Optimal Shape Design by Local Boundary Variations

Olivier Pironneau

University of Paris 6 - email: Olivier.Pironneau @ann.jussieu.fr

1. Introduction

Hadamard (1910) may have been the first applied mathematician to derive a formula for the sensitivity of a Partial Differential Equation (PDE) with respect to the shape of its domain. This opened the field of Optimal Shape Design (OSD). But the field as we know it now, really began with Cea et al (1973) as an offspring of optimal control theory (Lions (1968)) and the calcul of variation. So OSD has borrowed the vocabulary of control theory: the design is done by minimizing a *cost* function, which depends upon a *state* variable, i.e. the solution of the PDE, itself function of a *control*, the shape.

Among others, Pironneau (1973), Murat-Simon (1976), Cea (in Haug et al (1978) gave methods to derive optimality conditions for the continuous problems and Begis et al (1976) Morice (1976) and Marrocco et al (1978), in the same school, for the discretized problems.

Theoretical results on existence of solutions were obtained by Chenais (1975), Sverak (1992) Bucur et al. (1995) and Liu et al (1999); a counter example to existence was produced by Tartar (1975) in a key paper which linked optimal shape design with homogenization theory in what is now known as "topological optimization".

Most design engineers do their optimization by hand, intuitively. But it is generally believed that intuitive optimization is not possible beyond a handfold of degrees of freedom. When the design parameters are few, say less than a hundred, sensitivity with respect to shape can be obtained by finite difference approximation (take two $\epsilon-$close shapes and approximate the derivative by the difference of the values of the cost function divided by ϵ) and essentially no additional programming is needed beyond the state equation solver. But the precision may not be sufficient and stiff problens cannot be solved this way.

There are also commercial packages which find the minimum of a functional with respect to parameters and require from the user only a subroutine to evaluate the cost function for a given design. These packages are usally based on local variation methods (Powell(1970)), involving polynomial fits of the functional from point evaluations. They are expensive here because they require $O(P^2)$ solutions of the flow solver where P is the number of design variables.

But for 3D wings for example, there are hundreds of design parameters so that shape optimization requires a complete numerical treatment with a robust differentiable optimization package and a precise sensitivity analysis with respect to the shape of the wing.

A numerical fluid solver can be vewed as a C function with an input and an output , the design variables which define the wing shape and the drag for instance. Sensitivity analysis finds the gradient of the cost function with respect to the design variables. It is difficult when the fluid is compressible. An alternative is to let the computer do it for you by using a software for "Automatic Differentiation of programs" such as ADOL-C. This approach is extremely convenient and we shall give here a brief presentation. But to understand it fully it is better to know the analytical approach as well; this is the object of the paragraph on sensistivity analysis. More details can be found in Pironneau (1983), Neittanmaki (1991), and Banichuk (1990).

2. Examples

Before going to industrial examples let us present two laboratory examples which will serve to illustrate the method of solution chosen here.

2.1 Two Laboratory Test Cases: Nozzle Optimization

For clarity we will consider an optimization problem for incompressible irrotational inviscid flows

$$\min_{\partial\Omega}\{\int_D |\nabla\varphi - u_d|^2 : \quad -\Delta\varphi = 0 \ \text{ in } \ \Omega, \ \ \partial_n\varphi|_{\partial\Omega} = g\}$$

or with a stream function in 2D

$$\min_{\partial\Omega}\{\int_D |\nabla\psi - v_d|^2 : \quad -\Delta\psi = 0 \ \text{ in } \Omega, \ \ \psi|_{\partial\Omega} = \psi_\Gamma\}$$

In both problems one seeks for a shape which produces the closest velocity to u_d in the region D of Ω. In the second formulation the velocity of the flow is given by
$(\partial_2\psi, -\partial_1\psi)^T$ so $v_d = (u_{d2}, -u_{d1})^T$.

An application to wind tunnel or nozzle design for potential flow is obvious but it is laboratory because these are usually used with compressible flows.

2.2 Minimum weight of structures

In 2D linear elasticity, for a structure clamped in a part Γ_1 of its boundary $\Gamma = \partial\Omega$ and subject to volume forces F and surface shear g, the displacement $u = (u_1, u_2)$ is found by solving for u:

$$u \in V_0 = \{u \in H^1(\Omega)^2 : \quad u|_{\Gamma_1} = 0\}$$

$$\int_\omega [\partial_{tt}u \cdot v + \mu\epsilon_{ij}(u)\epsilon_{ij}(v) + \lambda\epsilon_{ii}(u)\epsilon_{jj}(v)] = \int_{\partial\Omega} g.v + \int_\Omega F.v \quad \forall v \in V_0$$

$$\text{where} \quad \epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i),$$

Many important problems of design arise when one wants to find the structure with minimum weight yet satisfying some inequality constraints for the stress such as in the design of light weight beams for strengthening of airplane floors, or for crank shaft optimization...

For all these problems the criteria for optimisation is the weight

$$J(\Omega) = \int_\Omega \rho,$$

where ρ is the density of the material.

But there are constraints on the maximum stress (itself a linear tensor function of the displacement tensor ϵ)

$$\tau(x) \cdot d < \tau_{dmax}$$

at some points x and for some directions d.

Indeed, a wing for instance, will behave differently under spanwise and chordwise load. Moreover, due to coupling between physical phenomena, the surface stresses come in part from fluid forces acting on the wing. This implies many additional constraints on the aerodynamical (drag, lift, moment) and structural (Lamé coefficients) characteristics of the wing. Therefore, the Lamé equations of the structure must be coupled with the equations for the fluid (fluid structure interactions). This is why most optimization problems nowadays require the solution of several state equations ("multiphysics").

2.3 Wing design

An important industrial problem is the optimization of the shape of a wing to reduce the drag. The drag is the reaction of the flow on the wing, its component in the direction of flight is the drag proper and the rest is the lift. A few percents of drag optimization means a great saving on commercial planes.

For viscous drag the Navier-Stokes equations must be used. For wave drag the Euler system is sufficient.

For a wing S moving at constant speed u_∞ the force acting on the wing is in a cartesian frame

$$F = (F_x, F_y, F_z)^T = \int_S [\mu(\nabla u + \nabla u^T) - \frac{2\mu}{3}\nabla.u]n - \int_S pn$$

The first integral is a viscous force, the so called viscous drag and the second is called the wave drag. In a frame attached to the wing, and with uniform flow at infinity, the drag is the component of F parallel to the velocity at infinity (i.e. $F.u_\infty$). The viscosity of the fluid is μ and p is its pressure.

The Navier-Stokes equations govern u the fluid velocity, θ the temperature, ρ the density and E the energy:

$$\partial_t \rho + \nabla.(\rho u) = 0$$
$$\partial_t(\rho u) + \nabla.(\rho u \otimes u) + \nabla p - \mu \Delta u - \frac{1}{3}\mu \nabla(\nabla.u) = 0,$$
$$\partial_t[rhoE] + \nabla \cdot [u\rho E] + \nabla \cdot (pu) = \nabla \cdot \{\kappa \nabla \theta + [\mu(\nabla u + \nabla u^T) - \frac{2}{3}\mu)\mathbf{I}\nabla \cdot u]u\}$$
$$\text{where } E = \frac{u^2}{2} + \theta \quad p = (\gamma - 1)\rho\theta$$

The problem is to minimize

$$J(S) = F.u_\infty$$

with respect to the shape of S.

There are several *constraints*:

- A geometrical constraint: the volume of S greater than a given value, else the solution will be a point.
- An aerodynamic constraint: the lift must be greater than a given value or the wing will not fly.

The problem is difficult because it involves the compressible Navier-Stokes equations at high Reynolds number. It can be simplified by considering only the wave drag i.e. the pressure term only in the definition of F (Jameson (1987)). When the viscous terms are dropped in the Navier-Stokes equations ($\mu = \kappa = 0$). Euler's equations remain. The problem is

$$\min_S \int_S pn \cdot u_\infty \qquad \text{subject to}$$

$$\partial_t \rho + \nabla.(\rho u) = 0$$
$$\partial_t(\rho u) + \nabla.(\rho u \otimes u) + \nabla p = 0,$$
$$\partial_t[rhoE] + \nabla \cdot [u\rho E] + \nabla \cdot (pu) = 0$$
$$\text{with } E = \frac{u^2}{2} + \theta \quad p = (\gamma - 1)\rho\theta$$

However, it is now well known that viscous effects have an important impact on the final shape (Mohammadi (1997)). Indeed, in transonic flows for instance the shock position is 30 percents chord upstream due to viscous effects.

Assuming irrotational flow an even greater simplication replaces the Euler equations by the compressible potential equation ($\gamma = 1.4$ for air):

$$u = \nabla\varphi, \quad \rho = (1 - |\nabla\varphi|^2)^{1/(\gamma-1)}, \quad p = \rho^\gamma, \quad \nabla.\rho u = 0.$$

Or even, if at low Mach number, by the incompressible potential flow equation:

$$u = \nabla\varphi, \qquad -\Delta\varphi = 0.$$

Constraints on admissible shapes are numerous:

- Minimal thickness, given length.
- Minimum admissible curvature
- Minimal angle at the trailing edge...

Another problem arises due to instability of optimal shapes with respect to data. It will be seen that the leading edge of the solution is a wedge. Thus if the incidence angle of u_∞ is changed the solution becomes bad. A multi-point functional must be used in the optimization, for some weighting factors β_i

$$J(S) = \sum \beta_i u^i_\infty F^i \quad \text{or} \quad J(S) = \max_i \{u^i_\infty F^i\}$$

at given lift $F^i \times u_\infty$ where the F^i are computed from Navier-Stokes equations with boundary conditions $u = u^i_\infty$.

2.4 Stealth Wings

2.4.1 Maxwell equations. The optimization of the far-field energy of a radar wave reflected by an airplane in flight requires the solution of Maxwell's equations for the electric field E and the magnetic field H:

$$\epsilon\partial_t E + \nabla \times H = 0 \quad \nabla.E = 0, \qquad \mu\partial_t H - \nabla \times E = 0 \quad \nabla.H = 0.$$

The dielectric and magnetic coefficient ϵ, μ are constant in air but not so in an absorbing medium. One variable, H for instance, can be eliminated by differentiating in t the first equation:

$$\epsilon\partial_{tt} E + \nabla \times (\frac{1}{\mu}\nabla \times E) = 0,$$

from which it is easy to see that $\nabla.E = 0$ is always zero if it is zero at initial time.

2.4.2 Helmholtz equation. Now if the geometry is cylindrical with axis z and if $E = (0, 0, E_z)^T$ then the equation becomes a scalar wave equation for E_z. Furthermore if the boundary conditions are periodic in time at infinity, $E_z = \mathcal{R}_e v_\infty e^{i\omega t}$ and compatible with the initial conditions then the solution has the form $E_z = \mathcal{R}_e v(x) e^{i\omega t}$ where v, the amplitude of the wave E_z of frequency ω , is solution of:

$$\nabla(\cdot\frac{1}{\mu}\nabla v) + \omega^2 \epsilon v = 0$$

Notice the wrong sign for ellipticity in the "Helmholtz" equation.

Remark

1. This equation arises naturally in accoustics. So the technics of this paragraph applies also there.

2. In vacuum $\mu\epsilon = c^2$,c the speed of light, so for numerical purposes it is a good idea to rescale the equation. The critical parameter is then the number of waves on the object, i.e. $\omega c/L$ where L is the size of the object.

2.4.3 Boundary conditions. The reflected signal on solid boundaries Γ satifies

$$v = 0 \quad \text{or} \quad \partial_n v = 0 \quad \text{on } \Gamma$$

depending on the type of waves (Transverse Magnetic polarization requires Dirichlet condition).

When there is no object this Helmholtz equation has a simple sinusoidal set of solutions which we call v_∞:

$$v_\infty(x) = \alpha \sin(k \cdot x) + \beta \cos(k \cdot x), \qquad \text{i.e. } E_z = \mathcal{R}_e(Ae^{i(k \cdot x + \omega t)})$$

where k is any vector of modulus $|k| = \omega c$. Radar waves are more complex but by Fourier decomposition, they can be viewed as a linear combination of such simple unidirectional waves.

Now if such a wave is sent on a object, it is reflected by it and the signal at infinity is the sum of the original wave with the reflected wave. So it is better to set an equation for the amplitude of the reflected wave only $u = v - v_\infty$.

A good boundary condition for u is difficult to set; one possibility is

$$\partial_n u + iau = 0.$$

Indeed when $u = e^{id \cdot x}$, $\partial_n u + iau = i(d \cdot n + a)u$, so that this boundary condition is "transparent" to waves of direction d when $a = -d \cdot n$. If we want this boundary condition to let all *outgoing* waves pass the boundary best when it is normal to it, we will set a=1.

To sumarize, we set for u the system in the complex plane:

$$\nabla \cdot (\frac{1}{\mu}\nabla u) + \omega^2 u = 0, \quad \text{in } \Omega,$$
$$\partial_n u + iu = 0 \quad \text{on } \Gamma_\infty$$
$$u = g \equiv -e^{ik\cdot x} \quad \text{on } \Gamma.$$

where $\partial\Omega = \Gamma \cup \Gamma_\infty$. It can be shown that the solution exists and is unique. Notice that the variables have been rescaled, ω is ωc, μ is μ/μ_{vacuum}.

Usually the criteria for optimization is a minimum amplitude for the reflected signal in a region of space D at infinity (hence D is an angular sector). For instance one can consider

$$\min_{S\in O}\{\int_{\Gamma_\infty\cap D}|\nabla u|^2 : \quad \omega^2 u + \nabla\cdot(\frac{1}{\mu}\nabla u) = 0, \quad u_{|\Gamma} = g, \quad iu + \partial_n u|_{\Gamma_\infty} = 0\}$$

where μ is different from one only in a region very near Γ and schematizes an absorbing paint.

But constraints are aerodynamical as well, (lift above a given lower limit for instance) and thus requires the solution of the fluid part as well. The design variables are:

- The shape of the wing
- The thickness of the paint
- The material characteristics (ϵ, μ) of the absorbing paint.

Here again, the theoretical complexity of the problem can be appreciated from the following question:

Would ribblets of the size of the radar wave improve the design?

Actually homogenization can answser the question as in Achdou (1991) (see also Artola (1991) and Achdou et al (1991)) It shows that indeed ribblets improve the design and in practice absorbing paints on the wing surface work in the same manner.

Homogenization shows that periodic surfacic irregularities are equivalent to new "effective" boundary conditions

$$u = 0 \quad \text{replaced by} \quad au + \partial_n u = 0$$

and so the optimization can be done with respect to a also. Hence the connections between OSD and topological optimization.

2.5 Optimal brake water

As a first approximation, the amplitude of sea waves satisfies Helmholtz' equation

$$\nabla(\mu\cdot\nabla u) + \epsilon u = 0$$

where μ is a function of the water depth and ϵ is proportional to the wave speed.

With approximate reflection and damping whenever the waves collide on a brake water S which is surrounded by rocks we have

$$\partial_n u + au = 0 \quad \text{on} \quad S.$$

At infinity a non reflecting boundary condition can be used

$$\partial_n(u - u_\infty) + ia(u - u_\infty) = 0$$

The problem is to find the best S with given length so that the waves have minimum amplitudes in a given harbour D:

$$\min_S \int_D u^2.$$

2.6 Ribblets

Consider a flat plate with groves dug on the surface parallel to the mean flow. It has been shown that such configurations have less drag per unit surface area than the flat plate (Figure 5).

The phenomenon is turbulent in its principle (Moin (1993)) because these groves or ribblets trap the large vortices and retard the formation of horse shoe vortices. It is beyond the limit of present computers to hope to solve such problems by optimal design methods. However even the laminar case leads to an optimization and it is not true that the flat plate is the best surface for drag per unit surface area for a Poiseuille flow.

Consider ribblets which are well within the logarithmic layer and near the viscous sublayer. Apply the Couette flow approximation. Then the problem is:

$$\min_\Sigma u_\infty \cdot \int_\Sigma [\nu(\nabla u + \nabla u^T) - pn]$$

with (u, p) solution of

$$\mathbf{u} = \begin{pmatrix} 0 \\ 0 \\ u(x,y) \end{pmatrix} \quad \text{and} \quad p = p(z)$$

$$-\nu \Delta u + \nabla p = \begin{pmatrix} 0 \\ 0 \\ \frac{\partial p}{\partial z} - \nu \Delta_{x,y} u \end{pmatrix} = 0$$

A solution with $p = kz$ is found and u solves

$$-\nu \Delta u + k = 0$$

The domain is 2D and with a periodic distribution of ribblets, the domain is one cell containing one ribblet Σ with $u|_\Sigma = 0$ and a Neumann condition on the upper artificial boundary which simulates the matching with the boundary layer S and periodic conditions on the lateral boundaries of the cell. The problem becomes:

$$\min_\Sigma(-\int_\Sigma \frac{\partial u}{\partial n})$$

subject to (u, k) solution of:

$$-\nu\Delta u + k = 0 \text{ in } \Omega$$
$$u = 0 \text{ on } \Sigma \quad \frac{\partial u}{\partial n} = 0 \text{ on } S$$
$$u = x - \text{periodic} \quad \int_\Omega u = d.$$

The last constraint on the flux has been added to fix k:

2.7 Sonic boom reduction

Some supersonic carrier are considered too noisy. An optimization of the shock wave jump and of the jet noise can be performed with respect to the far field noise. Again the full problem involves the Navier-Stokes equations but simpler approximations like Lighthill's turbulent noise source approximation can be used and in the far field it is the wave equation which is solved.

3. Existence of Solutions

3.1 Generalities

Assume that $\psi(\Omega)$ is the solution of

$$-\Delta\psi = f \;\text{ in }\; \Omega, \;\; \psi|_{\partial\Omega} = 0$$

and that

$$u_d \in L^2(\Omega), \quad f \in H^{-1}(\Omega)$$

For simplicity we have translated the nonhomogeneous boundary conditions of the laboratory examples above into a right hand side in the PDE ($f = \Delta\psi_\Gamma$).

Let $O \supset D$ be two given closed bounded sets in $R^d, d = 2, 3$ and consider

$$\min_{\Omega\in\mathcal{O}} J(\Omega) = \int_D |\nabla\psi(\Omega) - u_d|^2$$

with

$$\mathcal{O} = \{\Omega \subset R^d \;:\; O \supset \Omega \supset D, \;\; |\Omega| = 1\}.$$

where $|\Omega|$ denotes the area in 2D and the volume in 3D.

Chenais (1975) showed that there exists a solution provided that the class $\mathcal{O}$ is restricted to Ω which are:

1. locally on one side of their boundaries,
2. verifying the *Cone Property.*

Let $D_\epsilon(x,d)$ be the intersection with the sphere of radius ϵ and center x of the cone of vertex x direction d and angle ϵ.

Cone Property: *There exists ϵ such that for every $x \in \partial\Omega$ there exists d such that $\Omega \supset D_\epsilon(x,d)$.*

These two conditions imply that the boundary cannot oscillate too much.

Denote by $\mathcal{O}_\epsilon$ this set of admissible shapes.

Theorem:
The problem

$$\min_{\Omega\in\mathcal{O}_\epsilon} J(\Omega)$$

has at least one solution

Proof
The proof is done by considering a minimizing sequence Ω^n. The cone property implies that there exists Ω such that $\Omega^n \to \Omega$ in a sense sufficiently strong so that

$$\psi(\Omega^n)|_D \to \psi(\Omega)|_D, \quad \text{in } H^1(D)$$
$$\int_\Omega \nabla\psi(\Omega)\nabla w = \int_\Omega fw \quad \forall w \in H^1(\Omega).$$

Hence $J(\Omega^n) \to J(\Omega)$ and Ω is a solution.

In 2D an important result has been obtained by Sverak (1992):

Theorem .
If $\mathcal{O} = \mathcal{O}_N$ is the set of open sets containing D (possibly with a constraint on the area such as area ≥ 1) and whose number of connected component is bounded by N then

$$\min_{\mathcal{O}_N} J(\Omega) = \int_D |\nabla\psi(\Omega) - v_d|^2 \ : \ -\Delta\psi(\Omega) = f \ \ in \ \ \Omega, \ \ \psi(\Omega)|_{\partial\Omega} = 0\}$$

has a solution.

In other words, two things can happen to minimizing sequences:

- Either accumulation points are solutions
- Or the number of holes in the domain tends to infinity (and their size to zero).

This result is false in 3D as it is possible to make shapes with spikes such that a 2D cut will look like a surface with holes and yet the 3D surface remains singly connected. Bucur-Zolezio (1995) obtained an extension to 3D of the same idea by using capitance (see also Liu et al. (1999) for a result using equi-continuity for boundaries having the segment property (a segment of fixed size must fit in and out of the domain with one end on the boundary, at each boundary point) for the Neumann problem).

A corollary of their result can be summarized as:

If the boundary of the domain has the flat cone insertion property (each boundary point is the vertex of a fixed size 2D truncated cone which fits inside the domain) then the problem has at least one solution.

The proof of Sverak's theorem is sketched in Appendix A for the reader to see the kind of tools which are used in such studies.

3.2 Sketch of the proof of Sverak's Theorem

The proof relies on a compactness result for the Hausdorff topology and on a result of potential theory (capacitance).
The Hausdorff distance between 2 closed sets A, B is

$$\delta(A,B) = \max\{d(B,A), d(A,B)\} \quad \text{where } d(A,B) = \sup_{x\in A} d(x,B).$$

For this distance we have

Proposition
If F_n is a uniformly bounded sequence , then there is a closed bounded set F and a subsequence converging in the sense of Hausdorff to F.

Equivalently let Ω_n be a sequence of open sets in R^d with $\Omega_n \subset O$. Then one can extract a subsequence, also denoted by Ω_n converging in the sense of Hausdorff to a Ω, that is, verifying:

$$\forall C \subset \Omega, \exists m : C \subset \Omega_n \forall n \geq m \text{ and } \forall x \in O - \Omega, \exists x_n \in O - \Omega_n : x_n \to x.$$

So a minimizing subsequence for (2) will have the following properties

$$J(\Omega_n) \to \inf J(\Omega)$$
$$-\Delta\psi_n = f \text{ in } \Omega_n, \quad \psi \in H^1(\Omega_n) \text{ and } \psi_n \to \psi \quad \text{in } H^1(O) \text{ weakly with ,}$$
$$-\Delta\psi = f \text{ in } \Omega, \quad \inf J(\Omega) = \int_D |\nabla\psi - v_d|^2.$$

But we do not know how to show that

$$\psi = 0 \;\; in \;\; O - \Omega$$

For this an information on the characteristic function χ_n of $O - \Omega_n$ is needed because

$$0 = \chi_n \psi_n \to \chi\psi, \;\; \Rightarrow \;\; \psi(x) = 0 \; pp \; si \;\; \chi(x) \neq 0.$$

Sverak uses another argument. First he shows that it is sufficient to study the case $f = 1$. If Ω^n denotes the solution in $H^1_0(\Omega^n)$ of $-\Delta\Omega^n = 1$ then the convergence of Ω^n towards its weak limit is almost uniform (this is the difficult point) when the number of connected components is finite.

This result from the theory of sub-harmonic functions is true in 3D also with an hypothesis of capacitance. Hence a generalization can be found in Bucur et al (1995) where by existence is shown under the only restriction that one can fit a flat cone (a 2D cone as in Chesnais but for a 3D surface, so it is much more general) at each point of the boundary.

Corollary

Given N and the 2D-Navier-Stokes equations for incompressible flows there exists an optimal wing profile with given area in 2D in the class of uniformely bounded domains with less than N connected components

Proof

Let Ω^n be a minimizing sequence. Let u^n be the corresponding solution of the Navier-Stokes equations :

$$-\nu\Delta u^n + \nabla.(u^n \otimes u^n) + \nabla p^n = 0, \;\; \nabla \cdot u^n = 0 \;\; in \;\; \Omega^n, \;\; u^n|_S = 0, \;\; u|_{\Gamma_\infty} = u_\infty$$

By hypothesis Ω^n is bounded by O. From the Navier-Stokes equations it is easy to see that u^n extended by 0 in O is bounded in $H^1_0(O)^2$, so there exists a subsequence which converges weakly; let u be the limit. Now

$$f^n \equiv \nabla \cdot (u^n \otimes u^n) \to f \equiv \nabla \cdot (u \otimes u) \;\; \text{in } W^{-1,p}(O), \; \forall p,$$

But now if

$$-\Delta u^n + \nabla p^n = -f^n \quad \nabla \cdot u^n = 0$$
$$f^n \to f \;\; \text{in } W^{-1,p}(O),$$

then u is solution of the same Stokes problem with f instead of f^n. It remains to show that $u|_{\Omega - S} = 0$ but that is done for the Stokes problem exactly as for the Laplace equation since Stokes equation is a Laplacian in the space of solenoidal fields.

4. Solution By Optimization Methods

4.1 Gradient Methods

At the basis of gradient methods is the Taylor expansion of

$$J:\quad V \to \mathcal{R}$$

where, if V is a Hilbert space,

$$J(v+\lambda w) = J(v) + \lambda < \mathrm{Grad}_v J, w > + o(\lambda\|w\|), \quad \forall v, w \in V, \quad \forall \lambda \in \mathcal{R}.$$

where V is a Hilbert space with scalar product $< \cdot, \cdot >$ and $\mathrm{Grad}_v J$ is the element of V given by Ritz' theorem and defined by

$$< \mathrm{Grad}_v J, w >= J'_v w, \quad \forall w \in V.$$

By taking $w = -\rho \mathrm{Grad}_v J(v)$, with $0 < \rho << 1$ we find :

$$J(v+w) - J(v) = -\rho\|\mathrm{Grad}_v J(v)\|^2 + o(\rho\|\mathrm{Grad}_v J(v)\|)$$

Hence if ρ is small enough the first term on the right hand side will dominate the remainder and the sum will be negative:

$$\rho\|\mathrm{Grad}_v J(v)\|^2 > o(\rho\|\mathrm{Grad}_v J(v)\|) \quad \Rightarrow \quad J(v+w) < J(v)$$

Thus the sequence defined by :

$$v^{n+1} = v^n - \rho \mathrm{Grad}_v J(v), \quad n = 0, 1, 2, \ldots$$

makes $J(v^n)$ monotone decreasing. We have the following result:

Theorem: *If J is continuous, bounded from below, and $+\infty$ at infinity, then all accumulation points v^* of v^n satisfy*

$$\mathrm{Grad}_v J(v^*) = 0.$$

This is the so called *optimality condition* of the order 1 of the problem. If J is convex then it implies that v^* is a minimum; if J is strictly convex the minimum is unique.

By taking the best ρ in the *direction of descent* $w^n = -\mathrm{Grad}_v J(v^n)$,

$$\rho^n = arg\min_\rho J(v^n + \rho w^n) \text{ (meaning that } J(v^n + \rho^n w^n) = \min_\rho J(v^n + \rho w^n))$$

we obtain the so called *method of steepest descent with optimal step size*

We have to remark however, that minimizing a one parameter function is not all that simple. The exact minimum cannot be found in general, except for polynomial functions J. So in the general case, several evaluations of J are required for an approximate minimum only.

A closer look at the convergence proof of the method shows that it is enough to find ρ^n with the following property (Armijo rule):

Given $0 < \alpha < \beta < 1$, find ρ such that

$$-\rho\beta||\mathrm{Grad}_v J(v^n)||^2 < J(v^n - \rho \mathrm{Grad}_v J(v^n)) - J(v^n) < -\rho\alpha||\mathrm{Grad}_v J(v^n)||^2$$

It can be found by relating β to α, in the following fashion:

Choose two numbers $0 < \rho_0 < 1$, $\omega \in (0,1)$ and find $\rho = \rho_0^k$ where k is the first integer such that

$$\begin{aligned} J(v^n - \rho_0^{k+1}\mathrm{Grad}_v J(v^n)) - J(v^n) &< -\rho_0^{k+1}\omega||\mathrm{Grad}_v J(v^n)||^2 \\ -\rho_0^k\omega||\mathrm{Grad}_v J(v^n)||^2 &< J(v^n - \rho_0^k \mathrm{Grad}_v J(v^n)) - J(v^n) \end{aligned}$$

4.2 Newton Methods

Newton's method with optimal step size applied to the minization of J is

$$\begin{aligned} \text{Compute } w \text{ solution of } \quad J"_{vv}w &= -\mathrm{Grad}_v J(v^n), \\ \text{Set} \quad v^{n+1} &= v^n + \rho w \\ \text{with } \rho = arg \min_{\rho} J(v^n + \rho w) \end{aligned}$$

Near to the solution it can be shown that $\rho^n \to 1$ so that it is also the root finding Newton method applied to the optimality condition

$$\mathrm{Grad}_v J(v) = 0$$

It is quadratically convergent but it is expensive and usually $J"$ is difficult to compute, so a quasi-Newton, where an approximation of $J"$ is used, is prefered. For instance, a directional approximation can be found by:

$$\begin{aligned} &\text{Choose } 0 < \epsilon << 1, \quad w \text{ approximate solution of} \\ &\frac{1}{\varepsilon}(\mathrm{Grad}_v J(v^n + \epsilon w) - \mathrm{Grad}_v J(v^n)) = J"_{vv}(v^n).w, \end{aligned}$$

4.3 Constraints

In constrained optimization, we can have equality or inequality constraints on the optimization parameters or the state variables. When using gradient methods, equality constraints are usually taken into account by penalization in J while inequality constraints are treated by projection when they concern the optimization parameters directly. If they concern the state variables, usually they are transformed to equality constraint and then penalized.

Consider the following minimization problem under equality and inequality constraint on the parameters and state:

$$\min_x J(x, u(x)), \quad A(x, u(x)) = 0,$$

subject to

$$B(x, u(x)) \leq B_0, \quad C(x, u(x)) = C_0, \quad x_{\min} \leq x \leq x_{\max},$$

here A, B, C involve the parameters x and the state variable u (state constraints) while the last constraints is a box constraint on the parameters only. The problem can be approximated by "penalty"

$$\min_x J(x, u(x)) + \beta|(B - B_0)^+|^2 + \gamma|C - C_0|^2,$$

subject to

$$A(x, u(x)) = 0, \quad x_{\min} < x < x_{\max}.$$

β and γ are penalization parameters. They are usually difficult to choose.

At each iteration of the gradient method, the new prediction is kept inside this box x_min, x_max by projecting the gradient. To improve the treatment of constraints interior point algorithms can be used.

5. Sensitivity Analysis

Gradient and Newton methods require gradients of the cost function J and for this we need to identify an underlying Hilbert structure for the parameters of J, the shape. Two ways have been proposed:

- Assume that all admissible shapes are obtained by mapping a reference domain $\hat{\Omega}$: $\Omega = T(\hat{\Omega})$. Then the parameter of J is $T : R^d \to R^d$. A possible Hilbert space for T is the Sobolev space of order m and it seems that $m = 2$ is a good choice.
- What is important is a Hilbert structure for the tangent plane of the parameter space, meaning by this that the Hilbert structure is needed only for small variations of Ω, so that one works with local variations defined around a reference boundary Σ by

  $$\Gamma(\alpha) = \{x + \alpha(x)n_\Sigma(x) \ : \ x \in \Sigma\}$$

  where n_Σ is the normal to Σ at x and Ω is the domain which is on the left side of the oriented boundary $\Gamma(\alpha)$. Then the Hilbert structure is placed on α, for instance $H^m(\Sigma)$.

Comments It is generally believed that PDE-parameter optimization (here T) is more difficult than shape optimization numerically.

Before proceeding we need the following preliminary result. In most cases only one part of the boundary Γ is optimized, we call this part S.

Proposition
Consider a small perturbation S' of S given by

$$S' = \{x + \lambda \alpha n : x \in S\}$$

where α is a function of x via the curvilinear abscissa of x on S and λ is a positive number destined to tend to zero. Denote $\Omega' = \Omega(S')$. Then for any $f \in H^1(C), C \supset \Omega \cup \Omega'$

$$\int_{\Omega(S')} f - \int_{\Omega(S)} f = \int_{\Omega(S') - \Omega(S)\cap\Omega(S')} f - \int_{\Omega(S) - \Omega(S)\cap\Omega(S')} f$$
$$= \lambda \int_S \alpha f + o(\lambda\|\alpha\|)$$
$$\textit{and so} \quad \lim_{\lambda\to 0} \frac{1}{\lambda}[\int_{\Omega(S')} f - \int_{\Omega(S)} f] = \int_S \alpha f$$

Remark If S has an angle not all variations S' can defined by local variation on S but it can be shown that it is a sufficient class of variations.

Similarly the following can be proved (Pironneau(1983), p87).

Proposition
If $g \in H^1(S)$ and if R denotes the mean radius of curvature of S in any local basis ($1/R = 1/R_1 + 1/R_2$ in 3D) then

$$\lim_{\lambda\to 0} \frac{1}{\lambda}[\int_{S'} g - \int_S g] = \int_S \alpha(\partial_n g - \frac{g}{R})$$

5.1 Sensitivity Analysis for the nozzle problem

Consider

$$\min_{\partial\Omega\in\mathcal{O}} \int_D |\nabla\phi - u_d|^2$$
$$\text{subject to :}$$
$$-\Delta\phi = 0 \text{ in } \Omega, \quad a\phi + \partial_n\phi = g \text{ on } \partial\Omega,$$

the class of admissible shapes $\mathcal{O}$ being the set bounded domains with Lipschitz continuous boundaries containing D; but we will not worry about this constraint set for the time being and assume all constraints are verified by all variations encountered. In practice however we may have even additional constraints such as $\mathcal{O} \subset C$.

If $a = 0$ it is the potential flow formulation and if $a \to \infty, g = af$ it becomes the stream function formulation.

Assume that some part of $\Gamma = \partial\Omega$ is fixed, the unkown part being called S.

The variational formulation of the Laplace equation with Fourier boundary condition is

$$\text{Find } \phi \in H^1(\Omega) \text{ such that}$$
$$\int_\Omega \nabla\phi \cdot \nabla w + \int_\Gamma a\phi w = \int_\Gamma gw, \quad \forall w \in H^1(\Omega).$$

The Lagrangian of the problem is

$$L(\phi, w, S) = \int_D |\nabla\phi - u_d|^2 + \int_{\Omega(S)} \nabla\phi \cdot \nabla w + \int_\Gamma (a\phi w - gw)$$

and the minimization of J is equivalent to the min-max problem

$$\min_{S,\phi} \max_v L(\phi, v, S).$$

Recall that

$$J'_S(S, \phi) = L'_S(\phi, v, S) \text{ at the solution } \phi, v \text{ of the min-max}$$

Let us write that the solution is a saddle point of L. As L is linear in w and quadratic in ϕ, stationarity in these variables is simply

$$\begin{aligned}
\partial_\lambda L(\phi + \lambda\hat{\phi}, v, S) &= 2\int_D (\nabla\phi - u_d) \cdot \nabla\hat{\phi} + \int_{\Omega(S)} \nabla\hat{\phi} \cdot \nabla v \\
&+ \int_\Gamma a\hat{\phi} v = 0, \quad \forall\hat{\phi} \\
\partial_\lambda L(\phi, v + \lambda w, S) &= \int_{\Omega(S)} \nabla\phi \cdot \nabla w \\
&+ \int_\Gamma (a\phi w - gw) = 0 \quad \forall w
\end{aligned}$$

Acording to the 2 propositions above, stationarity with respect to S is

$$\begin{aligned}
\lim_{\lambda\to 0} \frac{1}{\lambda}[L(\phi, w, S') - L(\phi, w, S)] &= \\
\int_S \alpha[\nabla\phi \cdot \nabla w \quad &+ \quad \partial_n(a\phi w - gw) - \frac{1}{R}(a\phi w - gw)] = 0
\end{aligned}$$

and so we have shown that

Theorem : *The variation of J with respect to the shape deformation $S' = \{x + \alpha(x) n_S(x) \ : \ x \in S\}$ is*

$$\delta J \equiv J(S', \phi(S')) - J(S, \phi(S)) = \int_S \alpha \nabla\phi \cdot \nabla v$$

$$+ \int_S \alpha[\partial_n(a\phi v - gv) - \frac{1}{R}(a\phi v - gv)] + o(\|\alpha\|)$$

where $v \in H^1(\Omega(S))$ is the solution of

$$\int_{\Omega(S)} \nabla\hat{\phi} \cdot \nabla v + \int_\Gamma a\hat{\phi} v = 0, \quad \forall \hat{\phi} \in H^1(\Omega(S))$$

Notice that the boundary conditions for ϕ and v being

$$\partial_n \phi + a\phi = g, \quad \partial_n v + av = 0$$

we can eliminate a from the optimality conditions and find

$$\delta J = \int_S \alpha[\partial_s \phi \cdot \partial_s v - \partial_n \phi \cdot \partial_n v - \partial_n(gv) + \frac{1}{R} v \partial_n \phi].$$

where ∂_s denotes the derivative with respect to the curvilinear coordinate of S.

Corollary : *With homogeneous Neumann conditions ($a = g = 0$)*

$$\delta J = \int_S \alpha \partial_s \phi \cdot \partial_s v + o(\|\alpha\|)$$

and with homogeneous Dirichlet conditions on S ($a \to \infty, g = 0$)

$$\delta J = -\int_S \alpha \partial_n \phi \cdot \partial_n v + o(\|\alpha\|)$$

5.2 Discretization with Triangular Elements

For discretization let us use the simplest, a *Finite Element Method* of degree 1 on triangles. Unstructured meshes are better for OSD because they are easier to deform and adapt for a general shape deformation.

More precisely, Ω is approximated by $\Omega_h = \cup_{k=1}^{nT} T_k$ where the T_k are triangles such that

- The vertices of $\partial\Omega_h$ are on $\partial\Omega$ and the corners of $\partial\Omega$ are vertices of $\partial\Omega_h$.
- $T_k \cap T_l$, $(k \neq l)$ is either a vertex or an entire edge or empty.
- Triangulations are indexed on the longest edge, of size h, and as $h \to 0$ no angle should go to zero or π.

The Sobolev space $H^1(\Omega)$ is approximated by

$$H_h = \{w_h \in C^o(\bar{\Omega}_h) : w_h|_{T_k} \in P^1 \quad \forall k\}$$

where $P^1 = P^1(T_k)$ is the space of linear polynomials. The discrete problem in variational form is

$$\min_{\{(q^i)_{i=1}^{n_v} \in \mathcal{Q}\}} J(q^1, ..., q^{n_v}) = \int_D \|\nabla\phi_h - (u_h)_d\|^2$$
$$\text{subject to } \phi_h \in H_h \text{ solution of :}$$
$$\int_{\Omega_h} \nabla\phi_h \cdot \nabla w^j + \int_\Gamma a\phi w^j = \int_\Gamma g w^j, \forall j \in [1, ..., n_v]$$

The dimension of H_h equals n_v the number of vertices q^i of the triangulation and every function ϕ_h belonging to H_h is completely determined by its values on the vertices $\phi_h(q^i)$.

The canonical basis of H_h is the set of so-called *hat functions* defined by

$$w^i \in H_h, \quad w^i(q^j) = \delta_{ij}$$

Denoting by ϕ_i the coefficient of ϕ_h on that basis,

$$\phi_h(x) = \sum_1^{n_v} \phi_i w^i(x),$$

the PDE

$$\int_{\Omega_h} \nabla\phi_h \cdot \nabla w^j + \int_\Gamma a\phi w^j = \int_\Gamma g w^j, \forall j \in [1, ..., n_v]$$

yields a linear system for $\Phi = (\phi_i)$

$$A\Phi = F, \quad A_{ij} = \int_{\Omega_h} \nabla w^i \nabla w^j + \int_{\Gamma_h} a w^i w^j, \quad F_j = \int_{\Gamma_h} g w^j.$$

Hence in matrix form the problem is to find $Q = (q^i)$ solution of

$$\min_{Q \in \mathcal{Q}} \{J(Q) = \Phi^T B \Phi - 2U \cdot \Phi \ : \ A(Q)\Phi = F\}$$
$$\text{with } B_{ij} = \int_D \nabla w^i \nabla w^j, \quad U_j = \int_D u_d \cdot \nabla w^j.$$

where B and U are independent of Q if the triangulation is fixed within D. For simplicity we shall assume that F does not depend on Q, i.e. that $g = 0$ on S.

Remark

The method applies also to Dirichlet conditions treated by penality, as explained before. However, in practice it is necessary for numerical quality to use a lumped quadrature in the integral of the Fourier term, or equivalently to apply $\phi = \phi_\Gamma$ at all points of Γ by

$$A_{ij} = \int_{\Omega_h} \nabla w^i \nabla w^j + p\delta_{ij}\delta(q^i \in \Gamma_h), \quad F_j = p\phi_\Gamma(q^j)\delta(q^j \in \Gamma_h).$$

where p is a large number.

We present below a computation of discrete gradients for a Neumann problem but the method applies also to Dirichlet problems with this modification.

5.3 Discrete Gradients

A straightforward calculus of variation gives

$$\delta J = 2(B\Phi - U)\cdot\delta\Phi \quad \text{with } A\delta\Phi = -(\delta A)\Phi$$

Introducing Ψ solution of $A^T\Psi = 2(B\Phi - U)$ leads to

$$\delta J = (A^T\Psi)\cdot\delta\Phi = \Psi^T A\delta\Phi = -\Psi\cdot((\delta A)\Phi)$$

To evaluate δA we need 3 lemmas. If δQ is a variation of vertex positions (i.e. each vertex q^i moves by δq^i), we define

$$\delta q_h(x) = \sum_1^{n_v} \delta q^i w^i(x), \quad \forall x \in \Omega_h$$

and denote by Ω'_h the new domain.

Lemma 1 (see Figure 4)

$$\delta w^j = -\nabla w^j \cdot \delta q_h + o(\|\delta q_h\|)$$

Lemma 2

$$\int_{\delta\Omega_h} f \equiv \int_{\Omega'_h} f - \int_{\Omega_h} f = \int_{\Omega_h} \nabla\cdot(f\delta q_h) + o(\|\delta q_h\|)$$

Lemma 3

$$\int_{\delta\Gamma_h} g \equiv \int_{\Gamma'_h} g - \int_{\Gamma_h} g = \int_{\Gamma_h} gt\cdot\partial_s\delta q_h + \int_{\Gamma_h} \delta q_h \nabla g + o(\|\delta q_h\|)$$

where ∂_s denotes the derivative with respect to the curvilinear abscissa and t the oriented tangent vector of Γ_h.

In these the integrals are sums of integrals on triangles or edges and so f and g can be piecewise discontinuous across elements or edges.

Proofs

Proofs for Lemma 1 & 2 are in Pironneau (1983), so only the proof of Lemma 3 is given here.
Consider an edge $e_l = q^j - q^i$ and an integral on that edge

$$I_l = \|q^j - q^i\| \int_0^1 g(q^i + \lambda(q^j - q^i))d\lambda.$$

Then

$$\delta I_l = (\delta q^j - \delta q^i) \cdot (q^j - q^i)\|q^j - q^i\|^{-2} I_l$$
$$+\|q^j - q^i\| \int_0^1 ((1-\lambda)\delta q^i + \lambda \delta q^j)\nabla g(q^i + \lambda(q^j - q^i))d\lambda + o(\delta q_h)$$
$$= \int_{\Gamma_h} g t \cdot \partial_s \delta q_h + \int_{\Gamma_h} \delta q_h \nabla g + o(\delta q_h)$$

Now putting the pieces together (we omit to write the remainders $o(\ )$),

$$\delta \int_{\Omega_h} \nabla w^i \cdot \nabla w^j = \int_{\delta\Omega_h} \nabla w^i \cdot \nabla w^j + \int_{\Omega_h} [\nabla \delta w^i \cdot \nabla w^j + \nabla w^i \cdot \nabla \delta w^j]$$
$$= \int_{\Omega_h} [\nabla \cdot (\delta q_h \nabla w^i \cdot \nabla w^j) - \nabla(\nabla w^i \cdot \delta q_h) \cdot \nabla w^j - \nabla w^i \cdot \nabla(\nabla w^j \cdot \delta q_h)]$$

$$\delta \int_{\Gamma_h} w^i \cdot w^j = \int_{\delta\Gamma_h} w^i \cdot w^j + \int_{\Gamma_h} [\delta w^i \cdot w^j + w^i \cdot \delta w^j]$$
$$= \int_{\Gamma_h} w^i \cdot w^j t \cdot \partial_s \delta q_h + \int_{\Gamma_h} \delta q_h \nabla(w^i \cdot w^j)$$
$$- \int_{\Gamma_h} [(\nabla w^i \cdot \delta q_h) \cdot w^j + (\nabla w^j \cdot \delta q_h) \cdot w^i]$$

giving

Proposition

$$\delta J = \int_{\Omega_h} \nabla \psi_h^T (\nabla \cdot \delta q_h - \nabla \delta q_h - \nabla \delta q_h^T) \nabla \Phi_h + a \int_{\Gamma_h} \psi_h \cdot \Phi_h t^T \nabla \delta q_h t$$
$$+ o(\|\delta q_h\|)$$

where t is the tangent vector to Γ_h, $\psi_h = \sum \Psi_i w^i$ and Ψ is solution of $A^T \Psi = 2(B\Phi - U)$.

Consequently an iterative process like the method of steepest descent to compute the optimal shape will move each vertex of the triangulation in the direction opposite to the partial derivative of J with respect to the vertex coordinates (E^k is the k^{th} unit vector of R^d):

$$q_k^i := q_k^i - \rho[\int_{\Omega_h} \nabla\psi_h^T(\nabla\cdot(E^k w^i) - \nabla(E^k w^i) - \nabla(E^k w^i)^T)\nabla\phi_h$$
$$+a\int_{\Gamma_h} \psi_h \cdot \phi_h t^T \nabla(E^k w^i)t]$$

5.4 Implementation problems

Computation of discrete derivatives of cost functional is, as we have seen a crafty work, only reasonnable for simple problems.

Another difficulty is that for practical applications the optimization problem is changed all the time by the designer until a feasible situation is reached. A first cost function and constraint sets are set, the solution is found to violate certain unforeseen constraints so the constraint set is changed... Finally multipoint optimization is desired so the cost function and equations are changed... and each time the discrete gradients must be computed. *Automatic differentiation* is the cure but as we shall see it has its own difficulties.

Mesh distortion is also a big problem. After a few iterations the mesh is no longer feasible. A remeshing will induce interpolation errors which may cause divergence in the optimization process if done too often. *Automatic mesh adaption* and motion is the cure, it will also be explained in a coming chapter.

Finally boundary oscillation is also a frequent curse usually due to a wrong choice of scalar product in the optimization algorithm. We will give some elements of answer below.

5.5 Optimal shape design with Stokes flow

The drag and lift are the only forces at work in the absence of gravity. If the body is symmetric and its axis is aligned with the velocity at infinity then there is no lift and therefore we can equally well minimize the energy of the system, which for Stokes flow gives the following problem:

$$\min_{\Omega\in\mathcal{O}} J(\Omega) = \nu\int_{\Omega} |\nabla u|^2$$
$$\text{subject to :}$$
$$-\nu\Delta u + \nabla p = 0, \quad \nabla\cdot u = 0 \text{ in } \Omega$$
$$u|_S = 0, \quad u|_{\Gamma_\infty} = u_\infty$$

An example of $\mathcal{O}$ is :

$$\mathcal{O} = \{\Omega,\ \partial\Omega = S\cup\Gamma_\infty, |\tilde{S}| = 1\},$$

where $\tilde{S}$ is the domain inside the closed boundary S and $|\tilde{S}|$ is its volume or area in 2D.

Sensitivity analysis is as before; let $\Omega' \in \mathcal{O}$ be a domain "near" Ω defined by its boundary $\Gamma' = \partial\Omega'$, with

$$\Gamma' = \{x + \alpha(x)n(x), \text{ with } \alpha = \text{ regular, small, } \forall x \in \Gamma = \partial\Omega\}$$

Define also

$$\delta u = u(\Omega') - u(\Omega) \equiv u' - u$$

while extending u by zero in $\tilde{S}$. Then

$$\delta J = \nu\delta(\int_\Omega |\nabla u|^2) = \nu\int_{\delta\Omega}|\nabla u|^2 + 2\nu\int_\Omega \nabla\delta u : \nabla u + o(\delta\Omega, \delta u).$$

When ∇u is smooth, then

$$\nu\int_{\delta\Omega}|\nabla u|^2 = \nu\int_\Gamma \alpha|\nabla u|^2 + o(\|\alpha\|_{C^2}) = \nu\int_\Gamma \alpha|\partial_n u|^2 + o((\|\alpha\|_{C^2}).$$

Now $\delta u, \delta p$ satisfy

$$-\nu\Delta\delta u + \nabla\delta p = 0, \quad \nabla\cdot\delta u = 0 \text{ in } \Omega$$
$$\delta u|_{\Gamma_\infty} = 0, \quad \delta u|_S = -\alpha\partial_n u$$

Indeed the only non-obvious relation is the boundary condition on S. Now by a Taylor expansion

$$u'(x + \alpha n) = u'(x) + \alpha\partial_n u'|_{S'} + o(|\alpha|) = 0 \text{ since } u'|_{S'} = 0.$$

Now $u\,|_S = 0$ so,

$$\delta u|_S = -\alpha\partial_n u|_S.$$

Consequently ($A : B$ means $\sum_{ij} A_{ij}B_{ij}$)

$$\nu\int_\Omega \nabla\delta u : \nabla u = \nu\int_\Omega(-\Delta u)\cdot\delta u + \nu\int_\Gamma \partial_n u\cdot\delta u =$$
$$\int_\Omega p\nabla\cdot\delta u - \int_\Gamma p\delta u\cdot n + \nu\int_\Gamma \partial_n u\cdot\delta u =$$
$$\int_\Gamma(\nu\partial_n u - pn)\cdot\delta u = -\int_S \nu\alpha|\partial_n u|^2,$$

because, if s denotes the tangent component,

$$n\cdot\partial_n u = -s\cdot\partial_s u = 0 \text{ on } \Gamma.$$

We have proved the

Proposition 3 : *The variation of J with respect to Ω is :*

$$\delta J = -\nu\int_S \alpha|\partial_n u|^2 + o(\alpha)$$

Consequences

- If $\mathcal{O} = \{S : S \supset C\}$, as $|\partial_n u|^2 > 0$, then C is the solution (no fairing around C will decrease the drag in Stokes flow).
- If $\mathcal{O} = \{S : Vol\ \tilde{S} = 1\}$, then the object with minimum drag saisfies $\partial_n u \cdot s$ constant on S. Lighthill (cf. Pironneau (1973)) showed that near the leading and the trailing edge the only possible axisymmetric flow which can achieve this condition must have conical tips of half angle equal to 60^o.
- The method of steepest descent gave a shape near to the optimal shape after one iteration (cf. Pironneau (1973)), and it was confirmed in Bourot (1976) by a Newton method.

A similar analysis can be done for the Navier-Stokes equation for incompressible flows.

The Optimal shape undeer the constraint that the volume is fixed and that the shape be axisymmetric, is given on Figure 1.

5.6 OSD for laminar flow

Consider the minimum drag/energy problem with the Navier-Stokes equations.

$$\min_{S\in\mathcal{O}} J(\Omega) = \nu \int_\Omega |\nabla u|^2 \quad \text{subject to}$$
$$-\nu\Delta u + \nabla p + u\nabla u = 0, \quad \nabla\cdot u = 0, \quad \text{in } \Omega$$
$$u|_S = 0, \quad u|_{\Gamma_\infty} = u_\infty$$

and with $\mathcal{O} = \{S \ : \ |\tilde{S}| = 1\}$, $\Gamma = \partial\Omega = S_\infty \cup \Gamma$.

Let us express the variation of $J(\Omega)$ in terms of the variation α of Ω.

As for the Stokes problem,

$$\delta J = J(\Omega') - J(\Omega) = \nu \int_{\delta\Omega} |\nabla u|^2 + 2\nu \int_\Omega \nabla u \nabla \delta u + o(\delta u, \alpha).$$

but now the equation of δu is no longer self adjoint

$$-\nu\Delta\delta u + \nabla\delta p + u\nabla\delta u + \delta u\nabla u = o(\delta u),$$
$$\nabla\cdot\delta u = 0$$
$$\delta u|_{\Gamma_\infty} = 0, \quad \delta u|_S = -\alpha\partial_n u$$

So an adjoint equation is introduced with an adjoint state (P,q) :

$$-\nu\Delta P + \nabla q - u\nabla P - (\nabla P)u = -2\nu\Delta u, \quad \nabla\cdot P = 0 \ \text{ in } \Omega$$
$$P|_\Gamma = 0.$$

Proposition

The variation of J with respect to Ω is :

$$\delta J = \nu \int_S \alpha(\frac{\partial P}{\partial n} - \partial_n u) \cdot \partial_n u + o(\alpha)$$

For the chosen admissible set $\mathcal{O}$ we have that $\delta J \geq 0$ for every α with $\int_\Gamma \alpha = 0$. So, the optimality condition for this problem is :

$$\partial_n u \cdot (\partial_n P - \partial_n u) = \text{ constant on } S.$$

Proof

Multiply the equation for (P, q) by δu and integrate by parts

$$\int_\Omega \nu \nabla P : \nabla \delta u - \int_S \partial_n P \cdot \delta u - q \nabla \cdot \delta u + P \nabla \cdot (u \otimes \delta u + \delta u \otimes u)$$
$$= 2 \int_\Omega \nu \nabla u : \nabla \delta u - 2 \int_\Gamma \nu \partial_n u \cdot \delta u.$$

Then use the equation of δu multiplied by P and integrated on Ω

$$\int_\Omega \nu \nabla P : \nabla \delta u + P \nabla \cdot (u \otimes \delta u + \delta u \otimes u) = 0$$

So

$$\delta J = \nu \int_{\delta\Omega} |\nabla u|^2 + \int_S \alpha(\partial_n P - 2\partial_n u) \cdot \partial_n u$$
$$= \nu \int_S \alpha(|\partial_n u|^2 + (\partial_n P - 2\partial_n u) \cdot \partial_n u)$$

6. Alternative ways

An alternative method to obtain the discrete optimality conditions is to see that

$$A\Phi = F \quad \text{with} \quad A_{ij} = \int_\Omega \nabla w^i \cdot \nabla w^j$$

Therefore

$$A\delta\Phi = -(\delta A)\Phi + \delta F$$

with

$$\delta A = \int_{\delta\Omega} \nabla w^i \cdot \nabla w^j + \int_\Omega \nabla \delta w^i \cdot \nabla w^j + \int_\Omega \nabla w^i \cdot \nabla \delta w^j$$

Next use Lemma 4 for the first term and lemma 3 for the two others

$$\delta A = \int_\Omega \nabla w^i \cdot \nabla w^j \nabla \cdot \delta q - \int_\Omega (\nabla \delta q \nabla w^i) \cdot \nabla w^j - \int_\Omega (\nabla \delta q \nabla w^j) \cdot \nabla w^i$$

with the convention that the function of x, $\delta q = \sum \delta q^i w^i$.

7. Problems Connected With The Numerical Implementation

7.1 Independence from J

Note that the adjoint state p depends on the criterion t. On the other hand if the software is to be provided as a black box to the industry it must be such that it is easy to :

- change the design criterion
- add geometrical contraints.

Suppose that we minimize a functional of the general form :

$$J(\phi, \Omega) = \int_D f(\phi)dx, \quad \phi = \{\phi^j\}, j = 1, \dots, r.$$

Since the second member of the adjoint state equation is δE, we must be able to compute $\frac{\partial E}{\partial \phi_j}$ independently of $J(\phi, \Omega)$.

This computation can be done by finite differences because :

$$\frac{\partial E}{\partial \phi_j} \simeq \frac{J(\phi_h + \delta\phi_h, \Omega_h) - J(\phi_h, \Omega_h)}{\delta \phi_j}$$

This computation is not expensive. The number of elementary computations is of order N. Indeed, if N is the number of the mesh nodes, the calculation cost is of the order N, which is the same cost as the solution of a laplacian (cf. Arumugam(1989)).

7.1.1 Add geometrical constraints. To add geometrical constraints is easy if we give a parametrized description of the domain and its triangulation.

If the boundary to optimize is described by r parameters α_j, we can define it by a curve (ex. spline) defined by α_j and then generate the triangulation with vertices $\{q^i\}, i = 1, \dots, N$ on the curve.

Since in this case only the parameters α_j move independently, we must compute the variation of E with respect to α_j. But

$$\frac{\partial E}{\partial \alpha_j} = \sum_{k,i} \frac{\partial E}{\partial q_i^k} \cdot \frac{\partial q_i^k}{\partial \alpha_j}, i = 1, \dots, N, k = 1, 2.$$

Therefore, we must be able to compute $\frac{\partial q_i^k}{\partial \alpha_j}$ and this is done also by finite differences :

$$\frac{\partial q_i^k}{\partial \alpha_j} \simeq \frac{q_i^k(\alpha_j + \delta\alpha_j) - q_i^k(\alpha_j)}{\delta \alpha_j}$$

which is not computationaly expensive.

Remark : One could think that we can compute everything by finite differences, even

$$\frac{\partial E}{\partial q_i^k} \simeq \frac{J(q_i^k + \delta q_i^k) - J(q_i^k)}{\delta q_i^k}$$

but this is far too expensive, since we have to solve the state equation every time we compute $J(q_i^k)$. So, the computational cost is $2N * O(N) \simeq O(N^2)$ which is the cost of solution of N partial differential equations.

7.1.2 Other discretization methods. We have shown above that the finite element method is well suited to Optimal Shape Design because the same principles can be used on the discrete system. In Brackman (1987) and Makinen (1990) an extension to Iso-parametric elements can be found. Chenais (1993) shows also that with Cea's artificial domain velocity it is possible to have the discrete derivatives equal to the continuous derivatives discretized. Finally Finite Volume methods computations of derivatives can be found in Dervieux (1993).

7.1.3 Automatic Differentiation of Programs.. Usually the computer program for the PDE solver is written before hand and the optimal shape design analysis comes after.

The idea is to say that the PDE is known from a long sequence of equalities each of which is easy to differentiate. If each program line is thus differentiated a linearized solver is found. Then an adjoint equation is easier to found.

A review article on these methods can be found in (Gilbert et al (1991) for example).

Example

Consider the problem

$$\min_{u_1,u_2} \{J(u_1,u_2) = x_2^2 \ : \ x_1 = u_1; x_2 = ax_1^2 + u_2^2\}$$

Direct Method

The automatic differentier ADOLC of Griewank works as follows. The problem above is represented by the following program

$$\begin{aligned} x_1 &= u_1 \\ x_2 &= ax_1^2 + u_2^2 \\ J &= x_2^2 \end{aligned}$$

After each line one inserts the differentiated line and obtain

$$
\begin{aligned}
x_1 &= u_1 \\
dx_1 &= du_1 \\
x_2 &= ax_1^2 + u_2^2 \\
dx_2 &= 2ax_1 dx_1 + 2u_2 du_2 \\
J &= x_2^2 \\
dJ &= 2x_2 dx_2
\end{aligned}
$$

This is not too hard to do automatically because each line involves only usual functions whose derivative can be computed by symbolic computation. The resulting program gives, for prescribed du_i, the directional derivative

$$dJ = J'_{u_1} du_1 + J'_{u_2} du_2$$

Inverse method

From this it is possible to compute the partial derivatives J'_{u_i} by choosing $du_j = \delta_{ij}$, but the computing cost is prohibitive when the control space dimension is large. Then another strategy is possible.

Construct the Lagrangian by multiplying each line of the computer program by a lagrangian multiplier p_i:

$$L = J + p_1(x_1 - u_1) + p_2(x_2 - ax_1^2 + u_2^2)$$

Then as in control theory write that L has a saddle point at the solution:

$$
\begin{aligned}
L'_{x_1} &= p_1 - 2ax_1 p_2 = 0 \\
L'_{x_2} &= 2x_2 + p_2 = 0 \\
L'_{u_1} &= -p_1 \\
L'_{u_2} &= -2u_2 p_2
\end{aligned}
$$

At the solution $J'_{u_i} = L'_{u_i}$, so the last two lines gives us the anwser. Notice that the first lines define the adjoint of the problem and they must be computed from down up (hence the name reverse method). It is not easy to set up this strategy automatically. The program *Odyssee* implements the method for FORTRAN programs with some restrictions (no GOTO...).

Handling DO loops

Consider the equation

$$-\frac{d^2u}{dx^2}^2 + \sin u = 1, \quad \forall x \in]0,1[, \quad u(0) = u(1) = 0,$$

discretized by a finite difference method and a Gauss-Seidel solution of the linear system:

```
do  i=0..N
     u_{i}=0
do  k=1..M
  do  i=1..N-1
     v_{i}=sin  u_{i}
     u_{i} =(u_{i+1}  +u_{i-1}) - (v_{i}-1)/N^2)/2
end_do
end_do.
```

As is often the case, while programming, the intermediate variable v_i is introduced.

A DO loop being in fact identical to a long sequence of program statement let us introduced a lagrange multiplyier for each line and construct the Lagrangian:

$$L = \sum_{0}^{N} p_i^0 u_i + \sum_{k=1}^{M} \sum_{1}^{N-1} p_i^k (v_i - \sin u_i) + p_{N+i}^k (N^2(2u_i - u_{i+1} - u_{i-1}) + v_i - 1)$$

This Lagrangian contains only simple function so it can be differentiated with respect to u and v by any formal computation program (Maple, Mathematica...) Thus the adjoint program is obtained:

$$\frac{\partial L}{\partial u_0} = p_0^0 - \sum_{k=1}^{M} p_{N+1}^k N^2$$

$$\frac{\partial L}{\partial u_i} = p_i^0 + \sum_{k=1}^{M} [-p_i^k \cos u_i + N^2(2p_{N+i}^k - p_{N+i-1}^k - p_{N+i+1}^k)$$

$$\frac{\partial L}{\partial u_N} = p_N^0 - \sum_{k=1}^{M} p_{2N-1}^k N^2$$

$$\frac{\partial L}{\partial v_i} = \sum_{k=1}^{M} (p_i^k + p_{N+i}^k)$$

While there seems to be no conceptual difficulties, there is a dramatic increase of lagrangian variables due to DO loops.

The limit of the method is the memory of the computer.

Notice however that if we set $p_i' = \sum_{k=1}^{M} p_i^k$, the usual discrete adjoint equations are obtained, as if the linear system was solved in one go. This important remark can save us from trouble when handling iterative methods for systems.

Handling IF statements

Branching instructions are no problem. consider the case where $\sin u$ is replace by $\sin|u|$ and programmed as

$$\begin{aligned} &if\ u_i\ >\ 0\ then\ v_i = \sin u_i \\ &else\ \ v_i = \sin(-u_i) \end{aligned}$$

The idea is to consider that we have 2 programs, one for each result of the if statement. Then there will be two lagrangian and after differentiation one puts them back into the if structure and obtain

$$\begin{aligned} &if\ u_i\ >\ 0\ then\ \frac{\partial L}{\partial u_i} = -p_{i+1}\cos u_i + N^2(2p_{N+i} - p_{N+i-1} - p_{N+i+1}) \\ &else\ \frac{\partial L}{\partial u_i} = p_{i+1}\cos(-u_i) + N^2(2p_{N+i} - p_{N+i-1} - p_{N+i+1}) \end{aligned}$$

8. Regularity Problems

Consider an optimal shape design problem

$$\min_{S\in\mathcal{S}} J(S)$$

with admissible shapes defined locally around Σ fixed and smooth

$$\mathcal{S} = \{\mathbf{x} + \alpha(x)\mathbf{n}(x)\ :\ x\in\Sigma, \quad \alpha\in H_0^2(\Sigma)\ \}$$

Suppose we know a $\chi\in L^2(\Sigma)$ such that

$$J(S(\alpha+\delta\alpha)) = J(S(\alpha)) + \int_\Sigma \chi(s)\delta\alpha(s)\mathrm{d}s + o(\|\delta\alpha\|_2)$$

It is not a good idea to apply a gradient method in L^2 like

$$\alpha^{m+1} = \alpha^m - \rho\chi^m$$

because $\alpha^m\in H^2(\Sigma)$ does not imply $\alpha^{m+1}\in H^2(\Sigma)$ as one usually cannot expect $\chi\in H_0^2(\Sigma)$.

So let us define $\xi\in H_0^2(\Sigma)$ by

$$\frac{d^4\xi}{ds^4} = \chi, \text{ on } \Sigma, \quad \xi = \frac{d\xi}{ds} = 0 \text{ on } \partial\Sigma.$$

Then

$$\begin{aligned} J(S(\alpha+\delta\alpha)) &= J(S(\alpha)) + \int_\Sigma \chi(s)\delta\alpha(s)\mathrm{d}s + o(\|\delta\alpha\|_2) \\ &= J(S(\alpha)) + \int_\Sigma \frac{d^2\xi}{ds^2}\frac{d^2\alpha}{ds^2}\delta\alpha(s)\mathrm{d}s + o(\|\delta\alpha\|_2) \end{aligned}$$

Now we can do

$$\alpha^{m+1} = \alpha^m - \rho\xi^m$$

8.1 Application

Consider again the laboratory problem of Figure 2 and its discretization by the FInite Element Method (Figure 3).

$$J(S) = \int_D |u - u_d|^2 \quad : \quad -\Delta u = f, \quad u \in H_0^1(\Omega), \quad S \subset \partial\Omega$$

for which we know that for some $y(s) = x(s) + \theta\delta\alpha(s)$, $\theta \in]0,1[$ we have

$$\delta J = \int_\Sigma \frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\delta\alpha - \frac{1}{2}\int_\Sigma \frac{\partial p}{\partial n}(x(s))\frac{\partial^2 u}{\partial n^2}(y(s))\delta\alpha(s)^2 ds$$

with p solution of

$$p \in H_0^1(\Omega), \quad -\Delta p = 2(u - u_d)I_D$$

With the regularity $S \in H_0^2(\Sigma)$ we have $u, p \in H^2(\Omega)$, $\chi \in W^{\frac{1}{2},1}(\Sigma)$. Setting ξ by

$$\frac{d^4\xi}{ds^4} = \chi, \quad \text{on} \quad \Sigma, \quad \xi = \frac{d\xi}{ds} = 0 \quad \text{on} \quad \partial\Sigma.$$

might be difficult in practice, especially in 3D because PDEs on surfaces may be tricky to solve. Instead consider $\xi = v|_\Sigma$ with

$$-\Delta w = 0, \quad \frac{\partial w}{\partial n}|_\Sigma = \chi, \qquad -\Delta v = w, \quad \frac{\partial v}{\partial n}|_\Sigma = 0.$$

Lemma 1
The operator $\chi \to \xi \equiv A\chi$ is positive definite and $\chi \in L^2(\Sigma) \Rightarrow \xi \in H^2(\Sigma)$

Proof Let

$$-\Delta w' = 0, \quad \frac{\partial w'}{\partial n}|_\Sigma = \chi', \qquad -\Delta v' = w', \quad \frac{\partial v'}{\partial n}|_\Sigma = 0.$$

and note that

$$< \chi', A\chi > = \int_\Sigma \frac{\partial w'}{\partial n} v = \int_\Omega \nabla w' \nabla v = \int_\Omega w' w$$

Proposition
The following algorithm preserves the regularity of the variables:

$$\alpha^{m+1} = \alpha^m - \rho\xi^m$$

Remark
Oden et al suggested to use $\xi = \mathbf{u}\cdot\mathbf{n}|_\Sigma$ where

$$-\lambda\Delta\mathbf{u} + \mu\nabla(\nabla\cdot\mathbf{u}) = 0, \quad \sigma_{\mathbf{nn}}(\mathbf{u})|_\Sigma = \chi, \quad \mathbf{u}\cdot\mathbf{s} = 0$$

because

$$\int_\Sigma \xi\chi' = \int_\Sigma \sigma_{nn}(\mathbf{u}')\mathbf{u}\cdot\mathbf{n} = \int_\Omega (\lambda\nabla u\nabla v + \mu\nabla\cdot u\nabla\cdot v)$$

Although it is also a smoothing process it is less regualar than the one above.

8.2 Discretization

Recall that a finite element discretization of the problem is

$$J = \int_D (u - u_d)^2, \quad \int_\Omega \nabla u \nabla w^j + \frac{1}{\epsilon} u_j I_{q^j \in \Gamma} = \int_D f w^j$$

with $u = \sum_1^N u_j w^j$, $\quad \Omega = \cup T_k,\ T_k = \{q^{j_1}, q^{j_2}, q^{j_3}\}$.

Recall that

$$\delta w^j = -\nabla w^j \cdot \delta q_h, \quad \delta q_h = \sum_j \delta q^j w^j$$

and that

$$\int_{\Omega'} f - \int_\Omega f = \sum_k \int_{T_k} \nabla \cdot (f \delta q_h)$$

so that we have the

Proposition

$$\delta J = \int_\Omega \nabla u^T (\nabla \delta q_h + \nabla \delta q_h^T - I \nabla \cdot \delta q_h) \nabla p + o(|\delta q_h|)$$

Proof

$$\delta u = \sum_1^N \delta u_j w^j + u_j \delta w^j = \delta u_h - \nabla u_h \cdot \delta q_h$$

$$\int_\Omega \nabla(\delta u_h - \nabla u_h \cdot \delta q_h) \nabla w^j - \int_\Omega \nabla u \nabla w^j \nabla \delta q_h$$

$$+ \int_\Omega \nabla \cdot (\nabla u \nabla w^j \delta q_h) + \frac{1}{\epsilon} \delta u_j I_{q^j \in \Gamma} = 0$$

$$\delta J = \int_D 2 \delta u (u - u_d) = \int_\Omega \nabla p \nabla \delta u_h + \sum_{q^j \in \Gamma} p_j \delta u_j$$

Proposition

$$\delta J = \int_S \nabla u \cdot \nabla p\, \delta q_h \cdot n + \int_{Edges} [\nabla u \cdot \nabla p] \delta q_h \cdot n + o(|\delta q_h|)$$

This is because

$$\delta(\nabla Q_h \nabla Q_h^T \det Q_h^{-1}) = \nabla \delta q_h + \nabla \delta q_h^T - I \nabla \cdot \delta q_h + o(|\delta q_h|)$$

8.3 Consequence

• It is clear the the discrete optimization process tends to the continuous one. But... do we have the necessary regularity?
• It is not necessary to account for the motion of the inner mesh points if $h << 1$
• One should not use the gradient with respect to the inner points to move them because it is an order of magnitude smaller: $W^j = (w^j, w^j)^T$

$$q^j \leftarrow q^j - \rho \int_\Omega \nabla u^T (\nabla W^j + \nabla W^{jT} - I\nabla \cdot W^j)\nabla p$$

Use the smoothers, so the complete algorithm is

1. Solve
$$\int_\Omega \nabla u \nabla w^j + \frac{1}{\epsilon} u_j I_{q^j \in \Gamma} = \int_D f w^j$$
2. Solve
$$\int_\Omega \nabla p \nabla w^j + \frac{1}{\epsilon} p_j I_{q^j \in \Gamma} = 2\int_D (u - u_d) w^j$$
3. Solve
$$\int_\Omega \lambda \nabla U : \nabla W^j + \mu \nabla \cdot U \nabla \cdot W^j = \int_\Omega \nabla u^T (\nabla W^j + \nabla W^{jT} - \nabla \cdot W^j)\nabla p$$
4. Move the points of the mesh by
$$q^j \leftarrow q^j - \rho U^j$$

9. Consistent Approximations

OSD is expensive; there is a great economical advantage to combine the optimization algorithm with mesh refinement so as to obtain a speed up similar to multigrid.

For standard optimization, E. Polak (1998) developped a tool which he calls the theory of consistent approximation" which we apply here. The following is a summary of results obtained jointly with N. Dicesare and E. Polak. For more details see Dicesare et al (1998).

9.1 Algorithm

The problem is to minimize $J(z)$ in $\mathcal{O}$. The discrete problem is indexed by a discretization parameter h: minimize $J_h(z_h)$ in $\mathcal{O}_h$.

Assume that $\mathcal{O}$ is a Hilbert space. Let

$$\theta(x) = -||Grad_z J(z)|| \quad \text{and} \quad \theta_h(z) = ||Grad_z J_h(z)||$$

Algorithm 1

1. Choose a converging sequence of discretization spaces $\{\mathcal{O}_{h_n}\}$ with $\mathcal{O}_{h_n} \subset \mathcal{O}_{h_{n+1}}$ for all n. Choose $z^0, \epsilon^0, \beta \in]0,1[$.
2. Set $n = 0, \epsilon = \epsilon^0, h = h_0$
3. Compute z^n_m by performing m iterations of a descent algorithm on $\mathcal{P}_h$ from starting point z^n so as to achieve
$$\theta_h(z^n_m) > -\epsilon$$
4. Set $\epsilon = \beta\epsilon, h = h_{n+1}, z^{n+1} = z^n_m, n = n+1$ and go to Step 3.

The mathematical result is that if $\mathcal{P}_h$ epi-converge to $\mathcal{P}$ then any accumulation point z^* of $\{z^n\}$ generated by Algorithm 1 satisfies $\theta(z^*) = 0$.

9.2 Problem Statement

Consider a simple model problem where the shape is to be found that brings u, solution of a PDE, nearest to u_d in a subregion D of the entire domain Ω.

The unknown shape Γ is a portion of the entire boundary $\partial\Omega$: it is parametrized by its distance α to a reference smooth boundary Σ. To prevent an excess of oscillation the problem is regularized.

More concretely with the following notations ($\epsilon << 1$),

$$D \subset \Omega,\ u_d \in H^1(D),\ g \in H^1(\Omega),\ I \subset K \subset \mathcal{R},\ \ \Sigma = \{x(s)\ :\ s \in K\}$$

we consider

$$\min_{\alpha \in H^2_0(I)} J(\alpha) = \int_D (u - u_d)^2 + \epsilon \int_\Sigma |\frac{d^2\alpha}{ds^2}|^2$$
$$\text{subject to}\ \ u - \Delta u = 0\ \ \text{in}\ \ \Omega(\alpha),\quad \frac{\partial u}{\partial n}|_{\Gamma(\alpha)} = g|_{\Gamma(\alpha)},$$

$$\text{where}\ \ \Gamma(\alpha) = \partial\Omega(\alpha) = \{x(s) + \tilde{\alpha}(s) n(x(s))\ :\ s \in K\}$$

where $\tilde{\alpha}$ is the extension by zero in K of α which is only defined on I.

Recall that

$$H^2_0(I) = \{\alpha \in L^2(I)\ :\ \alpha', \alpha" \in L^2(I),\ \ \alpha(a) = \alpha'(a) = 0\ \ \forall a \in \partial I\}$$

and that $\|\alpha''\|_0 = \|d^2\alpha/ds^2\|_0$ is a norm in that space.

Let us denote the unknown part of the boundary by

$$S(\alpha) = \{x(s) + \alpha(s)n(x(s)) \ : \ s \in I\}$$

For simplicity let us assume that g is always zero on S.

9.3 Discretization

The discrete problem is

$$\min_{\alpha \in L_h \subset H_0^2(I)} J(\alpha) = \int_D (u - u_d)^2 + \epsilon \int_\Sigma |\frac{d^2\alpha}{ds^2}|^2$$

$$\text{subject to} \quad \int_{\Omega(\alpha)} (uv + \nabla u \nabla v) = \int_{\Gamma(\alpha)} gv \ \forall v \in V_h, \quad u \in V_h$$

where V_h is the usual Lagrange Finite Element space of degree 1 on triangles except that the boundary triangles have a curved side because $S(\alpha)$ is a cubic spline.

The space L_h is the finite dimensional subspace of $H_0^2(I)$ defined as the set of cubic splines which passes through the vertices which would we would have used otherwise to define a feasible polygonal approximation of the boundary. This means that the discretization of Ω is done as follows

1. Give a set of n_f boundary vertices $q^{i_1}, ..., q^{i_{nf}}$, construct a polygonal boundary near Σ
2. Construct a triangulation of the domain inside this boundary with an automatic mesh generator, i.e. Mathematically the inner nodes are theoretically linked to the outer ones by a map
$$q^j = Q^j(q^{i_1}, ..., q^{i_{nf}}), \quad nf < j < nv$$
3. Construct $\Gamma(\alpha)$, the cubic splines from the $q^{i_1}, ..., q^{i_{nf}}$, set α to be the normal distance from Σ to $\Gamma(\alpha)$.
4. Construct V_h by using triangular finite elements and overparametric curved triangular elements on the boundary.

This may seem complex but it is a handy construction because the discrete cost function J_h coincide with the continuous J and because L_h is a finite subspace of the (infinite) set of admissible parameters H_0^2.

We proceed and verify the hypothesis of the theorem to apply Algorithm 1.

9.4 Optimality Conditions: the continuous case

As before, by calculus of variations

$$\delta J = 2\int_D (u-u_d)\delta u + 2\epsilon\int_\Sigma \frac{d^2\alpha}{ds^2}\frac{d^2\delta\alpha}{ds^2}$$

with $\delta u \in H^1(\Omega(\alpha))$ and

$$\int_{\Omega(\alpha)}(\delta u v + \nabla\delta u\nabla v) + \int_\Sigma \delta\alpha(uv+\nabla u\nabla v) = 0 \; \forall v\in H^1(\Omega(\alpha)).$$

Introduce an adjoint $p\in H^1(\Omega(\alpha))$

$$\int_{\Omega(\alpha)}(pq+\nabla p\nabla q) = 2\int_D (u-u_d)q, \quad \forall q\in H^1$$

i.e.

$$p-\Delta p = I_D u, \quad \frac{\partial p}{\partial n}=0$$

Then

$$\delta J = -\int_\Sigma \delta\alpha(up+\nabla u\nabla p - 2\epsilon\frac{d^4\alpha}{ds^4})$$

9.4.1 Definition of θ. So we should take

$$\theta = -\|up+\nabla u\nabla p - 2\epsilon\frac{d^4\alpha}{ds^4}\|_{-2}$$

i.e. solve

$$\frac{d^4\theta}{ds^4} = up+\nabla u\nabla p - 2\epsilon\frac{d^4\alpha}{ds^4} \;\; on \;\; I, \quad \theta = \frac{d\theta}{ds} = 0 \;\; on \;\; \partial I$$

9.5 Optimality Conditions: the discrete case

Let w^j be the hat function attached to vertex q^j. If some vertices q^j vary by δq_j we define

$$\delta q_h(x) = \sum_j \delta q_j w^j(x)$$

and we know that (Pironneau[1983])

$$\delta w^k = -\nabla w^k\cdot\delta q_h$$

$$\int_{\delta\Omega} f = \int_\Omega \nabla\cdot(f\delta q_h) + o(|\delta q_h|)$$

Hence

$$J(\alpha+\delta\alpha) = 2\int_D (u_h-u_{dh})\delta u_h + 2\epsilon\int_\Sigma \frac{d^2\alpha}{ds^2}\frac{d^2\delta\alpha}{ds^2},$$

Furthermore and by definition of δu_h

$$\delta \sum_i u_i w^i = \sum_i (\delta u_i w^i + u_i \delta w^i) = \delta u_h + \delta q_h \cdot \nabla u_h$$

the partial variation δu_h is found by

$$\delta \int_{\Omega(\alpha)} (u_h w^j + \nabla u_h \nabla w^j) = \int_\Omega (\nabla \cdot (u w^j \delta q_h) + \delta u_h w^j + \nabla \delta u_h \nabla w^j)$$
$$+ \int_\Omega (u_h \delta q_h \cdot \nabla w^j + \nabla u_h \nabla \delta q_h \nabla w^j + u_h \delta w^j + \nabla u_h \nabla \delta w^j) = 0$$

Hence

$$\int_\Omega (\delta u_h w^j + \nabla \delta u_h \nabla w^j =$$
$$\int_\Omega (\nabla u_h (\nabla \delta q_h + \nabla \delta q_h^T) \nabla w^j - (u_h w^j + \nabla u_h \cdot \nabla w^j) \nabla \cdot \delta q_h)$$

So introduce an adjoint $p_h \in V_h$

$$\int_\Omega (p_h w^j + \nabla p_h \nabla w^j) = 2 \int_D (u_h - u_{dh}) w^j \quad \forall j$$

And finally

$$\delta J_h = \int_\Omega (\nabla u_h (\nabla \delta q_h + \nabla \delta q_h^T) \nabla p_h - (u_h p_h + \nabla u_h \cdot \nabla p_h) \nabla \cdot \delta q_h) + 2\epsilon \int_\Sigma \frac{d^2 \alpha}{ds^2} \frac{d^2 \delta \alpha}{ds^2}$$

9.6 Definition of θ_h

Let $e^1 = (1,0)^T$, $e^2 = (0,1)^T$ be the coordinate vectors of R^2, let χ^j be the vector of R^2 of components

$$\chi_k^j = \int_\Omega (\nabla u_h (\nabla w^j e^k + (\nabla w^j e^k)^T) \nabla p_h - (u_h p_u + \nabla u_h \cdot \nabla p_h) \nabla \cdot w^j e^k.$$

Because the inner vertices are linked to the boundary ones by the maps Q^j, let us introduce

$$\xi_k^j = \chi_k^j + \sum_{q^i \notin \Gamma} \chi^i \partial_{q_k^j} Q^i.$$

Then obviously

$$\delta J = \sum_1^{nf} \xi^j \cdot \delta q^j + 2\epsilon \int_\Sigma \frac{d^2 \alpha}{ds^2} \frac{d^2 \delta \alpha}{ds^2}$$

It is possible to find a β so as to express the first discrete sum as an integral on Σ of $\frac{d^2 \beta}{ds^2} \frac{d^2 \delta \alpha}{ds^2}$; it is some sort of variational problem in L_h:

$$\int_\Sigma \frac{d^2\beta}{ds^2}\frac{d^2\delta\lambda^j}{ds^2} = \xi^j \cdot n_\Sigma, \quad j = 1,...,nf; \quad \beta \in L_h$$

where λ^j is the cubic spline obtained by a unit normal variation of the boundary vertex q^j only.
Then the "derivative" of J_h is the function $s \in I \to \beta(s) + 2\epsilon\alpha(s)$ and the function θ_h is

$$\theta_h = -||\beta||_{H_0^2(I)}$$

Remark This may be unnecessarily complicated in practice. A pragmatic summary of the above is that β is solution of a fourth order problem, so why not set a discrete fourth order problem on the normal component of the vertex themselves. In the case $\epsilon = 0$ this would be

$$\frac{1}{h^4}[q'^{j+2}_n - 4q'^{j+1}_n + 6q'^j_n - 4q'^{j-1}_n + q'^{j-2}_n] = \xi^j,$$

$$q'^0_n = q'^1_n = q'^{nf-1}_n = q'^{nf}_n = 0$$

and then the norm of the second derivative of the result for θ_h

$$\theta_h \approx -(\sum_j \frac{1}{h^2}[q^{j+1}_n - 2q^j_n + q^{j-1}_n]^2)^{\frac{1}{2}}$$

9.7 Hypothesis of the Theorem

The following is shown in Dicesera et al (1999)

- *Inclusion* $h' < h \Rightarrow \mathcal{O}_h \subset \mathcal{O}_h$.
- it Continuity The cost functions are continuous in z

$$\alpha^n \xrightarrow{H_0^2(I)} \alpha, \quad \Rightarrow J^n \to J.$$

  Similarly in the discrete case, the spline is continuous with respect to the vertex position so

$$q^{i\ n} \to q^i \Rightarrow \alpha_h^n \xrightarrow{H_0^2(I)} \alpha_h, \quad \Rightarrow J_h^n \to J_h.$$

- *Consistency* $\forall\alpha$, $\exists\alpha_h \to \alpha$ with $J_h \to J$.
  if the following is observed:
  - Corners of the continuous curve are vertices of the discrete curves
  - the distance between boundary vertices converges uniformly to zero.
- *Continuity of θ Conjecture* : There exists ε such that $\alpha \in H_0^2 \quad \Rightarrow u \in H^{3/2+\epsilon}(\Omega)$.
  Arguments: We know that $\alpha \in C^{0,1} \quad \Rightarrow u \in H^{3/2}$(Jerisson and Kenig [???]) and $\alpha \in C^{1,1} \quad \Rightarrow u \in H^2$(Grisvard [???]).
  This technical point of functional analysis is need for the continuity of θ.

$$\alpha^n \xrightarrow{H^2} \alpha, \quad \Rightarrow \nabla u^n \nabla p^n|_\Sigma \xrightarrow{L^2} \nabla u \nabla p|_\Sigma$$

- *Continuity of* $\theta_h(\alpha_h)$
  Recall that a variation $\delta\alpha_h$ (i.e. a boundary vertex variation $\delta q^j, j \in \Sigma$) implies variations of all inner vertices $\delta\alpha, \delta q^k, \forall k$
  The problem is that θ is a boundary integral on Σ and θ_h is a volume integral! We must explain why

$$\delta J_h = \int_\Omega (\nabla u_h(\nabla \delta q_h + \nabla \delta q_h^T)\nabla p_h - \nabla u_h \cdot \nabla p_h \nabla \cdot q_h$$

$$+2\epsilon \int_\Sigma \frac{d^2\alpha}{ds^2}\frac{d^2\delta\alpha}{ds^2} \xrightarrow{?} \delta J = -\int_\Sigma \delta\alpha(up + \nabla u \nabla p + 2\epsilon \frac{d^4\alpha}{ds^4})$$

This is due to the fact that if $\nabla X = I + \nabla Q$, the jacobian matrix of the mapping $x \to X = x + Q(x)$ of $\mathcal{R}^2 \to \mathcal{R}^2$ is the linearization of the operator which appears in the change of variable $x \to X(x)$:

$$\delta(\nabla X^T \nabla X \det X^{-1}) = \nabla Q + \nabla Q^T - I\nabla \cdot Q + o(\|Q\|).$$

So δJ_h is almost a surface integral:

$$\delta J_h = -\int_\Sigma (\delta q_h \cdot n_\Sigma(u_h p_h + \nabla u_h \nabla p_h) + 2\epsilon \frac{d^4\alpha_h}{ds^4})$$

$$-\int_E [\delta q_h \cdot n_E(u_h p_h + \nabla u_h \nabla p_h)] + o(\delta q_h) + o(h)$$

where E is the set of edges of the triangulation, [.] the jump across the edges and n_E the normal to the edge E (the sign of this expression depends on the choice of the normal n_E).

9.8 Algorithm 3

An adaptation of Algorithm 1 to this case is

1. Choose an initial set of boundary vertices.
2. Construct a finite element mesh, construct the spline of the boundary.
3. Solve the discrete PDE and the discrete adjoint PDE.
4. Compute θ_h (or its approximation (cf. remark above))
5. if $\theta_h > -\epsilon$ add points to the boundary mesh, update the parameters and go back to Step 2.

There are still several hypothesis to verify to make sure that Algorithm 3 converges. We proceed in a loose fashion and give only the general idea of the proof.

9.9 Convergence

It comes from the theory of Finite Element Error Analysis (Ciarlet[1975]):
Lemma

$$\mid \int_{\Sigma} \nabla u_h \nabla p_h - \nabla u \nabla p \mid \leq C h^{1/2} (\|p\|_2 + \|u\|_2)$$

and the following triangular inequalities

- $|a_h b_h - ab| = (a_h - a)(b_h - b) + b(a_h - a) + (b_h - b)a$
  $\leq |b||a_h - a| + |a||b_h - b| + |a_h - a|^2 + |b_h - b|^2$
- $|\nabla u_h - \nabla u|_{0,\Sigma} \leq |\nabla(u_h - \Pi_h u)|_{0,\Sigma} + |\nabla(\Pi_h u - u)|_{0,\Sigma}$

plus an inverse inequality for the first term and an interpolation for the second.

10. Numerical Results

Numerical results with the local boundary variation method just described have been obtained my PhD students. For details we send the reader to their thesis, mostly at the Université Paris 6:

- F. Angrand for a wing optimization with the transonic equation
- G. Arumugam for the optimization of ribblets in laminar flow
- A. Vossinis for the choice of a numerical algorithm, Newtown, GMRES or Conjugate Gradient.
- F. Baron for the stealth wing problem and the harbour optimization

But very impressive results have been obained by Marrocco for the design of an electromagnet and by Mohammadi for the design of 3D aircrafts and wings by using automatic differentiation of programs.

Thanks to this last piece of work the method is now mature and efficient.

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