac{1}{\varepsilon}(1-\chi^h_{ij})p^\varepsilon_{ij} = 2(\Phi^\varepsilon_{ij} - \Phi_{dij})\chi(\mathrm{D})|_{ih,jh}, \qquad i,j = 1,\ldots,N-1, \tag{98}$$

$$p^\varepsilon_{ij} = 0 \quad on\ \partial\mathbb{C}. \tag{99}$$

Proof. Again the proof is very similar; so we need only verify the transformation of (91) to (92):

$$\delta E = \sum_{i,j=1,\ldots,N-1}\left[-\Delta^h_{ij}p^\varepsilon\,\delta\Phi_{ij} + \frac{1}{\varepsilon}(1-\chi^h_{ij})p^\varepsilon_{ij}\,\delta\Phi_{ij}\right]h^2. \tag{100}$$

From (93), we see that

$$\sum -(\Delta^h_{ij} p^\varepsilon)\,\delta\Phi_{ij} = \sum -(\Delta^h_{ij}\,\delta\Phi)\,p^\varepsilon_{ij}; \tag{101}$$

thus the result is derived as in Proposition 3. □

To obtain an idea of the form of the solution, we use the algorithm presented in [18].

Algorithm 2

[0. Set $\chi^0_{ij} = 1$ if $\{ih, jh\} \in D$, 0 elsewhere. Choose M.

For $m = 0, \ldots, M$ do

1. Compute $\{\Phi^\varepsilon_{ij}\}$ by solving (94) and (95).
2. Compute $\{p^\varepsilon_{ij}\}$ by solving (98) and (99).
3. Set $\chi^{m+1}_{ij} = \chi^m_{ij}$, except at the following points:

$$\chi^{m+1}_{ij} = \begin{cases} 1 & \text{if} \quad \chi^m_{ij}\Phi^\varepsilon_{ij}p^\varepsilon_{ij} > 0 & (102) \\ 0 & \text{if} \quad (1 - \chi^m_{ij})\Phi^\varepsilon_{ij}p^\varepsilon_{ij} < 0 \text{ and } \{ih, jh\} \notin D. & (103) \end{cases}$$

Convergence: By (97) we know only that

$$E(\chi^{m+1}) < E(\chi^m) + o\left(\frac{1}{\varepsilon}(\chi^{m+1} - \chi^m)\right). \tag{104}$$

Since there is a finite number of possibilities for χ, Algorithm 2 generates cluster points. However, such points may not be satisfactory. For instance, if Ω has too many holes inside; this is related to the convergence of the penalized problem when $\varepsilon \to 0$ and this point remains unanswered. □

Now that we know the approximate shape of Ω, we may discretize Γ_1 by a curve Γ_h (in two dimensions) made of straightline segments connecting the nodes $\{q^i\}^m$ (see Figure 8.5). Then, we define χ_{ij} by

$$\chi_{ij} = \frac{\text{area}(\Omega_h \cap](i-1)h, (i+1)h[\times (j-1)h, (j+1)h[)}{4h^2}, \tag{105}$$

for example.

It is possible to prove that

$$\Phi^\varepsilon_i \to \Phi \quad \text{strongly in } L^2, \text{ when } \varepsilon \to 0, h \to 0 \tag{106}$$

(see [2]). For other methods of solving this type of problem, see also [65]. The explicit computation of χ_{ij} as a function of $\{q^i\}$ is somewhat complicated because of the many possible cases. However, if $n \ll N$, the "corners" can be neglected, and the computation of (105) reduces to one of finding the two intersections of a segment $\{q^l, q^{l+1}\}$ with

$$](i-1)h, (i+1)h[\times](j-1)h, (j+1)h[\qquad \text{(see Figure 8.5).}$$

Now the variables of the problem given in (94) to (96) are the $\{q^i\}^N_1$, but $\partial E/\partial q^i$ is

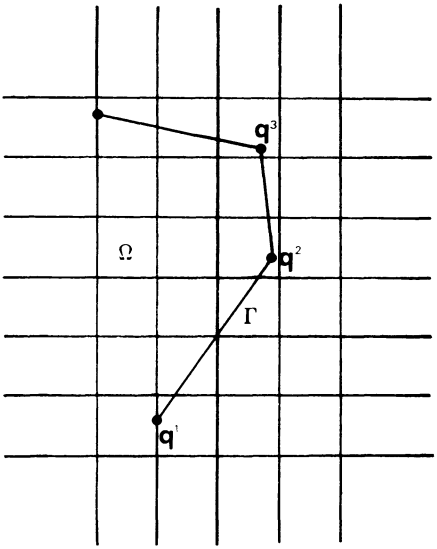


Fig. 8.5 With the penalty method the vertices of the boundary need not be grid points.

easily obtained from $\partial E/\partial \chi$ given by (97) and $\partial \chi/\partial q$ given by (105); so a gradient algorithm may be used.

Comments. This last method is not as precise as the other methods studied in this book because of the penalization; however, as the reader has noticed, there are no moving meshes or complicated mappings. If the curve Γ_h becomes very oscillating, the only difficulty is deciding whether a point is inside or outside Ω. Nevertheless, this method coupled with Algorithm 2 above is perhaps as close as we can get to a universal method of optimum design, that is, a method that does not require any *a priori* information on the shape of the solution.

8.5 Discretization by the Boundary Element Method

8.5.1 Problem position

The boundary element method (reviewed in Section 1.5) has an advantage over other methods, when it can be applied: it does not require any triangulation of the domain, only of its boundary. Therefore, it is also becomes a possible solution to the complicated problem of moving meshes. However, it is efficient only if the solution of the PDE is needed on the boundary. Thus, it is more or less limited to a problem of the type

$$\min_{\Omega \in \mathcal{O}} E(\Omega) = \int_\Gamma |\Phi - \Phi_d|^2 \, d\Gamma, \tag{107}$$

$$-\Delta\Phi = 0 \quad \text{in } \Omega, \left.\frac{\partial \Phi}{\partial n}\right|_\Gamma = g. \tag{108}$$

Recall from Eq. (71) of Chapter 2 that Φ is approximated by a piecewise constant function Φ_k on the element $\{T_k\}_1^N$ of Γ and it is computed from the linear system

$$2\pi\Phi_k + \sum_{l=1,\dots,N} \Phi_l \int_{T_l} \frac{\partial}{\partial n} |x - x^k|^{-1}\, d\Gamma = \sum_{l=1,\dots,N} \int_{T_l} g|x - x^k|^{-1}\, d\Gamma \qquad \forall k = 1,\dots,N, \quad (109)$$

where x^k is a point in T_k. Similarly, the criteria may be approximated by

$$E_h(\Gamma) = \sum_{k=1,\dots,N} |\Phi_k - \Phi_d(x^k)|^2 S_k, \quad (110)$$

where S_k is the area of T_k.

8.5.2 Optimality conditions

Without examining the details of the calculation of the above integrals, we can still give the form of the optimality conditions.

Proposition 5. *Assume that the elements $\{T_k\}$ are triangles defined by their vertices $\{q^l\}$ and that x^k is the barycenter of T_k; then*

$$\begin{aligned}\frac{\partial E_h}{\partial q_i^l} = \sum_{T_k \supset \{q^l\}} -\tfrac{2}{3}\frac{\partial \Phi_d}{\partial x_i}(x^k)(\Phi_k - \Phi_d(x^k))S_k + |\Phi_k - \Phi_d(x^k)|^2 \frac{\partial S_k}{\partial q_i^l} \\ + \sum_k p_k \left[\frac{\partial}{\partial q_i^l}\int_{\Gamma_h} g|x - x^k|^{-1}\, d\Gamma - \sum_{m,k} \Phi_m p_k \frac{\partial}{\partial q_i^l} \right. \\ \left. \times \int_{T_m} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma\right],\end{aligned} \quad (111)$$

where $\{p_k\}$ is the solution of

$$2\pi p_k + \sum_{l=1,\dots,N} p_l \int_{T_k} \frac{\partial}{\partial n}|x - x^l|^{-1}\, d\Gamma = 2(\Phi_k - \Phi_d(x^k))S_k, \qquad k = 1,\dots,N. \quad (112)$$

PROOF. Differentiating E_h, we obtain

$$\begin{aligned}\frac{\partial E}{\partial q_i^l} = \sum_{T_k \supset \{q^l\}} -\tfrac{2}{3}\frac{\partial \Phi_d}{\partial x_i}(x^k)(\Phi_k - \Phi_d(x^k))S_k + |\Phi_k - \Phi_d(x^k)|^2 \frac{\partial S_k}{\partial q_i^l} \\ + 2\sum_k (\Phi_k - \Phi_d(x^k))\frac{\partial \Phi_k}{\partial q_i^l} S_k.\end{aligned} \quad (113)$$

Now differentiate the equation that gives Φ_k:

$$\begin{aligned}2\pi\Phi_k' + \sum_l \Phi_l' \int_{T_l} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma = \frac{\partial}{\partial q_i^l}\int_{\Gamma_h} g|x - x^k|^{-1}\, d\Gamma \\ -\sum_m \Phi_m \frac{\partial}{\partial q_i^l}\int_{T_m} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma,\end{aligned} \quad (114)$$

where Φ'_k is short for $\partial\Phi_k/\partial q_i^l$. If it is multiplied by p_k and summed over k, it becomes

$$\sum_k 2\pi\Phi'_k p_k + \sum_{m,k} \Phi'_m p_k \int_{T_m} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma$$

$$= \sum_k p_k \frac{\partial}{\partial q_i^l} \int_\Gamma g|x - x^k|^{-1}\, d\Gamma - \sum_{m,k} \Phi_m p_k \frac{\partial}{\partial q_i^l} \int_{T_m} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma, \tag{115}$$

and by definition of p_k the first member is also

$$2\sum_m (\Phi_m - \Phi_d(x^m))\frac{\partial \Phi_m}{\partial q_i^l} S_m \qquad \square$$

Up to this point, we have encountered no difficulties except perhaps the fact that the linear system that gives $\{p_k\}$ is not the same as the one that gives $\{\Phi_k\}$. However, the computations of

$$\frac{\partial}{\partial q_i^l} \int_{T_m} \frac{\partial}{\partial n}|x - x^k|^{-1}\, d\Gamma,$$

and the similar computation for $q^l, q^k \in T_m$, are quite lengthy because we must differentiate the precise expressions. The lazy programmer may find that it is sufficient to approximate them from their finite difference equivalent, i.e.,

$$\frac{\partial}{\partial q_i^l} f(q^l) \simeq \frac{f(q_i^l + \delta q_i^l) - f(q_i^l)}{\delta q_i^l} \tag{116}$$

with $\delta q \simeq \frac{1}{1000}$; this is usually close enough, and at worst it is only twice as expensive on the computer as computing the exact expressions. We summarize the method below.

8.5.3 Algorithm 3

[0. Choose $\{T_k\}_1^N, M$.

For $k = 0, \ldots, M$ do

1. Solve (109).
2. Solve (112).
3. Compute $\partial E_h/\partial q_i^l$ by (111) and (116).
4. Compute an approximation of (see Chapter 4)

$$\rho^* = \arg\min E_h\left(\left\{q^l - \rho\frac{\partial E_h}{\partial q_i^l}\right\}\right). \tag{117}$$

5. Set $q_i^l := q_i^l - \rho^*\, \partial E_h/\partial q_i^l, \qquad i = 1, \ldots, 3, \quad l = 1, \ldots, N.$

8.5.4 Application

In potential approximation, the aerodynamic characteristics, lift l and pressure distribution C_p; of an airplane S flying at moderate speed may be found by solving for ϕ and l in the system

$$\Delta\phi = 0 \quad \text{in } \mathbb{R}^3 - S,$$

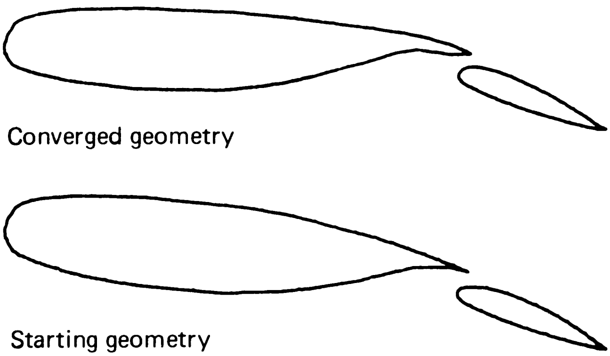
$$\left.\frac{\partial\phi}{\partial n}\right|_{\partial S} = 0, \qquad \phi(x \to \infty) \simeq u_\infty x + l; \tag{118}$$

$\nabla\phi$ parallel to the wake at the trailing edge.

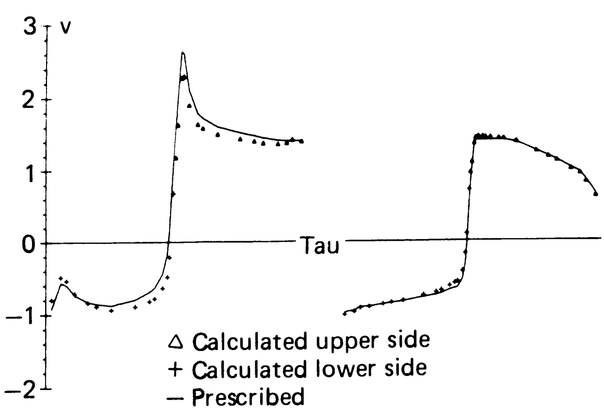
This system is currently solved by the boundary element method (panel method in three dimensions) in aeronautical engineering. The reduced pressure distribution C_p on the surface ∂S of the airplane is

$$C_p(x) = k_1 - k_2|\nabla\Phi|^2, \qquad x \in \partial S, \tag{119}$$

where k_1 and k_2 are the physical constraints.



(a) Airfoil shapes



(b) Velocity distribution

Fig. 8.6 Optimization of an airfoil by the boundary element method (from Labrujere [37]).

If a wing with a desired C_{pd} is to be designed, we may solve

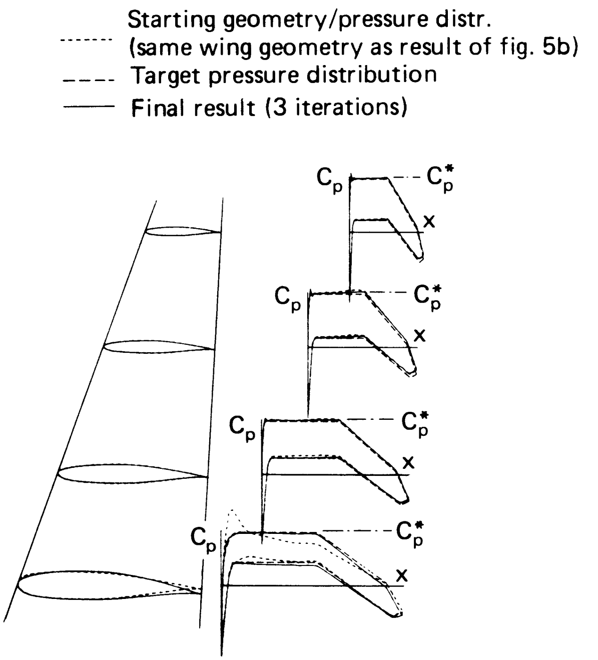
$$\min_{S \in \mathcal{O}} E(S) = \int_{\partial S} (C_p(S) - C_{pd})^2 \, d\Gamma. \tag{120}$$

In [37] and [28], this problem is not formulated as in (120); however, the problem is treated as the inverse problem. Namely, find S such that

$$C_p(S) = C_{pd}, \tag{121}$$

and (121) is solved by a Newton-type algorithm.

To compare results obtained from these two methods, we reproduce the shapes obtained by Labrujere *et al* [37] using the latter method (Figure 8.6) and those obtained by Fray and Slooff [28] for the former method, a compressible version of (118) in three dimensions (Figure 8.7).



a) • High weight on trailing–edge angle (10°)
• Low weight on leading–edge radius (2.5%)
• Zero weight on thickness and twist

Fig. 8.7 Optimization of a wing by the boundary element method (from Fray and Sloof [28]).

CHAPTER 9

Two Industrial Examples

9.1 Introduction

We present two applications of the solution methods, developed in previous chapters. Our purpose here is not only to illustrate the methods but also to show how certain implementation problems can be resolved when the solution methods are used. These implementation problems are:

- Effect of nonlinearities
- The relation between the motions of internal nodes and boundary nodes
- The oscillations of the unknown boundaries
- Nondifferentiable criteria

The examples are taken from [46] and [4]. The first one is the optimization of an electromagnet (see Figure 9.1). The second one is the optimization of an airfoil.

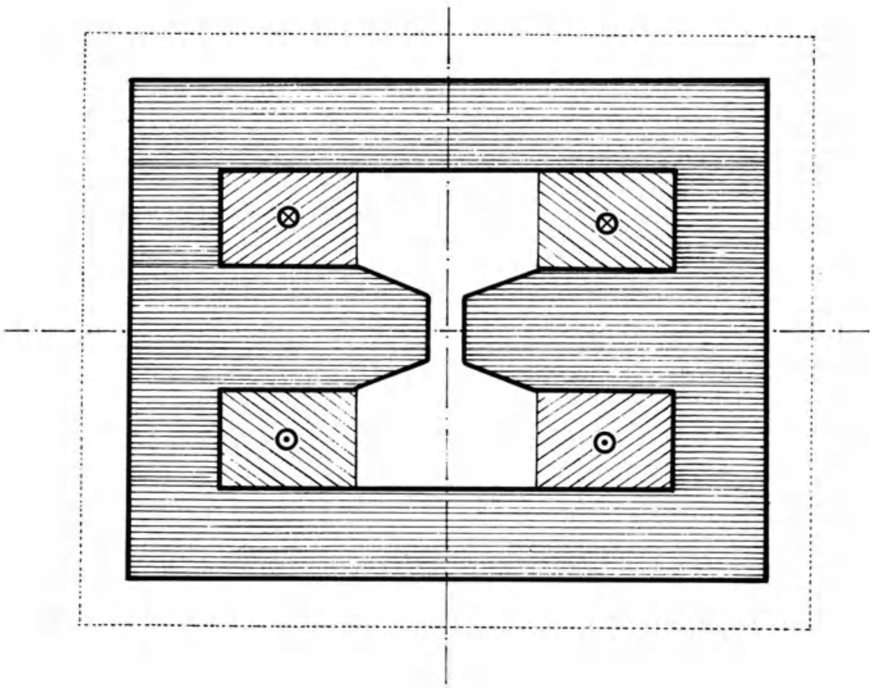


Fig. 9.1 Cross section of the electromagnet.

Finally, we summarize and determine the feasibility of these techniques for the future of industrial design.

9.2 Optimization of Electromagnets

9.2.1 Problem statement

The problem arises in connection with computer tape-reader heads for which a very constant magnetic field is desired in the polar region of the electromagnet. After some simplifications, Figure 9.1 shows a two-dimensional approximation of the physical domain shown in Figure 2.3. By symmetry we can restrict the analysis to one-fourth of the domain only (Figure 9.2):

$$C =]AB[\times]AD[, \qquad \partial C = \Gamma_0 \cup \Gamma_1, \qquad \Gamma_0 = DC \cup CB \cup BA, \qquad \Gamma_1 = DA. \quad (1)$$

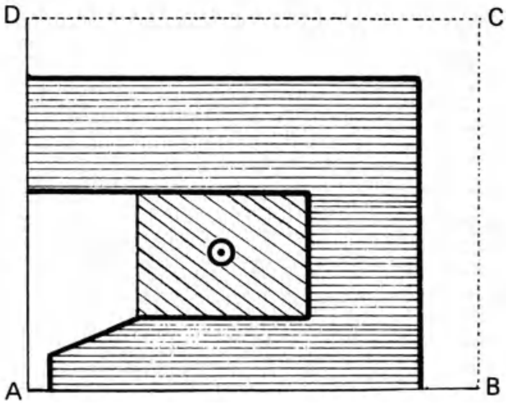


Fig. 9.2 Computational domain.

As explained in Section 1.6.3, the electromagnetic vector potential A satisfies an equation involving the current density $j(\cdot)$ in copper:

$$\nabla \cdot [\rho(|\nabla A|^2, x)\nabla A] = j \quad \text{in } C, \tag{2}$$

where ρ is defined by

$$\rho(|\nabla A|^2, x) = \begin{cases} \nu_a = \dfrac{10^7}{4\pi} \text{ MKSA} & \forall x \in C - \Omega_f \cup \Omega_c, \quad \forall A, \\ \nu_c = \dfrac{10^7}{4\pi} \text{ MKSA} & \forall x \in \Omega_c, \quad \forall A, \\ \nu_f = a + (b-a)\dfrac{|\nabla A|^{2\alpha}}{|\nabla A|^{2\alpha} + c} & \forall x \in \Omega_f, \quad \forall A. \end{cases} \tag{3}$$

The last equation is a numerical "fit" of experimental data (without hysteresis). Figure 9.3 shows the precision for the following values:

$$a = 5.164 \times 10^{-4}, \qquad b = 0.175775, \qquad c = 8758.756, \qquad \alpha = 5.4192. \tag{4}$$

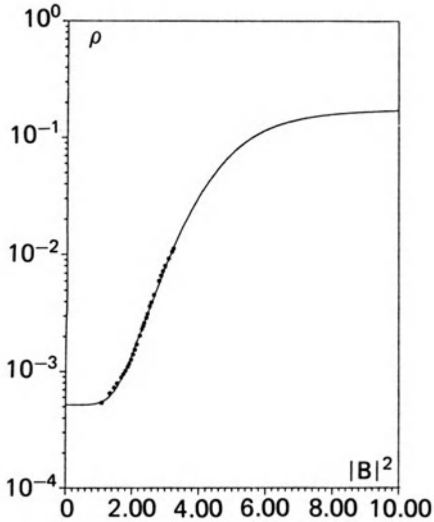


Fig. 9.3 Reluctivity ρ as a function of $|B|^2 = |\nabla \times A|^2$:"." experimental points;—fitting by (3).

The boundary conditions are

$$A = 0 \quad \text{on } \Gamma_0 \qquad \text{(symmetry)}, \tag{5}$$

$$\frac{\partial A}{\partial n} = 0 \quad \text{on } \Gamma_1 \qquad \text{(decay at infinity and symmetry)}. \tag{6}$$

By (3) ρ is a nondecreasing function of $|\nabla A|$, $\forall x \in C$; so (2), (5), and (6) define $A(\Omega_f)$ uniquely (see also Proposition 5 of Chapter 1).

We wish to find Ω_f such that the electromagnetic field $\nabla \times A$ is constant and equal to E_d in the interpolar region $D \subset C - \Omega_f \cup \Omega_c$; so we solve

$$\min_{\Omega_f \in \mathcal{O}} E(\Omega_f) = \int_D |\nabla A(\Omega_f) - u_d|^2 \, dx, \tag{7}$$

$$\mathcal{O} = \{\Omega_f : \Omega_f \subset C - \Omega_c - D, \ \Omega_f \text{ open set of } \mathbb{R}^2\}, \tag{8}$$

$$u_{d_1} = E_{d_2}, \qquad u_{d_2} = -E_{d_1}. \tag{9}$$

We consider two cases:

Problem A:	$D = D'$	(D fixed)
Problem B:	$D = D' \cap \Omega_f$	(D varies with Ω_f)

for a given fixed D'.

Remark. *Even if $\mathcal{O}$ is restricted to the sets Ω_k with Lipchitz boundaries of constant $k > 0$, it is difficult to prove that both problem A and problem B have at least one solution, (which may depend on k).*

9.2.2 Optimality conditions: continuous case

Proposition 1. *Suppose Ω'_f is defined from Ω_f and $\alpha \in C^1(\partial\Omega_f)$ by*

$$\partial\Omega'_f = \{x + \alpha(x)n(x) : x \in \partial\Omega_f\}. \tag{10}$$

Then the variation $\delta E = E(\Omega'_f) - E(\Omega_f)$ is given by

$$\delta E = \int_{\partial\Omega_f} [v_f(|\nabla A(\Omega_f)|^2, x) - v_a](\nabla A(\Omega_f) \cdot \nabla P)\alpha \, d\Gamma$$

$$+ \delta(B) \int_{\partial\Omega_f \cap D'} \alpha|\nabla A - u_d|^2 \, d\Gamma + o(\|\alpha\|_{C^1}), \tag{11}$$

where $\delta(B) = 1$ for problem B and 0 for problem A, and where P is the solution of

$$\nabla \cdot [\rho(|\nabla A|^2, x)\nabla P + 2\dot\rho(|\nabla A|^2, x)\nabla A \cdot \nabla P \nabla A] = \nabla \cdot [\chi_D(\nabla A - u_d)] \quad \text{in } C, \tag{12}$$

$$P = 0 \quad \text{on } \Gamma_0, \qquad \frac{\partial P}{\partial n} = 0 \quad \text{on } \Gamma_1, \tag{13}$$

and $\dot\rho$ is the derivative of ρ with respect to the argument $|\nabla A|^2$.

Proof. The symbol $\simeq$ stands for equality up to higher-order terms. By (7)

$$\delta E \simeq \int_{\delta D} |\nabla A - u_d|^2 \, dx + 2\int_D (\nabla A - u_d)\nabla\delta A \, dx. \tag{14}$$

The first integral gives the last integral in (11). By (2), (5), and (6)

$$\nabla \cdot (\rho(|\nabla A|^2, x)\nabla\delta A) + \nabla \cdot (\delta\rho\nabla A) \simeq 0 \quad \text{in } C, \tag{15}$$

$$\delta A = 0 \quad \text{on } \Gamma_0, \qquad \frac{\partial\delta A}{\partial n} = 0 \quad \text{on } \Gamma_1. \tag{16}$$

However, (15) and (16) in variational form are

$$\int_C (\rho\nabla\delta A\nabla w + \delta\rho \, \nabla A \cdot \nabla w) \, dx \simeq 0 \qquad \forall w \in H^1_{00}(C), \tag{17}$$

$$\delta A \in H^1_{00}(C) = \{w \in H^1(C) : w|_{\Gamma_0} = 0\}, \tag{18}$$

and (12) is

$$\int_C \rho\nabla P\nabla w + 2\dot\rho\nabla A \cdot \nabla P\nabla A \cdot \nabla w) \, dx = \int_D (\nabla A - u_d)\nabla w \, dx \qquad \forall w \in H^1_{00}(C), \tag{19}$$

$$P \in H^1_{00}(C). \tag{20}$$

So, as before, let $w = P$ in (17) and $w = \delta A$ in (19):

$$\int_D (\nabla A - u_d)\nabla\delta A\, dx \simeq \int_C [2\dot{\rho}\nabla A \cdot \nabla\delta A - \delta\rho]\nabla A \cdot \nabla P\, dx \tag{21}$$

Now by (3)

$$\delta\rho = \begin{cases} \nu_f - \nu_a & \forall x \in \Omega'_f \cap (C - \Omega_f \cup \Omega_c), \\ \nu_a - \nu_f & \forall x \in \Omega_f \cap (C - \Omega'_f \cup \Omega_c), \\ 2\dot{\rho}\nabla A\nabla\delta A & \forall x \in \Omega_f \cap \Omega'_f, \\ 0 & \text{elsewhere.} \end{cases} \tag{22}$$

Figure 9.4 shows that the first two cases are present in a region of thickness α; therefore,

$$\int_C \delta\rho\ \nabla A\nabla P\, dx \simeq \int_{\partial\Omega_f} \alpha(\nu_f - \nu_a)\nabla A \cdot \nabla P\, dx + \int_{\Omega_f} 2\dot{\rho}\nabla A \cdot \nabla\delta A\nabla A \cdot \nabla P\, dx, \tag{23}$$

which ends the proof, at least formally. As previously, we ought to check that the higher-order terms are $o(\|\alpha\|_{C^1})$ as in Chapter 6. □

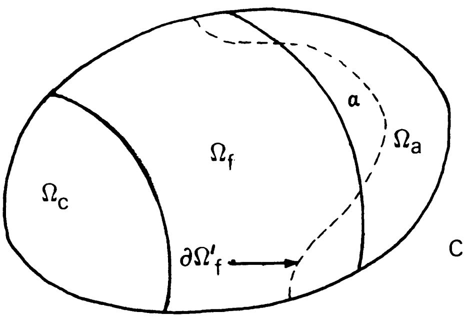


Fig. 9.4 Variation of the ferrous region Ω_f and of Ω_a.

9.2.3 Discretization

As there is no obvious Ω_f which gives

$$(\nu_f - \nu_a)\nabla A \cdot \nabla P + \delta(B)|\nabla A - u_d|^2 = 0, \tag{24}$$

we may use a computer to evaluate the optimization algorithms to solve (2) to (6), (12), (13), and (24). We have chosen to apply the finite element of degree 1 on triangular elements:

$$H_h^1 = \{w_h \in C^0(C_h): w_h|T_j \in P^1 \qquad \forall\, T_j \in \mathscr{T}_h\} \tag{25}$$

for a triangulation $\mathcal{T}_h$ of C_h on which the interfaces $\partial\Omega_f$ and $\partial\Omega_c$ are the sides of triangles. Then (2) to (6) are approximated by the following nonlinear system of finite dimension:

$$\int_C \rho_h(|\nabla A_h|^2, x)\nabla A_h \cdot \nabla w_h \, dx = \int_C j_h w_h \, dx \qquad \forall\, w_h \in V_h, \tag{26}$$

$$A_h \in V_h = \{w_h \in H_h^1 : w_h|\Gamma_{0h} = 0\}, \tag{27}$$

where ρ_h is piecewise constant on the triangles and is determined by $\rho(|\nabla A_h|^2, q^c)$, where q^c is the center of gravity of the triangle. If D_h is an approximation of D made of triangles and u_{dh} is a piecewise constant approximation of u_d, then we solve

$$\min_{\Omega_{fh} \in \mathcal{O}_h} E(\Omega_{fh}) = \int_{D_h} |\nabla A_h - u_{dh}|^2 \, dx. \tag{28}$$

Knowing the initial triangulation of Figure 9.5, we allow Ω_f to move by varying the vertices of the interpolar boundary on the lines of discretization as shown on Figure 7.6. Then in order to keep the triangulation regular, the nonboundary vertices are linked to the boundary vertices by an affine mapping, keeping the vertices of the two vertical lines of Figure 9.6 fixed.

9.2.4 Computation of derivatives in the discrete case

Let vertex q^k translates to $q^k + \delta q^k$; then from (28),

$$\delta E \simeq \int_{\delta D_h} |\nabla A_h - u_h|^2 \, dx + 2\int_{D_h} \nabla\delta A_h(\nabla A_h - u_{dh}) \, dx.$$

By Proposition 7.3,

$$\int_{\delta D_h} |\nabla A_h - u_h|^2 \, dx \simeq \int_{D_h} \delta q^k \nabla(w^k|\nabla A_h - u_{dh}|^2) \, dx. \tag{29}$$

Recall that $\delta A_h \simeq \Sigma\, \delta A_i w^i + A_i\, \delta w^i \simeq \delta\tilde{A}_h - w^k \nabla A_h \cdot \delta q^k$. So from (26), $\delta\tilde{A}_h \in V_h$ and

$$\begin{aligned}\sum_j \int_{T_j \cap T'_j} & [\delta\rho_h\, \nabla A_h \nabla w_h + \rho_h(\nabla\delta A_h \cdot \nabla w_h + \nabla A_h \nabla\delta w_h)] \, dx \\ & + \sum_j \int_{T'_j - T'_j \cap T_j} \rho'_h\, \nabla A'_h \nabla w'_h \, dx - \int_{T_j - T_j \cap T'_j} \rho_h \nabla A_h \nabla w_h \, dx \\ & \simeq 0 \qquad \forall\, w_h \in V_h.\end{aligned} \tag{30}$$

The prime refers to the quantities evaluated on the triangulation associated with $q^k + \delta q^k$.

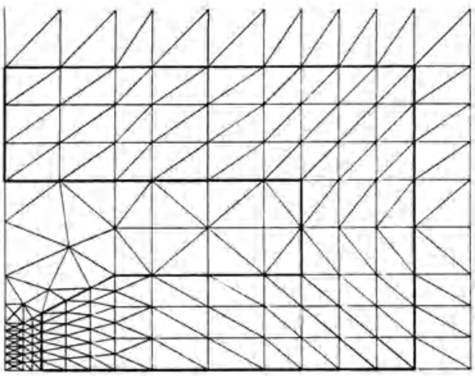


Fig. 9.5 An initial triangulation (158 nodes. 267 elements).

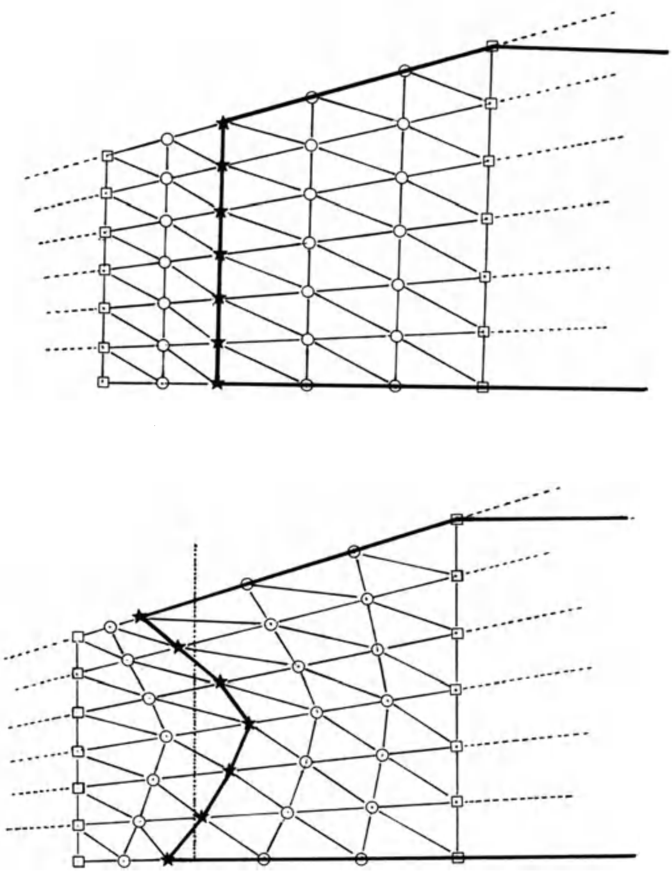


Fig. 9.6 Triangulation of the poles: □ fixed nodes, * principal moving nodes, ○ associated moving nodes.

Proposition 2 of Chapter 7 gives us δw_h, and Proposition 3 of Chapter 7 allows us to simplify the last two sets of integrals; thus, (30) becomes

$$\int_C 2\dot{\rho}_h \nabla A_h \cdot \nabla\delta\tilde{A}_h \nabla A_h \nabla w_h + \rho_h(\nabla\delta\tilde{A}_h \cdot \nabla w_h - \nabla A_h \cdot \nabla w^k \delta w_h \cdot \nabla q^k)\,dx$$

$$- \int_C (2\dot{\rho}_h \nabla A_h \cdot \nabla w^k \nabla A_h \cdot \delta q^k \nabla A_h \cdot \nabla w_h + \rho_h \nabla w^k \cdot \nabla w_h \nabla A_h \cdot \delta p^k)\,dx$$

$$+ \int_C \delta q^k \cdot \nabla(w^k \rho_h \nabla A_h \cdot \nabla w_h)\,dx \simeq 0. \tag{31}$$

Thus, the adjoint equation ought to be $P_h \in V_h$ and

$$\int_C (\rho_h \nabla P_h \cdot \nabla w_h + 2\dot{\rho}_h \nabla A_h \cdot \nabla w_h \nabla A_h \cdot \nabla P_h)\,dx$$

$$\simeq 2\int_{D_h} (\nabla A_h - u_{dh}) \cdot \nabla w_h\,dx \qquad \forall\, w_h \in V_h. \tag{32}$$

Then (31) and (32) imply

$$\begin{aligned} 2\int_{D_h} (\nabla A_h - u_{dh}) \cdot \nabla\delta\tilde{A}_h\,dx \simeq & \int_C (\rho_h \nabla A_h \cdot \nabla w^k \nabla P_h \cdot \delta q^k \\ & - \rho_h \nabla A_h \cdot \nabla P_h \nabla w^k \cdot \delta q^k \\ & + 2\dot{\rho}_h \nabla A_h \cdot \nabla w^k \nabla A_h \cdot \delta q^k \nabla A_h \cdot \nabla P_h \\ & + \rho_h \nabla w^k \cdot \nabla P_h \nabla A_h \cdot \delta q^k)\,dx \\ & + \int_{Dh} ((|\nabla A_h - u_{dh}|)^2 \nabla w^k \cdot \delta q^k \\ & - 2(\nabla A_h - u_{dh}) \cdot \nabla w^k \nabla A_h \cdot \delta q^k)\,dx. \end{aligned} \tag{33}$$

We summarize this result in Proposition 2.

Proposition 2. *If $P_h \in V_h$ is the solution of (32), then*

$$\begin{aligned} \frac{\partial E}{\partial q_l^k} = & \int_C \Bigg[\rho_h(|\nabla A_h|^2)\left(\nabla A_h \cdot \nabla w^k \frac{\partial P_h}{\partial x_l} - \nabla A_h \cdot \nabla P_h \frac{\partial w^k}{\partial x_l} + \nabla w^k \cdot \nabla P_h \frac{\partial A_h}{\partial x_l}\right) \\ & + 2\dot{\rho}_h(|\nabla A_h|^2) \nabla A_h \cdot \nabla w^k \nabla A_h \cdot \nabla P_h \frac{\partial A_h}{\partial x_l}\Bigg]\,dx \\ & + \int_{D_h} \left[|\nabla A_h - u_{dh}|^2 \frac{\partial w^k}{\partial x_l} - 2(\nabla A_h - u_{dh}) \cdot \nabla w^k \frac{\partial A_h}{\partial x_l}\right] dx. \end{aligned} \tag{34}$$

This formula does not take into account the links between the nodes of $\partial\Omega_{fh}$ and the internal nodes. Recall that if there are N' moving nodes and N independent motions,

$$q^k = X^k(t_1, \ldots, t_N), \qquad k = 1, \ldots, N' \tag{35}$$

implies

$$\frac{\partial E}{\partial t_i} = \sum_{k,l} \frac{\partial E}{\partial q_l^k} \frac{\partial X_l^k}{\partial t_i}. \tag{36}$$

Here $\{t_i\}$ are the curvilinear abscissas of the vertices of $\partial\Omega_{fh}$ on the lines of discretization along which they move.

9.2.5 Algorithms and Numerical Examples

The method of steepest descent has been chosen to develop the following algorithm.

Algorithm 1

[0. Choose $\{t_i^0\}$ (i.e., build $\mathcal{T}_h$; choose M.

For $m = 0, \ldots, M$ do

1. Compute A_h and P_h by (26) and (32).
2. Compute $\partial E/\partial t_i$ by (36) to (34).
3. Compute by Algorithm 3 of Chapter 4 an approximation ρ of the minima of E with respect to $\rho > 0$, when the vertices $\{q^k\}$ move as described by (35) with the t_i replaced by $t_i^m - \rho\partial E/\partial t_i$:

$$\frac{1}{\rho}\delta q^k = \sum_i \frac{\partial X^k}{\partial t_i}\frac{\partial E}{\partial t_i}; \tag{37}$$

where ρ is subject to a box constraint $\rho \in \,]a, b[$ since each vertex must stay within the domain of Figure 9.6.

4. Set $t_i^{m+1} = t_i^m - \rho\, \partial E/\partial t_i$, compute the new triangulation by (35).

The computer program to do this algorithm consists of five modules:

1. A module for solving (26) by the overrelaxation method
2. A module for solving (32) by Cholesky factorization
3. A module that computes the "direction of descent (37)" of each vertex of $\mathcal{T}_h$, when A_h and P_h are known
4. A module for the computation of ρ (step 3 of algorithm)
5. A plotting module

Numerical Experiment 1: $D_h = D'_h$ *fixed*

Let D_h be the union of all triangles between the first two vertical lines on the left and the first seven horizontal lines from the bottom left of the triangulation of Figure 9.5.
The current density $j = 5 \times 10^5$ MKSA. When $u_d = \{0, 1.3\}$, the initial value for the criteria and its value after nine iterations are

$$E(\Omega_f^0) = 0.6116 \times 10^{-5} \quad \text{and} \quad E(\Omega_f^9) = 0.3445 \times 10^{-5}.$$

Figure 9.7 shows $E(\Omega_f^m)$ versus m for four different values of j and u_d. Figure 9.8 shows the shape of Ω_f^9.

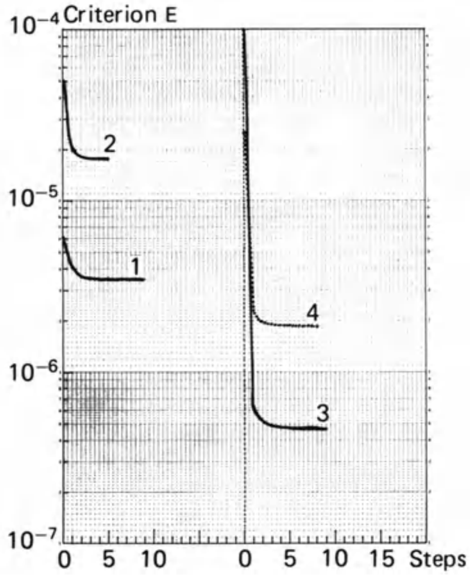
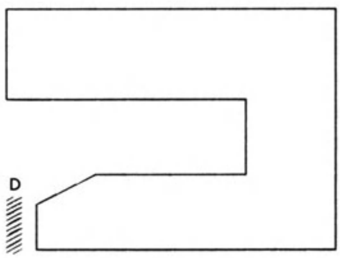


Fig. 9.7 Variation of the criterion with the iteration index for four values of j and u_h. (1) $j = 5\ 10^6$; $u_h = \{1.3, 0\}$. (2) $j = 5\ 10^6$; $u_h = \{1.6, 0\}$. (3) $j = 20\ 10^6$; $u_h = \{1.3, 0\}$. (4) $j = 20\ 10^6$; $u_h = \{1.6, 0\}$.



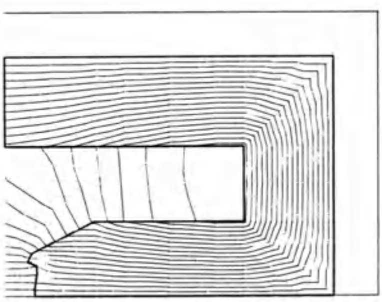


Fig. 9.8 D and Ω^9 for $u_d = \{1.3, 0\}$, $j = 5 \times 10^6$ MKSA (from [46]).

Numerical Experiment 2. For $D_h = D'_h \cap \Omega_f$, take $j = 2 \times 10^7$ MKSA and $u_d = \{0, 1.3\}$. D_h is shown in Figure 9.9. Figures 9.10 to 9.12 show Ω_f^{10}, Ω_f^{16}, and Ω_f^{56}, respectively. These were obtained by smoothing the oscillations (reinitialization) at iterations 17 and 37. (The total computing time was 3 minutes on an IBM 370/168.) Figure 9.13 shows $E(\Omega_f^m)$ versus m.

It seems that the discrete problem has an oscillating boundary for its solution; if the triangulation size is divided by 2, then the number of oscillations is doubled. This problem can be solved another way, as we shall see, by allowing free movement for all other vertices, restricting only the movement of $q^k = (q^{k+1} + q^{k-1})/2$, $\forall\, k$ odd, for example.

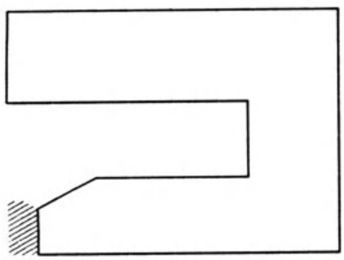


Fig. 9.9 The shaded region is $D' \cap \Omega$.

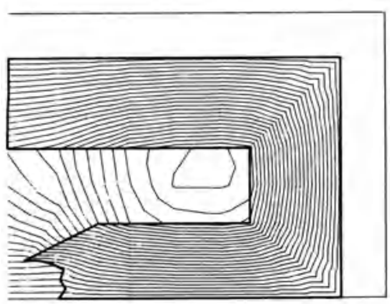


Fig. 9.10 Shape $\Omega^{10} \cdot u_d = \{0, 1.3\}$; $j = 20 \times 10^6$ MKSA.

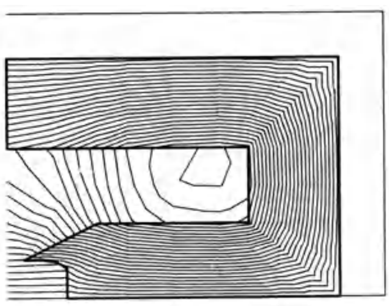


Fig. 9.11 Shape Ω^{16} after smoothing.

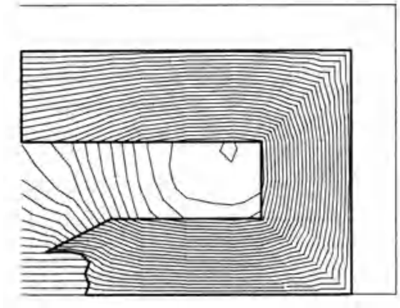


Fig. 9.12 Shape Ω^{56}.

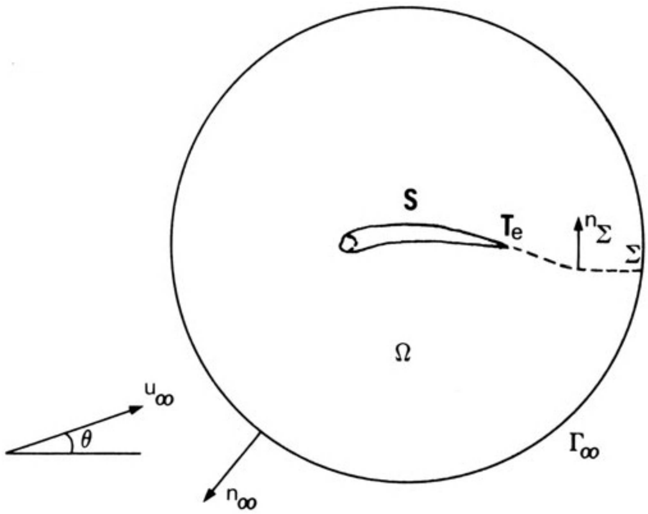


Fig. 9.13 Airfoil S in a flow limited by Γ_∞. The wake is simulated by $\sum$. The angle of attack Θ may vary.

9.3 Optimization of Airfoils

9.3.1 Problem statement

The design of airfoils, or wings, with good aerodynamical properties is an important problem of aeronautical engineering. Although the real problem is three-dimensional and in the transonic regime, we present results for the two-dimensional subsonic case only. The basic design problem is to find a wing of given lift and minimum drag at "crusing" speed u_∞ that is acceptable at other crusing speeds near u_∞ and that can be built mechanically.

The problem can be simplified by assuming that the drag is proportional to the distance d between the trailing edge and the point where the boundary layer separates. In turn, a smooth, flat pressure distribution $p|_S$ on the surface of the airfoil gives a small d. So, for some known p_d (to make the problem more general), we may consider the problem

$$\min_S |p - p_d|_{\infty,S}. \tag{38}$$

However, these criteria are nondifferentiable; so that L^∞ norm is approximated by the L^q norm, $q \gg 1$, and we consider the problem

$$\min_S E(\Omega) = \int_S |p - p_d|^q \, d\Gamma. \tag{39}$$

In the potential approximation of the compressible Navier–Stokes equation, the velocity $u(x)$ is the gradient $\nabla\Phi(x)$ of a potential Φ which is a solution of

$$\nabla \cdot [(1 - |\nabla\Phi|^2)^{1/(\gamma-1)}\nabla\Phi] = 0, \tag{40}$$

and the pressure is

$$p = p_1(1 - |\nabla\Phi|^2)^{\gamma/(\gamma-1)} \tag{41}$$

(for air $\gamma = 1.4$); p_1 is a given constant. As shown in Figure 9.10, Γ_∞ approximates the boundary at infinity $\Gamma = \partial\Omega = S \cup \Gamma_\infty$, and the boundary conditions are of the Neumann type:

$$\frac{\partial\Phi}{\partial n} = g \quad \text{on } \Gamma, \tag{42}$$

where $g = 0$ on S, and $g = u_\infty \cdot n$ on Γ_∞. From Proposition 6 of Chapter 1, (40) and (42) have a unique solution in $H^1(\Omega)$ (up to a constant because $\Gamma_1 = \varnothing$) if

$$(1 - |\nabla\Phi|^2)^{1/(\gamma-1)} - \frac{2}{\gamma-1}|\nabla\Phi|^2(1 - |\nabla\Phi|^2)^{1/(\gamma-1)-1} > 0,$$

i.e.,

$$|\nabla\Phi|^2 \leq \frac{\gamma-1}{\gamma+1}, \tag{43}$$

In physical terms this means that the flow would be subsonic. If (41) does not hold, then the solution is not unique. Another condition is needed; namely, the entropy condition ($\Delta\Phi \neq +\infty$ for the case of shocks).

Unfortunately, the solution of (40), (42), and (43) is unacceptable because it usually rotates around the trailing edge. Therefore, the constraint $\Phi \in H^1(\Omega)$ is relaxed, a line of discontinuity Σ is introduced to simulate the wake of the profile, and

$$\Phi|_{\Sigma^+} - \Phi|_{\Sigma^-} = \alpha \qquad \text{(constant)}, \tag{44}$$

where α is adjusted so that the flow is tangent to the wake Σ at the trailing edge T_e:

$$\frac{\partial \Phi}{\partial n_\Sigma} \text{ continuous at } T_e. \tag{45}$$

Again, at least in two dimensions, one can show that (40) to (45) have a unique solution if g is not too large [*cf.* (43)].

So we assume that g is such that (43) is satisfied for any S in the set of allowable profiles. We also assume that α is given (because α is proportional to the lift) but that the angle of incidence θ is not known and that

$$g|_{\Gamma_\infty} = |u_\infty|(n_{\infty 1}\cos\theta + n_{\infty 2}\sin\theta), \tag{46}$$

where $(n_{\infty 1}, n_{\infty 2})$ is the normal of Γ_∞. Then we denote by $\Phi(S,\theta)$ the solution of (40), (42) plus (46), and (44). We set

$$E(S,\theta) = \int_S [(1 - |\nabla\Phi(S,\theta)|^2)^{\gamma/(\gamma-1)} - p_d]^q \, d\Gamma, \tag{47}$$

$$F(S,\theta) = \left[\frac{\partial}{\partial n_\Sigma}\Phi(S,\theta)^+ - \frac{\partial}{\partial n_\Sigma}\Phi(S,\theta)^-\right]\bigg|_{x=T_e}, \tag{48}$$

and we solve

$$\min_{\substack{S\in\mathcal{S}\\ \theta\in[0,\pi/2]}} \{E(S,\theta) : F(S,\theta) = 0\}. \tag{49}$$

There are many constraints on S in practice. In particular, to define θ independently of S, all trailing edges should be at T_e, and all S should be tangent at their leading edge to some circle of radius μ and center L_e, and this circle should be contained in the domain delimited by S (Figure 9.13). To rule out flat airfoils, we also require that the area delimited by S remains constant.

9.3.2 Discretization

We use the simple P^1 finite element method to solve our problem. Let

$$H_h^1(\alpha) = \{w_h \in C^0(\Omega_h - \Sigma) : w_h|_{T_j} \in P^1 \quad \forall\, T_j \in \mathcal{T}_h;\ w_h|_{\Sigma^+} - w_h|_{\Sigma^-} = \alpha\}, \tag{50}$$

where $\mathcal{T}_h$ is a triangulation of Ω such that Σ is made of sides of triangles and

$$\Omega = \bigcup_j T_j. \tag{51}$$

Let $\Phi_h(S,\theta) \in H_h^1(\alpha)$ be the solution of

$$\int_\Omega (1 - |\nabla\Phi_h|^2)^r\, \nabla\Phi_h \cdot \nabla w_h \, dx = \int_{\Gamma_\infty} |u_\infty|(\cos\theta\, n_{\infty 1} + \sin\theta\, n_{\infty 2}) w_h \, d\Gamma \qquad \forall\, w_h \in H_h^1(0). \tag{52}$$

where

$$r = \frac{1}{\gamma - 1}. \tag{53}$$

Let

$$D_h = \bigcup_{j \in J} T_j; \qquad J = \{j : T_j \cap S = 1 \text{ side}\}. \tag{54}$$

Then $E(S, \theta)$ is approximated by

$$E_h(S, \theta) = \int_{D_h} ((1 - |\nabla \Phi_h|^2)^{r+1} - p_d)^q \, dx \tag{55}$$

and

$$F_h(S, \theta) = |\nabla \Phi_h|^2|_{T^+} - |\nabla \Phi_h|^2|_{T^-}, \tag{56}$$

where T^+ and T^- are the two triangles of D_h containing the point T_e.

9.3.3 Computation of the Derivatives

We proceed as before: one vertex of S, q^k, translates to $q^k + \delta q^k$, and we compute the changes $\delta\Phi_h$, δE_h, and δF_h. Then θ is changed to $\theta + \delta\theta$, and the corresponding changes are also computed.

Proposition 3. *Let $\delta\tilde{\Phi}_h \in H_h^1(0)$ be the solution of*

$$\begin{aligned}
&\int_\Omega [(1 - |\nabla\Phi_h|^2)^r \nabla\delta\tilde{\Phi}_h \nabla w_h - 2r\nabla\Phi_h \cdot \nabla\delta\tilde{\Phi}_h (1 - |\nabla\Phi_h|^2)^{r-1} \nabla\Phi_h \cdot \nabla w_h] \, dx \\
&\quad = \delta\theta \int_{\Gamma_\infty} |u_\infty|(-\sin\theta \, n_{\infty 1} + \cos\theta \, n_{\infty 2}) w_h \, d\Gamma \\
&\quad\quad - \int_\Omega \delta q^k \cdot \nabla[(1 - |\nabla\Phi_h|^2)^r \nabla\Phi_h \nabla w_h w^k] \, dx \\
&\quad\quad + \int_\Omega [(1 - |\nabla\Phi_h|^2)^r \nabla w^k \cdot \nabla w_h \nabla\Phi_h \cdot \delta q^k \\
&\quad\quad - 2r\nabla\Phi_h \cdot \nabla w^k (1 - |\nabla\Phi_h|^2)^{r-1} \nabla\Phi_h \cdot \nabla w_h \nabla\Phi_h \cdot \delta q^k \\
&\quad\quad + (1 - |\nabla\Phi_h|^2)^r \nabla\Phi_h \cdot \nabla w^k \nabla w_h \cdot \delta q^k] \, dx - \int_{\Gamma_\infty} u_\infty n w^k \nabla w_h \cdot \delta q^k \, d\Gamma, \\
&\qquad\qquad\qquad\qquad\qquad\qquad \forall\, w_h \in H_h^1(0).
\end{aligned} \tag{57}$$

Then

$$\delta\Phi_h \simeq \delta\tilde{\Phi}_h - w^k \nabla\Phi_h \cdot \delta q^k, \qquad \forall\, \delta q^k, q^k \notin \Gamma_\infty. \tag{58}$$

PROOF. To simplify the formulas, we introduce the notation

$$\rho_h = (1 - |\nabla\Phi_h|^2)^r, \qquad \dot{\rho}_h = -r(1 - |\nabla\Phi_h|^2)^{r-1}. \tag{59}$$

Then we differentiate (52),

$$\begin{aligned}\int_{\delta\Omega} \rho_h \nabla\Phi_h \cdot \nabla w_h \, dx &+ \int_\Omega (\delta\rho_h \nabla\Phi_h \cdot \nabla w_h + \rho_h \nabla\delta\Phi_h \cdot \nabla w_h + \rho_h \nabla\Phi_h \cdot \nabla\delta w_h) \, dx \\ &= \int_{\Gamma_\infty} [|u_\infty|(-\sin\theta\, n_{\infty 1} + \cos\theta\, n_{\infty 2})\delta\theta w_h \\ &\quad + |u_\infty|(\cos\theta\, n_{\infty 1} + \sin\theta\, n_{\infty 2})]\delta w_h \, d\Gamma,\end{aligned} \tag{60}$$

and use the results of Chapter 7:

$$\int_{\delta\Omega} f dx = \int_\Omega \delta q^k \nabla(w^k f) \, dx, \tag{61}$$

$$\delta w_h = -w^k \nabla w_h(q^k) \cdot \delta q^k, \tag{62}$$

$$\delta\Phi_h = \Sigma\, \delta\Phi_i w^i + \delta w^i \Phi_i = \delta\tilde{\Phi}_h - w^k \nabla\Phi_h(q^k) \cdot \delta q^k. \tag{63}$$

Proposition 4. *With the notation of (59);*

$$\begin{aligned}\delta E_h(S,\theta) = &\int_{D_h} [\delta q^k \cdot \nabla\{[(1 - |\nabla\Phi_h|^2)^{r+1} - p_d]^q w^k\} \\ &+ q[(1 - |\nabla\Phi_h|^2)^{r+1} - p_d]^{q-1} \\ &\times (2(r+1)\rho_h \nabla\Phi_h \cdot \nabla w^k \nabla\Phi_h \cdot \delta q^k - \nabla p_d \cdot \delta q^k)] \, dx \\ &+ \delta\theta \int_{\Gamma_\infty} |u_\infty|(-\sin\theta\, n_{\infty 1} + \cos\theta\, n_{\infty 2}) p_h \, d\Gamma \\ &- \int_\Omega \delta q^k \cdot \nabla(\rho_h \nabla\Phi_h \cdot \nabla p_h w^k) \, dx + \int_\Omega [\rho_h \nabla w^k \cdot \nabla p_h \nabla\Phi_h \cdot \delta q^k \\ &+ 2\nabla\Phi_h \cdot \nabla w^k \dot{\rho}_h \nabla\Phi_h \cdot \nabla p_h \nabla\Phi_h \cdot \delta q^k \\ &+ \rho_h \nabla\Phi_h \cdot \nabla w^k \nabla p_h \cdot \delta q^k] \, dx - \int_{\Gamma_\infty} u_\infty \cdot n w^k \nabla p_h \cdot \delta q^k \, d\Gamma,\end{aligned} \tag{64}$$

where $p_h \in H_h^1(0)$ is the solution of

$$\begin{aligned}\int_\Omega &(\rho_h \nabla w_h \cdot \nabla p_h + 2\dot{\rho}_h \nabla\Phi_h \cdot \nabla w_h \nabla\Phi_h \cdot \nabla p_h) \, dx \\ &= -2(r+1)q \int_{D_h} ((1 - |\nabla\Phi_h|^2)^{r+1} - p_d)^{q-1} \rho_h \nabla\Phi_h \nabla w_h \, dx \qquad \forall\, w_h \in H_h^1(0).\end{aligned} \tag{65}$$

PROOF. From (55)

$$\delta E = \int_{\delta D_h} ((1 - |\nabla\Phi_h|^2)^{r+1} - p_d)^q \, dx$$
$$+ \int_{D_h} q((1 - |\nabla\Phi_h|^2)^{r+1} - p_d)^{q-1}[-2(r+1)\nabla\Phi_h \cdot \nabla\delta\Phi_h(1 - |\nabla\Phi_h|^2)^r$$
$$- \nabla p_d \cdot \delta q^k] \, dx \tag{66}$$

Thus from (61) through (63), we obtain the first integral of the right hand side of (64) plus the remaining term:

$$-\int_{D_h} 2(r+1)q\big((1 - |\nabla\Phi_h|^2)^{r+1} - p_d)^{q-1} \nabla\Phi_h \cdot \nabla\delta\tilde{\Phi}_h\rho_h \, dx.$$

Therefore, p_h is defined by (65). Now take $w_h = p_h$ in (57) and $w_h = \delta\Phi_h$ in (65) to give (64). □

Proposition 5.

$$\delta F_h = \delta\theta \int_{\Gamma_\infty} |u_\infty|(-\sin\theta \, n_{\infty 1} + \cos\theta \, n_{\infty 2}) r_h \, d\Gamma - \int_{\Gamma_\infty} u_\infty \cdot n w^k \nabla r_h \cdot \delta q^k \, d\Gamma$$
$$+ \int_\Omega [\rho_h(\nabla w^k \cdot \nabla r_h \nabla\Phi_h \cdot \delta q^k + \nabla\Phi_h \cdot \nabla w^k \nabla r_h \cdot \delta q^k)$$
$$+ 2\dot{\rho}_h \nabla\Phi_h \cdot \nabla w^k \nabla\Phi_h \cdot \nabla r_h \nabla\Phi_h \cdot \delta q^k] \, dx$$
$$- 2[\nabla\Phi_h \cdot \nabla w^k \nabla\Phi_h \cdot \delta q^k|_{T^+} - \nabla\Phi_h \cdot \nabla w^k \nabla\Phi_h \cdot \delta q^k|_{T^-}]$$
$$- \int_\Omega \delta q^k \cdot \nabla(\rho_h \nabla\Phi_h \cdot \nabla p_h w^k) \, dx \tag{67}$$

where $r_h \in H_h^1(0)$ is the solution of

$$\int_\Omega [\rho_h \nabla w_h \cdot \nabla r_h + 2\dot{\rho}_h \nabla\Phi_h \cdot \nabla w_h \nabla\Phi_h \cdot \nabla r_h] \, dx = 2(\nabla\Phi_h \cdot \nabla w_h|_{T^+} - \nabla\Phi_h \cdot \nabla w_h|_{T^-})$$
$$\forall\, w_h \in H_h^1(0). \tag{68}$$

PROOF. By differentiating (56), we obtain

$$\delta F_h = 2\nabla\Phi_h \nabla\delta\Phi_h|_{T^+} - 2\nabla\Phi_h \nabla\delta\Phi_h|_{T^-}. \tag{69}$$

Now use (62) to obtain the last term in (67) and a remaining term, which is the right-hand side of (68).

The rest of the proof is similar to that of Proposition 4. □

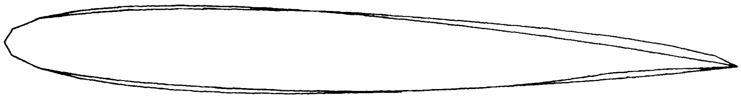


Fig. 9.14 Initial and final airfoil S^0, S^{30} (from [4]).

9.3.4 Numerical tests

To avoid oscillations, it is important to restrict the movement of all points on the airfoil by

$$\delta q^{2n} = \tfrac{1}{2}(\delta q^{2n-1} + \delta q^{2n+1}), \tag{70}$$

with the provision that all other vertices can move freely subject to the usual constraints, i.e., that they remain in the domain of Figure 7.2.

There is an additional constraint: the trailing edge should remain physically sound. It is this last constraint that limits the step size (ρ of the one-dimensional minimization) of the algorithm. The reduced gradient method is used (Algorithm 6 of Chapter 4). The initial S is shown on Figure 9.14; $\alpha = 0.04$, $u_\infty = 0.5$; $p_d = 0$, $m = 4$; nine points are fixed at the leading edge; $E(S^0, \theta^0) = 1$. S^0 is shown in Figures 9.14, S^{30} on 9.15, and Figure 9.16 shows the pressure on S^0 and S^{30}. The computing time is 1 hour cpu time on an IBM 3033, and the criteria are given as $E(S^{30}, \theta^{30}) = 0.53$.

9.3.5 Nondifferentiable criteria

Consider the case

$$E(S, \theta) = \sup_S \,(1 - |\nabla\Phi|^2)^{r+1}. \tag{71}$$

The gradient of E with respect to S or θ does not exist everywhere; however, it is still possible to derive optimality conditions, as is explained in [60].

In the discrete case,

$$E_h(S, \theta) = \sup_{T_j \in D_h} \,(1 - |\nabla\Phi_h|^2)^{r+1}|_{T_j}; \tag{72}$$

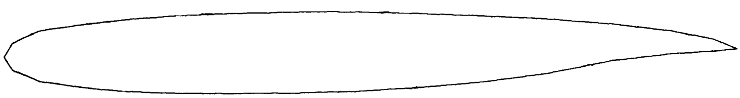


Fig. 9.15 Final airfoil S^{30}.

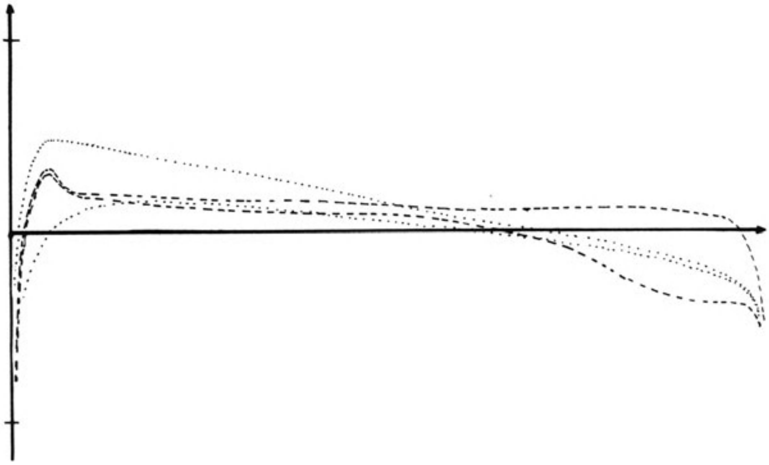


Fig. 9.16 Pressure distribution on the skin of S^0(...) and S^{30}(---).

thus there exists i such that

$$E_h(S, \theta) = (1 - |\nabla\Phi_h|^2)^{r+1}|_{T_i}, \tag{73}$$

and therefore,

$$\delta E_h = -2(r + 1)\rho_h \nabla\Phi_h \nabla\delta\Phi_h|_{T_i} \tag{74}$$

except if q^k is such that any small variation in one direction makes T_i become $T_{i'}$. In otherwords, E_h is almost everywhere differentiable. Experience shows that in such circumstances the gradient can be computed as usual from (74), and the optimization algorithms can be used as if normal conditions existed.

9.4 Conclusion

The two examples treated in this chapter illustrate the feasibility of optimal shape design by the finite element method: the formulae for the derivatives of the criteria and constraints are rather straightforward; the adjoint equations are usually no more difficult to solve than the state equations since they are linear and of the same type. The amount of programming needed is determined by the moving meshes, and programming the simulation of moving meshes, we must admit, is a rather time-consuming task. On the other hand, the finite difference methods have their own difficulties: the mapping of domains and the complicated formulae for the derivatives. Finally, we must note that in an industrial setting time is spent setting up the allowable set of shapes in order to get a feasible solution.

Examining these problems from the mathematical point of view, we find there is still work to be done on the problem of the existence of solutions and on the problem of convergence properties of algorithms. Nonetheless, when it is necessary to find the optimal shape, these difficulties can be overcome as we have shown. Thus interesting developments and new applications in three-dimensional shape optimization studies in industry are likely to develop in the near future.

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