

SHAPE OPTIMIZATION IN FLUID MECHANICS

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Key Words shape design, complexity, adaptation, aerodynamics, sensitivity

■ **Abstract** This paper is a short and nonexhaustive survey of some recent developments in optimal shape design (OSD) for fluids. OSD is an interesting field both mathematically and for industrial applications. Existence, sensitivity, and compatibility of discretizations are important theoretical issues. Efficient algorithmic implementations with low complexity are also critical. In this paper we discuss topological optimization, algorithmic differentiation, gradient smoothers, Computer Aided Design (CAD)-free platforms and shock differentiation; all these are applied to a multicriterion optimization for a supersonic business jet.

1. INTRODUCTION

The applications of optimal shape design (OSD) are uncountable. For systems governed by partial differential equations, they range from structure mechanics to electromagnetism and fluid mechanics and, more recently, to a combination of the three. For instance, the design of a harbor that minimizes the incoming waves can be done at little cost by standard optimization methods once the numerical simulation of Helmholtz equation is mastered (Baron et al. 1993); microfluidic technologies, large paper machines, etc., can also be optimized this way (Mohammadi et al. 2001, Hamalainen et al. 1999), yet the biggest demand is still for airplane optimization, for which even a small drag decrease means a lot of savings (Jameson 2003, Alonso et al. 2002, Reuter et al. 1996), but multidisciplinary requirements grow. Among the applications to fluids known to the authors are (a) weight reduction and aerodynamic design of engines, cars, airplanes, and even music instruments (Becache et al. 2001); (b) electromagnetically optimal shapes, such as in stealth objects with aerodynamic constraints; (c) wave cancelling in boat design (Lohner 2001, Jameson et al. 1998); and (d) drag reduction in air and water by static or active mechanisms (Moin et al. 1992). In industry, optimum design is not a once and for all solution tool because engineering design is made of compromises owing to the multidisciplinary aspects of the problems (see Figure 1) and the necessity of doing multipoint constrained design.

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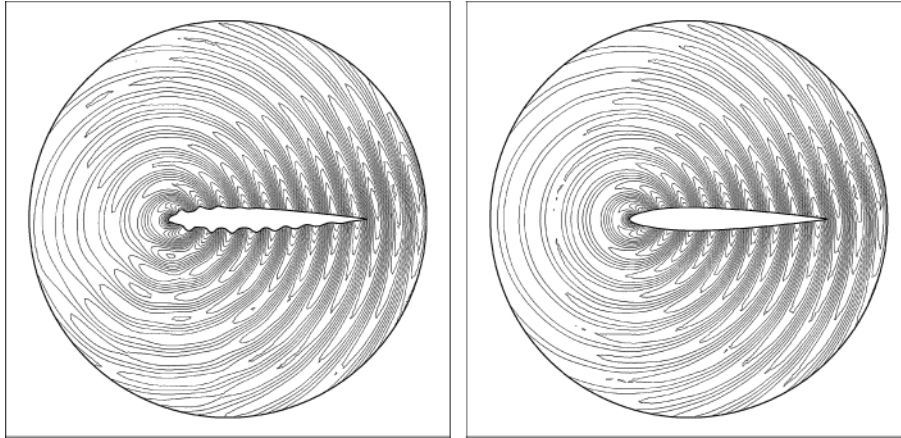


Figure 1 Optimal design of an airfoil to minimize in a sector (angle between 180–225 degrees) the reflection of a monochromatic incident radar wave. The optimal shape on the left is not admissible from the aerodynamic view point; a multidisciplinary optimization is necessary and an almost as efficient result is obtained with a constraint on the lift. Computed by A. Baron.

OSD is a branch of differentiable optimization and more precisely of optimal control for distributed systems (Lions 1968); as such, gradient and Newton methods are natural numerical tools. Existence of solutions and differentiability of the criteria with respect to shape deformation occupied most of the 1980s (Pironneau 1984, Delfour et al. 2001, Sokolowski et al. 1991, Haslinger et al. 2003). It became clear (Tartar 1974) that oscillations of shapes could lead to nonphysical solutions of the optimization problem in the limit, a phenomenon known as homogenization, which has also led to a new class of problems called topological optimization (for instance, are many pipes better than a single pipe to transport fluids?).

Numerical algorithms developed in a number of ways (see Section 2) and answered questions like (a) should optimization algorithms be applied to the continuous or to the discretized problem? The answer is: to the discrete problem if the conjugate gradient method is used [unless combined with mesh refinement (Lemarchand et al. 2002)] and to either if Newton's method is used (Marrocco et al. 1978, Kim et al. 1999). (b) Should one treat the partial differential equations as constraints or add them to the cost function? One-shot methods (Arian et al. 1995) advocate the latter but these are rather unstable on problems involving the full Navier-Stokes equations. (c) Should one optimize the position of all mesh points, of boundary points only, or try a reduced representation of the surfaces by splines or other? This last point is still a research area even though a number of approaches have been proposed: parametrization via a surface response, as used by experimentalists (Giunta 1997), hierarchical basis (Beux et al. 1993) as with

multigrids, Computer Aided Design (CAD)-free parametrization (Mohammadi et al. 2001), etc.

Real aeronautical applications began in the 1990s (Jameson 1988, Elliott et al. 1996); it is now possible to optimize an entire airplane for a criterion such as drag, under geometric and aerodynamic constraints such as volume and lift. The latest application is for the design of silent (with respect to sonic boom) supersonic airplanes (Nadarajah et al. 2002, Mohammadi 2002); we discuss this problem in the last section.

But OSD is still numerically difficult because it is computer intensive and because in practice one has to make compromises between shapes that are good with respect to more than one criteria. One approach is via Pareto optimality; there is a mathematical theorem that says in simple situations Pareto optimal points are minimizers of some convex combination of all the criteria, and the converse is also true. The trouble is that such linear combinations lead to stiff problems with many suboptima, requiring global optimization tools such as genetic algorithms.

Genetic algorithms are simple but very slow and cannot be used presently with more than a few parameters (Obayashi 1997, Makinen et al. 1999); the solution is probably in a yet to be found combination of gradient and evolutionary methods (Quagliarella et al. 1997, Peri 2003).

2. FORMULATIONS

Consider the academic problem of designing one boundary S of a wind tunnel Ω with required properties (such as uniform flow) in some region of space D (see Figure 2). This is a typical yet simple design problem which will serve our purpose to introduce most of the tools of differentiable optimizations also used for more complex industrial designs.

Assume that the flow is potential and two dimensional. With a stream function formulation this would be

$$\min_{S \in \mathcal{S}_d} \left\{ j(S) := \int_D |\psi - \psi_d|^2 : -\Delta\psi = 0, \text{ in } \Omega \quad \psi|_S = 0 \quad \psi|_C = \psi_d \right\}, \quad (1)$$

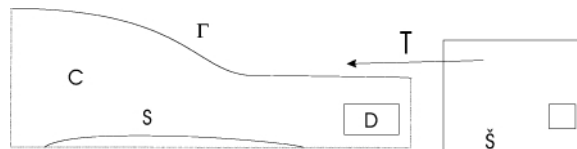


Figure 2 Inverse design for a wind tunnel with desired properties ψ_d in D .

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where $C = \Gamma \setminus S$ and $\Gamma = \partial\Omega$. It can be discretized by

$$\min_{\mathcal{T}_h} \left\{ j_h := \int_D |\psi - \psi_d|^2 : \int_{\Omega} \nabla \psi_h \nabla w_h + \frac{1}{\epsilon} \int_C (\psi_h - \psi_d) w_h = 0 \quad \forall w_h \in V_h \right\}, \tag{2}$$

where V_h is the finite element space of piecewise linear continuous functions on the triangulation \mathcal{T}_h of Ω ; h denotes the average edge length in the triangulation. If w^i denotes the function of V_h , which is one at vertex q^i and zero at all other vertices, then with $\Psi_j := \psi_h(q^j)$,

$$\psi_h(x) = \psi_d(x) + \sum_{i \notin \Gamma} \Psi_i w^i(x)$$

and Equation 2 is of the form

$$\min_{\vec{q}} \Psi^T B(\vec{q}) \Psi : A(\vec{q}) \Psi = F(\vec{q}), \tag{3}$$

where $A_{ij} = (\nabla w^i, \nabla w^j)$, $B_{ij} = (w^i, w^j)$, and F is the discrete Laplacian of ψ_d . It is clear that these depend on the position of all the vertices (stored here in the vector \vec{q}) and not just of the S vertices.

At first sight, Equation 3 looks like a large optimization problem and it is hard to see any connection with standard optimal control theory, yet an optimal time control problem on which the same discretization procedure is applied yields an optimization problem of similar structure. Thus, many tools of control theory and of the Calculus of Variations have been extended to Partial Differential Equations (PDE) and we shall use them to solve Equation 3 numerically (except the Pontryagin principle, which plays no part here).

Before attempting any numerical simulation we can study the existence of solutions. These are by no means impractical questions because many of these OSD problems do not have solutions. For example, if $\psi_d \in L^2(\Omega)$ but $\psi_d \notin H^1(\Omega)$, Equation 1 does not have a solution because $\psi \rightarrow \psi_d$ is possible and $\psi = \psi_d$ is not possible.

Existence can be studied in several ways and it is interesting that each way gives rise to a different numerical method. The first possibility occurs by using continuity results with respect to domain boundaries (Pironneau 1984, Delfour et al. 2001); the unknown is an implicit or explicit parametrization of the boundary. Although the set of admissible boundaries is not easily endowed with a vector space structure, one can define boundary variations, which have a Hilbertian structure. For instance, normal variations by $\alpha(x)$, $x \in S$ around a reference boundary S of normal $\vec{n}(x)$ would be

$$S(\alpha) = \{x + \alpha(x)\vec{n}(x) : x \in S\}. \tag{4}$$

One can also map the unknown domain Ω from a fixed domain O and consider that the unknown is the mapping $T:O \rightarrow \Omega$. Denote by T' its Jacobian matrix, let $\hat{\psi}_d$

be $\psi_d \circ T$ with ψ_d extending the given boundary conditions and the requirement in D (recall that $\psi_d = 0$ on S and is constant on the upper wall of the nozzle). Then we can solve

$$\min_{T \in \mathcal{T}_d} \left\{ \int_{\hat{D}} |\hat{\psi} - \hat{\psi}_d|^2 : \nabla \cdot [A \nabla \hat{\psi}] = 0 \text{ in } O \right. \\ \left. \hat{\psi}|_{\partial \hat{O}} = \hat{\psi}_d, A = T'^{-1T} T'^{-1} \det(T') \right\} \quad (5)$$

As for Equation 1, it is also possible to work with a local (tangent) variation $tV(x)$ and set

$$\Omega(tV) = \{x + tV(x) : x \in \Omega\} \quad t \text{ small and constant.} \quad (6)$$

The third way is to extend the operators by zero below S and take the characteristic function of Ω , χ , for unknown

$$\min_{\chi \in X_d} \left\{ \int_D |\psi - \psi_d|^2 : -\nabla \cdot [\chi \nabla \psi] = 0, \quad \psi(1 - \chi) = 0, \quad \psi|_{\partial \Omega} = \psi_d \right\}. \quad (7)$$

This last approach, suggested by Tartar (1974), has led to what is now called topological optimization. It may be difficult to work with the function χ , then, following Allaire et al. (2002), the function χ can be defined through a smooth function η by $\chi(x) = \text{bool}(\eta(x) > 0)$ and in the algorithm we can work with a smooth η as in the level-set methods where the shape is identified as being the location in the space where a distance type functional vanishes.

Most existence results are obtained by considering minimizing sequences S^n , or T^n , or χ^n and, in the case of our academic example, showing that $\psi^n \rightarrow \psi$ for some ψ (resp $T^n \rightarrow T$ or $\chi^n \rightarrow \chi$), and that the PDE is satisfied at the limit.

Using regularity results with respect to the domain (Chesnais 1987) (see also Neittaanmaki 1991 and Delfour et al. 2001) showed that in the class of all S uniformly Lipschitz, Equation 1 has a solution. However, the solution could depend on the Lipschitz constant. Similarly, working with Equation 5 showed that in the class of $T \in W^{1,\infty}$ uniformly, the solution exists (Murat et al. 1976).

However, working with Equation 7 generally leads to weaker results because if $\chi^n \rightarrow \chi$, χ may not be a characteristic function; this leads to a relaxed problem, namely Equation 7 with

$$X_d = \{\chi : 0 \leq \chi(x) \leq 1\} \text{ instead of } \tilde{X}_d = \{\chi : \chi(x) = 0 \text{ or } 1\}. \quad (8)$$

These relaxed problems usually have a solution and it is often possible to show that if the solution is not in \tilde{X}_d then it is the limit of composite domains made of mixtures of smaller and smaller subdomains and holes (Murat et al. 1987).

In dimension two, and for Dirichlet problems like Equation 1, there is a very elegant result due to Sverak (1992, 1993) that shows that either there is no solution

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Figure 3 Borwall & Petersson solved the problem of the cheapest (drag) transmission of fluid from left to right for a given volume of pipe. Topological optimization was used so as to handle topological changes such as seen here between the initial guess and the computed solution (Borwall et al. 2001).

because the minimizing sequences converge to a composite domain or there is a regular solution; more precisely, if a maximum number of connected components for the complement of Ω is imposed as an inequality constraint for the set of admissible domains then the solution exists.

For fluids it is hard to imagine that any minimal drag geometry would be the limit of many small solids objects surrounded by fluids. Nevertheless, in some cases the approach is quite powerful because it can answer topological questions that are embarrassing for the formulations Equation 1 and Equation 5, such as: Is it better to have a long wing or two short wings for an airplane (see Figure 3)?

2.1. Well-Posed Regularized Formulations

Another way to ensure well posedness is to regularize the problem by changing the criterion and adding a “cost” to the control. For Equation 1,

$$J(\Omega) = \int_D (\psi - \psi_d)^2 + \epsilon \int_S dx$$

ensures existence.

More generally, one may consider working with

$$J(\Omega) = \int_D (\psi - \psi_d)^2 + \epsilon \|S\|^2,$$

but the choice of norm is delicate. In general, for second-order problems anything related to the second derivatives (i.e., radius of curvature) would likely work, but it is not known if weaker norms would work also. For computer solutions, regularization is easier than constraint on the smoothness of the unknowns.

Such “Tychonov regularizations” are extremely important in other fields (data assimilation in meteorology, inverse imaging, etc.). Here the mathematical results

justify the precise form of the regularization to use and make the problem well posed. For applications, once the type of penalty is chosen through mathematical analysis, the choice of the parameter ϵ remains a problem. One solution is to consider ϵ as an additional (positive) control.

After existence, derivability must be studied because derivatives with respect to shapes are needed to apply gradient or Newton methods (this is explained in Section 3). One could say that derivatives are needed only for the discrete system and that these are differentiable almost everywhere because there are finite dimensional models. Automatic differentiation of computer programs (presented briefly below) use that property, but it pushes the difficulty at the convergence level when the mesh size vanishes.

3. SHAPE DERIVATIVES

It is wise to check differentiability analytically. For each formulation (Equations 1, 5, 7) there is a canonical method. For Equation 1 it occurs by using normal variations around a reference shape (see Equation 4 and Figure 4). If Gateau differentiability in $L^2(S)$ can be established, $\zeta \in L^2(S)$ exists with

$$j(S(t\alpha)) - j(S) = t \int_S \zeta \alpha + o(t).$$

Frechet differentiability will hold if, in addition, $o(t)$ is $o(t|\alpha|_0)$, where $|\cdot|_0$ denotes the norm of $L^2(S)$. Then ζ is the L^2 -gradient, denoted by $\text{grad}_\alpha j(S)$ and we have

$$j(S(\alpha)) - j(S) = \int_S \text{grad}_\alpha j(S) \alpha \, ds + o(|\alpha|_0),$$

so $\text{grad}_\alpha j(S)$ must be zero at the solution of Equation 1 and $\bar{\alpha} = -\text{grad}_\alpha j(S)$ is a direction of descent in the sense that if S is not the solution, $j(S(t\bar{\alpha})) < j(S)$ for a small enough positive constant t . Following Cea (1980) and Delfour et al. (2001) one may consider a velocity of deformation $V(x)$ and define a time-dependent shape

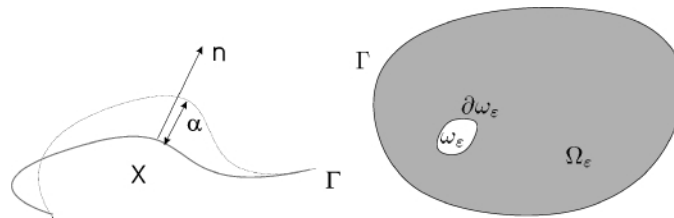


Figure 4 Normal variations on a reference shape (*left*). Topological variation on the shape (*right*).

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$$\Omega(t) = \{x + V(x)t : x \in \Omega\}$$

and compute $\frac{dJ}{dt}$, known as the material derivative of J .

Recently, the concept of topological derivative was introduced by Sokolowski (Sokolowski et al. 1991) and also by Masmoudi (Garreau et al. 2001). One replaces an area of fluid by a small solid disk of center x and radius ϵ in the domain and studies the limit of $\frac{1}{\epsilon^m}(\psi^\epsilon - \psi)$, for the right power m , where ψ^ϵ is the solution of the PDE with the disk and ψ the solution without the disk (see Figure 4).

3.1. Sensitivity: An Example

Consider the problem of finding the derivatives with respect to the domain parameter $t \in \mathbb{R}$ of the solution of the Laplace equation with Dirichlet conditions

$$-\Delta \psi^{t\alpha} = 0 \text{ in } \Omega^{t\alpha} \quad \psi^{t\alpha} = \psi_d \text{ on } \Gamma^{t\alpha} = \{\bar{x} + t\alpha\bar{n} : x \in \Gamma\}, \quad (9)$$

where $\Omega^{t\alpha}$ is the set of boundary $\Gamma^{t\alpha}$. The function α plays the role of a direction of differentiation whereas t (which could have been $\|\alpha\|$) is the parameter that tends to zero. The derivative with respect to t in the direction α is calculated by assuming enough regularity so as to have

$$\psi^{t\alpha} = \psi + t\psi' + \frac{t^2}{2}\psi'' + \dots \text{ at } t = 0.$$

By linearity, ψ' and ψ'' also satisfy the Laplace equation. By a Taylor expansion in x ,

$$\psi^{t\alpha}(x + t\alpha n) = \psi^{t\alpha}(x) + t\alpha \frac{\partial \psi^{t\alpha}}{\partial n}(x) + \frac{t^2 \alpha^2}{2} \frac{\partial^2 \psi^{t\alpha}}{\partial n^2}(x) + \dots$$

By definition, $\psi^{t\alpha}(x + t\alpha n) = 0$ because $x + t\alpha n \in \Gamma^{t\alpha}$; therefore

$$-\Delta \psi' = -\Delta \psi'' = 0 \quad \psi'|_\Gamma = -\alpha \frac{\partial \psi}{\partial n} \quad \psi''|_\Gamma = -2\alpha \frac{\partial \psi'}{\partial n} - \alpha^2 \frac{\partial^2 \psi}{\partial n^2}.$$

Notice that ψ is not only Gateau-differentiable, as shown above, but also Frechet-differentiable because ψ' is linear in α .

3.2. The Minimum Drag Problem for Viscous Incompressible Flows

For an object in an incompressible fluid, minimizing the viscous drag can be performed by minimizing the energy, so one may consider

$$\min_{\Omega \in \mathcal{C}} E(u, \Omega) = \int_{\Omega} \frac{1}{2} |\nabla u|^2 dx \text{ subject to}$$

$$u|_{\partial\Omega} = u_\Gamma, \quad \nabla \cdot (u \otimes u) + \nabla p - \nu \Delta u = 0, \quad \nabla \cdot u = 0.$$

Let $S \subset \Gamma$ be an airfoil and $u_\Gamma = 0$ on S . Sensitivity analysis by local normal variations (Equation 4) is fairly straightforward when the Dirichlet conditions are treated by penalty. Consider the space H of solenoidal functions with square integrable first derivatives and the Navier-Stokes equations in variational form

$$NS(u, w) = \int_{\Omega} (u \otimes u : \nabla w + v \nabla u : \nabla w) + \frac{1}{\epsilon} \int_{\Gamma} (u - u_\Gamma) w = 0 \quad \forall w \in H.$$

The notation $A : B$ stands for the trace of the matrix product AB . The optimality conditions, which characterize the solution S , are obtained by writing that the Lagrangian $L(u, w, S(t)) = NS + E$ is stationary in u and t :

$$\begin{aligned} \partial_\tau L(u + \tau v, w, S)|_{\tau=0} &= \int_{\Omega} (u \otimes v + v \otimes u) : \nabla w \\ &\quad + \int_{\Omega} (v(\nabla v : \nabla w + \nabla w : \nabla v)) + \frac{1}{\epsilon} \int_{\Gamma} v \cdot w \quad \forall v \in H \\ \partial_t L(u, w, S(t)) &= \int_S (v \nabla u : \nabla w) \alpha + \frac{1}{\epsilon} \int_S \alpha \partial_n u \cdot w \\ &\quad + \frac{1}{2} \int_S \alpha |\nabla u|^2 \quad \forall \alpha \in \mathbb{R} \end{aligned}$$

because $u|_S = 0$, $dS(t) = dS + o(|\alpha|)$, and because (Pironneau 1984)

$$\frac{d}{dt} \int_{\Omega(t)} f = \int_S f \alpha \quad \frac{d}{dt} \int_{S(t)} g = \frac{d}{dt} \int_S g(x(s) + t\alpha(s)n(s)) ds = \int_S \alpha \partial_n g.$$

The derivative of E is $\partial_t L(u, v, S(t))$ at $t = 0$:

$$\begin{aligned} \partial_t E(S(t))|_{t=0} &= \int_S \alpha \partial_n u \cdot \partial_n \left(v + \frac{u}{2} \right) \text{ where } (v, q) \text{ is the solution of} \\ &\quad -\nabla \cdot (v \otimes u + u \otimes v) + \nabla q - v \Delta v = \Delta u \quad \nabla \cdot v = 0, \quad v|_\Gamma = 0. \quad (10) \end{aligned}$$

This ‘‘Calculus of Variations’’ can be justified mathematically (i.e., small functions are indeed small) (Pironneau 1973).

In the next section, we analyze a frequent situation with fluids, which is mathematically difficult because shocks when differentiated yield Dirac functions.

3.3. Sensitivity in the Presence of Shocks

As Godlewski et al. (1998) pointed out in a pioneering paper, there are serious difficulties of analysis with the Calculus of Variations when the solution of the partial differential equation has a discontinuity. As analyzed below, optimizing an airplane with respect to its sonic boom is precisely a problem in that class, so these difficulties must be investigated. For illustration, we consider the Burgers

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equation and expose the problem and the results known so far. Suppose we seek the minimum with respect to a parameter a (scalar for clarity) of $j(u, a)$ with u solution of

$$\partial_t u(x, t) + \partial_x \left(\frac{u^2}{2} \right) (x, t) = 0, \quad u(x, 0) = u^0(x, a), \quad \forall (x, t) \in R \times (0, T). \tag{11}$$

Consider an initial data u^0 , with a discontinuity at $x = 0$ satisfying the entropy condition $u^-(0) > u^+(0)$; then $u(x, t)$ has a discontinuity at $x = s(t)$ which depends on a , of course, and propagates at a velocity given by the Rankine-Hugoniot condition $\dot{s} = \bar{u} = (u^+ + u^-)/2$, where u^\pm denotes its values before and after the shock.

Let H denote the Heavyside function and δ its derivative, the Dirac function; let $s' = \frac{\partial s}{\partial a}$ and $[u] = u^+ - u^-$ the jump of u across the shock. We have

$$\begin{aligned} u(x, t) &= u^-(x, t) + (u^+(x, t) - u^-(x, t))H(x - s(t)) \\ &\Rightarrow u' = u^{-'} - s'(t)[u]\delta(x - s(t)), \end{aligned} \tag{12}$$

where $u^{-'}$ is the pointwise derivative of u^- with respect to a .

One would like to write that Equation 11 implies

$$\partial_t u'(x, t) + \partial_x (uu')(x, t) = 0, \quad u'(x, 0) = u^{0'}(x, a). \tag{13}$$

Unfortunately, uu' in Equation 13 has no meaning at $s(t)$ because it involves the product of a Dirac function by a discontinuous function! The classical solution to this riddle is to say that Equation 12 is valid at all points except at $(t, s(t))$, and that the Rankine-Hugoniot condition, differentiated, gives the missing equation:

$$\dot{s}'(t) = \bar{u}'(s(t), t) + s'(t)\partial_x \bar{u}(t, s(t)). \tag{14}$$

However such strategy would be difficult to generalize to complex systems such as Euler's equations. The question then is to embed these results into a variational framework so as to compute the derivative of j as usual by using weak forms of the PDEs and adjoint states. It turns out that Equation 13 is true even at the shock (Bardos et al. 2002), but in the sense of distribution theory and with the convention that whenever uu' occurs it means $\bar{u}u'$ at the shock, where $\bar{u} = (u^+ + u^-)/2$.

Furthermore, Equation 13 in the sense of distribution contains a jump condition which, of course, is Equation 14. This apparently technical result has a useful corollary: Integrations by parts are valid and the calculus of variations can be extended. For instance, the derivative of $j = \int_{R \times (0, T)} J(x, t, u, a)$ with respect to a is $j' = j'_a + \int_{R \times (0, T)} J'_u u'$ and when a is multidimensional, to transform $\int_{R \times (0, T)} J'_u u'$ one may introduce an adjoint state v solution of

$$\partial_t v + u \partial_x v = J'_u(x, t), \quad v(x, T) = 0 \tag{15}$$

and write that

$$\int_{R \times (0,T)} J'_u u' = \int_{R \times (0,T)} (\partial_t v + \bar{u} \partial_x v) u' = - \int_R u^{0'} v(0) dx. \quad (16)$$

Notice that the adjoint state v has no shock because its time boundary condition is continuous and the characteristics integrated backward never cross the shock. Giles (2001) observed this fact in the more general context of the Euler equations for perfect gas. He also showed that artificial viscosity is a valid method to handle the problem numerically.

4. PRINCIPLES OF ALGORITHMIC DIFFERENTIATION

We would like to give a brief description of automatic or rather algorithmic differentiation (AD) methods because of its practical importance. This technique should be seen as complementary to the analytical approaches. It makes the computation of shape derivatives automatic, for the discrete systems at least, but it has also its own dangers.

When a function $j(u)$ is given by a computer program each line of the program can be differentiated automatically and exactly (with Maple, Mathematica, Reduce, etc.). Thus j'_u can be computed by differentiating every line and adding the result to the computer program above the original line. To illustrate the idea, consider the problem of stabilizing near a given state $z_d(t)$ Lorenz' (1963) chaotic system $x(t), y(t), z(t)$ by a control $u(t)$. After an explicit discretization in time the system is programmed as below ($a, b, c, d, e, \delta t$ are numerical constants) and any gradient or Newton method to find a u^n , which drives j to zero, would require j'_u .

Program for j(u)	Lines to add
$j = 0 \quad x^0 = a \quad y^0 = b \quad z^0 = d$	$dj = 0 \quad dx^0 = 0 \quad dy^0 = 0 \quad dz^0 = 0$
for(n=0; n<N; n++)	
$\{x^{n+1} = x^n + \delta t e(x^n - y^n)$	$dx^{n+1} = dx^n + \delta t e(dx^n - dy^n)$
$y^{n+1} = y^n - \delta t(x^n z^n - y^n)$	$dy^{n+1} = dy^n - \delta t(dx^n z^n + x^n dz^n - dy^n)$
$z^{n+1} = z^n + \delta t(x^n y^n - z^n - u^n)$	$dz^{n+1} = dz^n$
	$+ \delta t(dx^n y^n + x^n dy^n - dz^n - du^n)$
$j = j + \delta t (z^n - z_d^n)^2 \}$	$dj = dj + 2\delta t (z^n - z_d^n) dz^n$

If this new program is run with $u = u_0$, $du^n = \delta_{mn}$ (Kronecker's symbol) then dj is the derivative of j with respect to u^m at u_0 . This is called the direct mode of AD. The reverse mode of AD is similar to the continuous adjoint method and aims

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to provide the gradient with a cost independent of the number of optimization variables in the program. In the reverse mode one builds the Lagrangian of the program by associating a dual variable to each line of the program (each line of a computer code is seen as an equality constraint and the final line as the cost function) except the one associated with the criteria.

$$L = \sum p^n(-x^{n+1} + x^n + \delta t e(x^n - y^n)) + q^n(-y^{n+1} + y^n - \delta t(x^n z^n - y^n)) \\ + r^n(-z^{n+1} + z^n + \delta t(x^n y^n - z^n - u^n)) + j - \delta t \sum (z^n - z_d^n)^2$$

Stationarity of L with respect to the state variables should be written in reverse order ($z^n, y^n, x^n, z^{n-1} \dots$). For instance,

$$\frac{\partial L}{\partial z^n} = 0 \quad \Rightarrow \quad -\delta t q^n x^n - r^{n-1} + r^n - \delta t - 2\delta t (z^n - z_d^n).$$

This is a discrete form of the first adjoint equation, which gives r^{n-1} in terms of r^n . Then the stationarity of L with respect to u gives the derivative of j :

$$j'_{u^n} = \frac{\partial L}{\partial u^n} = f \delta t r^n.$$

The reverse mode is capable of computing all the derivatives j'_{u^n} at once while in the direct mode it is necessary to run the computer program n times with different values of du^n . However, the reverse mode is difficult to automatize because it requires a symbolic manipulation of the lines of the program, a reversal of the loops, etc. (Griewank 2000). A variant known as reverse accumulation is used in the *odyssey* software; for each assignment $y = y + f(x)$, the dual expression is $p_x = p_x + f' p_y$ with p_x and p_y the dual variables of x and y . Hence, if initialized by ($p_x = 0, p_y = 1$) it gives $p_x = f'$. This method is often used to write directly (even by hand) the adjoint code. Our experience is that in many cases it is even more efficient than deriving analytically the continuous adjoint and discretizing it.

4.0.1. SOFTWARE However, differentiating each line by hand or by an external program can be cumbersome. It can be done with tools such as *adol-C* (Griewank 2000), *adifor* (Bischof et al. 1992), and *odyssey* (Gilbert et al. 1991, Faure 1996, Rostaing 1993), or even by any C++ compiler by overloading the arithmetic operators and the functions of the standard C-library. For instance the multiplication as in $x * y$ will be overloaded to perform both $x * y$ and $dx * y + x * dy$. This yields a remarkably simple procedure as one needs only to replace the standard type `float` (or `double`) by a new type `dfloat` and add the line `#include dfloat.h` to link to this new class. This is extremely convenient for prototyping an applications, however it does not use the reverse mode and so its efficiency decrease with the number of parameters.

5. INCOMPLETE SENSITIVITY

Another direction of research is to try to simplify the formulae for the gradients and keep only the dominant terms. Generically, the design of a shape S , defined by a set of parameters x usually involve intermediate parameters $q(x)$ (mesh related informations), state or flow variables $U(q(x))$, and a criterion or cost function for optimization j :

$$j(x): x \rightarrow q(x) \rightarrow U(q(x)) \rightarrow j(x, q(x), U(q(x))) \quad (17)$$

The derivative of j with respect to x is

$$\frac{dj}{dx} = \frac{\partial j}{\partial x} + \frac{\partial j}{\partial q} \frac{\partial q}{\partial x} + \frac{\partial j}{\partial U} \frac{\partial U}{\partial x}. \quad (18)$$

Most of the computing time to evaluate Equation 18 is spent on $\partial U/\partial x$ in the last term.

We observed (no theoretical justification) that the last term is small when:

- (a) j is of the form $j(x) = \int_S f(x, q(x))g(U)$,
- (b) the local curvature of S is not too large, and
- (c) f and g are such that formally we can verify $\frac{1}{|f|} \left| \frac{\partial f}{\partial n} \right| \gg \frac{1}{|g|} \left| \frac{\partial g}{\partial U} \right|$, where n is the normal to S , while $\left| \frac{\partial U}{\partial n} \right|$ is of $O(1)$.

If these requirements are met, then local variations about S , $S' = \{x + t\alpha n : x \in S\}$ give (Pironneau 1984)

$$\int_{S'} fg - \int_S fg = t \int_S \alpha \left(\frac{\partial fg}{\partial n} - \frac{fg}{R} \right) + o(t) \sim t \int_S \alpha g \frac{\partial f}{\partial n}.$$

Our experience is that $\frac{\partial g}{\partial U}$ is small indeed, whereas geometrical quantities, such as n , have much greater variations. An optimization method using an incomplete sensitivity is a suboptimal gradient method and in that sense has limitations, but the gain in computing time is so large (no adjoint state) that it is worth pursuing.

5.0.1. EXAMPLES Consider $j = \epsilon^m u_x(\epsilon)$ as cost function (hence $f = \epsilon^n$ and $g = u_x$) and the following Dirichlet problem

$$-u_{xx} = 1, \text{ on }]\epsilon, 1[, \quad u(\epsilon) = 0, \quad u(1) = 0$$

as the state equation which has as a solution $u(x) = -x^2/2 + (\epsilon + 1)x/2 - \epsilon/2$. The gradient of j with respect to ϵ is

$$j'_\epsilon(\epsilon) = \epsilon^{m-1}(m u_x(\epsilon) + \epsilon u_{x\epsilon}(\epsilon)) = \frac{\epsilon^{m-1}}{2}(-n(\epsilon - 1) - \epsilon).$$

Incomplete sensitivity gives

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$$j'_\epsilon \approx m\epsilon^{m-1}u_x(\epsilon) = \frac{\epsilon^{m-1}}{2}(-n(\epsilon - 1)),$$

which is correct for large m . Note also that the sign of the gradient is always correct and this will be true with any state equations giving $u_x(\epsilon) < 0$.

The next example concerns a Poiseuille flow in a channel driven by a constant pressure gradient p_x . The walls are at $y = \pm a$. The flow velocity satisfies

$$u_{yy} = \frac{p_x}{\nu}, \quad u(-a) = u(a) = 0. \tag{19}$$

The analytical solution is $u(a, y) = \frac{p_x}{2\nu}(y^2 - a^2)$. We are interested in the sensitivity of the flow rate when the channel thickness changes. The flow rate is given by $j_1(a) = \int_{-a}^a u(a, y)dy$, which is not in the domain of validity of incomplete sensitivity. Indeed, the gradient is

$$\frac{dj_1}{da} = \int_{-a}^a \partial_a u(a, y)dy = \frac{-2a^2 p_x}{\nu},$$

whereas incomplete sensitivity gives zero.

Now consider the cost function $j_2(a) = a^m j_1(a)$. Then

$$\frac{dj_2}{da} = ma^{m-1}j_1(a) + a^m \frac{dj_1}{da} = -\frac{4ma^{m+2}p_x}{6\nu} - \frac{a^{m+2}p_x}{\nu}.$$

The two contributions have the same sign and are of the same order, and for large values of n incomplete sensitivity is correct.

Another interesting example leading to a functional reformulation concerns shape optimization to improve blade efficiency involving the difference of pressure between inlet and outlet boundaries Δp . This is an important industrial problem; the blade efficiency is defined by $j = \frac{q\Delta p}{\omega T_R}$ with q the flow rate, ω the angular velocity, and T_R the torque. Hence, freezing q , Δp , and ω and reducing the torque improves the efficiency. But Δp is not in the validity domain of incomplete sensitivities (it is a function evaluated away from the unknown surface). From the momentum equation, after integrating by part, we have

$$\int_{\Gamma} u(u.n) d\sigma + \int_{\Gamma} \tau n d\sigma = 0,$$

where τ is the Newtonian stress tensor and Γ the boundary of the domain. To simplify the presentation, suppose $n_{inlet/outlet} = (\pm 1, 0, 0)$, neglecting viscous terms on the in and outlet boundaries and using periodicity on the other external boundaries we have

$$\int_{\Gamma_i} \left(p + \frac{u^2}{2} \right) - \int_{\Gamma_o} \left(p + \frac{u^2}{2} \right) = \int_{\Gamma_w} \left(-p + \nu \frac{\partial u}{\partial n} \right) = C_d.$$

Therefore, if the inlet and outlet are far enough so that u is constant, from $\nabla \cdot u = 0$ we have $\Delta p = C_d$. We have linked the pressure variations away from the wall to

the drag coefficient. In the general case, the analysis involves a combination of lift and drag coefficients (Mohammadi et al. 2001).

5.0.2. REDUCED COMPLEXITY AND INCOMPLETE SENSITIVITIES Note that in a computer implementation we can always try incomplete sensitivity, check that the cost function decreases, and if it does not we can add the missing term. A middle path is to use a reduced complexity formula that provides an inexpensive approximation of the missing term. Assume we have an approximation $\tilde{U}(x) \sim U(x)$. For example, if we are dealing with the Navier-Stokes equations, \tilde{U} could come from the Newton formula for the pressure combined with the Euler equations. In the context of Equation 17 the following approximation can be used (see Equation 21)

$$\frac{dj}{dx} \approx \frac{\partial j}{\partial x} + \frac{\partial j}{\partial q} \frac{\partial q}{\partial x} + \frac{\partial j}{\partial U} \frac{\partial \tilde{U}}{\partial x}. \quad (20)$$

\tilde{U} is an approximation of U used here only to simplify the computation of $\partial \tilde{U} / \partial x$. Note that the reduced model needs to be valid only at points where it is used.

A further improvement is obtained by writing in place of Equation 17

$$x \rightarrow q(x) \rightarrow \tilde{U}(q(x)) \left(\frac{U(x)}{\tilde{U}(x)} \right).$$

$$\frac{dj}{dx} \approx \frac{\partial j(U)}{\partial x} + \frac{\partial j(U)}{\partial q} \frac{\partial q}{\partial x} + \frac{\partial j(U)}{\partial U} \frac{\partial \tilde{U}}{\partial x} \frac{U(x)}{\tilde{U}(x)}. \quad (21)$$

Fluid dynamics provides a wide range of reduced models: the Newton formula for the pressure, the Poiseuille flow approximation, boundary-layer models, wall functions for velocity, and temperature for laminar and turbulent flows, etc. Of course, these have to be used only in their respective validity domains.

In our numerical tests we obtained considerable speed up by using Equation 21 with the following wall law in place of the full turbulence model:

$$\frac{\partial}{\partial y_w} \left(\frac{\partial}{\partial y} \left((v + v_t) \frac{\partial u}{\partial y} \right) \right) = \frac{\partial}{\partial y} \left(\frac{\partial}{\partial y_w} \left((v + v_t) \frac{\partial u}{\partial y} \right) \right) = \frac{-2u_\tau}{0.4(y - y_w)^3}, \quad (22)$$

where y denotes the distance normal to the wall, y_w the shape location, u is the tangential velocity, v and v_t the kinematic flow and eddy viscosities. For simplicity we have considered a wall function of the form $u = u_\tau f(y^+)$ with $u_\tau^2 = v \left(\frac{\partial u}{\partial y} \right)_w$ the local friction velocity, $y^+ = \frac{(y - y_w)u_\tau}{v}$ and $f(y^+) = \frac{\ln(y^+)}{0.4} + 5$.

6. LINK WITH CAD

In industries, shapes are defined and stored in CAD systems (such as Catia) in databases, as a set of Bezier, or other patches with infinite details for screws and bolts irrelevant to a computer simulation of aerodynamics properties. Furthermore, CAD data are usually proprietary and cannot leave the physical area of the industry.

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There is a large scientific literature on OSD with the design variables of the CAD systems. However, our experience is that the mesh generation modules of the CAD systems are usually not powerful enough for aerodynamics and certainly not for mesh adaptation at this time. For accurate results, it is essential to abstract the optimization from the CAD system so as to use advanced mesh generation and mesh adaptation tools (George 1991).

In our industrial cooperation, we ask the engineer for any surface mesh, even a bad one (but a conforming mesh, i.e., no holes or overlapping elements) to define the initial design. The strategy is then what we call a CAD-free optimization platform: it (a) generates any surface mesh from the CAD data, (b) applies a visual- C^1 (Farin 1987, Gopalsamy et al. 1989) reconstruction with edge recognition to generate an appropriate surface mesh for CFD, (c) applies a 3D volumic automatic mesh generator from the surface mesh [we use the modules developed at INRIA (George 1991)], (d) performs the optimization with mesh refinement using the same module as in (b) couples with the PDE solver (Mohammadi et al. 2001), and (e) feeds the result back into the CAD system after optimization.

6.1. CAD-Free Shape Parameterization

In this approach all the nodes of the surface mesh over the shape are control parameters. One particular aspect of this parameterization comes from the fact that regularity requirements must be specified and handled by the user, unlike in a CAD-based parameter space.

From a practical point of view, this inconvenience is compensated for by the fact that a CAD-based parameter space might not be suitable for optimization. In fact, our experience shows that optimization in the CAD-free framework helps improve the CAD definition of the shape. The final shape has to be expressed through CAD in all cases. Concerning mesh dependency of the optimization, the same remark holds when using a CAD-based parameter space. It is obvious that the optimization might converge to different shapes in different CAD-based parameter spaces. Finally, new generations of CAD tools can fit CAD parameters into a surface mesh if one knows the initial correspondence between CAD parameters and surface mesh.

We discussed regularization mathematically in the first section; the practical importance of a smoothing step can also be understood by the following argument.

Suppose Γ is a surface in a domain $\Omega \in R^3$ and we want shape variations $\delta x \in C^1(\Gamma)$. From Sobolev inclusions, we know that in 2D $H^{5/2}(\Gamma) \subset C^1(\Gamma)$. In the context of shape optimization, applying to a C^1 shape a gradient method does not necessarily produce a new $C^1(\Gamma)$ shape because the variation δx are in $L^2(\Gamma)$ only (Mohammadi & Pironneau 2001) (see Figure 5) and therefore we need to project δx into $H^{5/2}(\Gamma)$, for instance.

A projection on $H^{2m}(\Gamma)$ can be achieved by solving a PDE of order $2m$ on Γ , such as (in 2D) $\tilde{\delta}^m = \delta \tilde{x}$. Analysis suggests using a fourth-order operator



Figure 5 Sketch of a CAD-free deformation without and with the regularization operator. The initial deformation is only $C^0(\Gamma)$ and to have a $C^1(\Gamma)$ variation, one needs to project it, for instance, into $H^{5/2}(\Gamma)$ if Γ is a surface in \mathbb{R}^3 .

(Mohammadi & Pironneau 2001). Numerically, a second-order elliptic system with a discontinuity capturing operator for the definition of the viscosity gives satisfactory results. Furthermore, it is a good idea to use an operator that leaves unchanged regions where the deformation is already smooth enough.

6.2. Regularity and the Iterative Algorithms

Here we would like to point out some loss of regularity issues appearing at this occasion and some available cures.

Here is a simple example to illustrate the loss of regularity in the construction of minimizing sequences in infinite dimension. The loss of regularity is related to the fact that the gradient of the functional has necessarily less regularity than the parameter.

Suppose that the functional $J(x)$ is a quadratic function of a parameter x $J(x) = |Ax - b|^2$ with $x \in H_0^1(\Omega)$, $b \in L^2(\Omega)$ and $A : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$, $\Omega \subset \mathbb{R}^n$.

The gradient $\text{grad}_x J = 2A^T(Ax - b) \in H^{-1}(\Omega)$ has less regularity than x ; therefore, an iterative scheme like the method of descent with step size ρ , $x^{m+1} - x^m = -\rho \text{grad}_x J = -2\rho A^T(Ax - b)$ deteriorates the regularity of x . We need to project or smooth the variation into $H^1(\Omega)$. This situation is similar to what happens with the CAD-free parameterization where a surface is represented by an infinite number of independent points.

Suppose the parameter belongs to a finite dimensional parameter space, for instance with a polynomial definition of a surface. When considering the coefficient of the polynomial as parameter, changes in the polynomial coefficients do not change the regularity because the new parameter will always belong to the same polynomial space. If the surface is parameterized by two (or several) polynomials, it is necessary to add regularity conditions for the junctions between the polynomials. We then recover the link introduced by the smoothing operator between parameter coefficients. This is similar to what happens with a CAD-based parameterization when the number of CAD parameters grows.

The smoothing can also be seen as a modification of the scalar product $(\cdot, \cdot)_0$ natural to Calculus of Variation [i.e., the scalar product of L^2 by a more elaborate one, such as $(\nabla \cdot, \nabla \cdot)_0$]. It has a preconditioning effect in that it dissipates localized high frequencies. From this standpoint, at the discrete level, smoothing replaces a descent algorithm such as

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$$j^{n+1} = j^n - \rho(\text{grad}_x j^n, \text{grad}_x j^n)_0$$

by

$$j^{n+1} = j^n - \rho(\text{grad}_x j^n, \text{grad}_x j^n)_M,$$

where M is a positive definite preconditioning matrix.

6.2.1. SHAPE REGULARITY AND PENALIZATION Another way to treat the problem reported above is to consider a regularized criterion. With the notation of Section 3 (dots denote the derivatives in the tangential direction)

$$j_\mu = j + \frac{\mu}{2} \int_S \dot{\alpha}^2, \\ j_\mu(S(t)) = j_\mu(S) + t \int_S \alpha \left(\partial_n u \cdot \partial_n \left(v + \frac{u}{2} \right) - t\mu\ddot{\alpha} \right) + o(t|\alpha|). \quad (23)$$

Although it is a second-order term, $\alpha\ddot{\alpha}$ is kept to prevent numerical oscillations. One starts with a smooth shape, moves it in its normal direction by

$$\alpha = t \left(\partial_n u \cdot \partial_n \left(v + \frac{u}{2} \right) - t\mu\ddot{\alpha} \right)$$

and iterates. This gradient method will decrease j_μ at each step, and the smoothness of S is preserved by the last term. A similar and mathematically more correct result is obtained by applying the gradient method on j in a different metric by using the scalar product of the Sobolev space $H^1(S)$ for α , i.e., find β such that

$$j(S(t)) = j(S) + t \int_S \dot{\beta}\dot{\alpha} + o(t\|\alpha\|).$$

β is found by solving on S

$$-\ddot{\beta} = \partial_n u \cdot \partial_n \left(v + \frac{u}{2} \right).$$

Then S is moved proportionally to β in its normal direction and j decreases.

Again, this differential equation on S acts as a smoother, an old idea for such moving boundary problems where numerical oscillations develop if nothing is there to kill them; but here we have a mathematical justification in that S is moved by a quantity that has the same smoothness because $\beta \in H^1(S)$, at least. If more smoothness is required, the second derivative can be replaced by a $2m$ -th derivative. There are also ways to replace the differential equation on the surface S by a system of partial differential equations in Ω , which are much easier to implement (see Lemarchand et al. 2002).

7. AN EXAMPLE OF MULTICRITERIA SHAPE OPTIMIZATION

We present a shape optimization problem under acoustic, aerodynamic, and geometric constraints using some of the ingredients presented above. The acoustic concerns the sonic boom of an airplane (Whitham 1952). In shape design for transonic aircraft in cruise conditions, multicriteria aspects mainly concern the aerodynamic and elastic characteristics of the aircraft. For instance, the aim can be to reduce the drag at given lift and with given maximum by-section thickness, which would ensure structural realizability. Shape optimization for civil supersonic transport includes another important objective: the control of the sonic boom. This makes the problem harder than in the transonic case, as drag and sonic boom reductions are naturally incompatible (in supersonic regime low-drag geometries are sharp and have a high boom level because shocks are attached then).

In principle, supersonic civil transport in cruise condition only involves N-waves. The N-wave is generated by steady flight conditions and its pressure wave is shaped like the letter “N.” N-waves have a front shock with a positive peak overpressure, which is followed by a linear decrease in pressure until the rear shock returns to ambient pressure.

The flow in regions close to the aircraft, or the near field, is evaluated using the Euler system for gas dynamics in conservation form. The solution method is based on a finite volume Galerkin method (Mohammadi 1994). The variables at the lower boundary of this computational domain are then used to define waveform parameters, which are propagated to the ground using the waveform parameter method (Thomas 1972) (see Figure 6).

7.1. Cost Function Definition

Consider the problem of drag C_d minimization with constraints on the lift C_l , volume V , maximum by-section thickness d defined for each node and smooth pressure gradient on the ground to minimize the sonic boom. In our approach the mesh is unstructured and the surface mesh is made of triangles. In the by-section definition of the shape from its CAD-free definition, the number of sections is arbitrary and depends on the complexity of the geometry. The sections are obtained as intersections of vertical planes with the shape. The maximum airfoil thickness d of each section is evaluated. Each node in the surface mesh is associated with two sections and linear interpolation is used to define the maximum thickness associated to this node. The cost function is given by

$$j(x) = C_d + (C_l^0 - C_l)_+ + (V^0 - V)_+ \\ + \int_S (d - d_0)^2 d\gamma + \int_{\text{ground}} (\nabla p_g \cdot U_\infty)^2 d\gamma.$$

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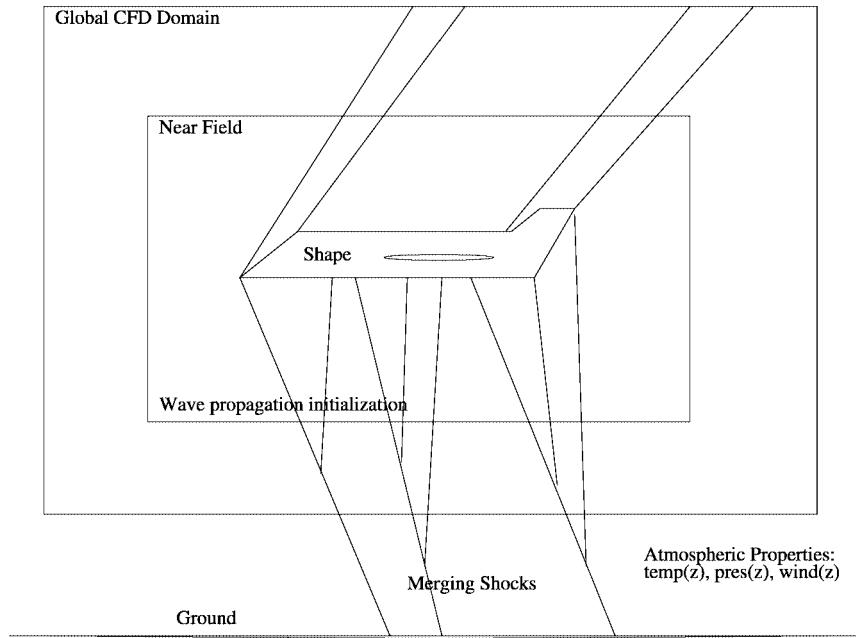


Figure 6 Shock wave pattern and illustration of the near field computational domain and the initialization of the wave propagation method with the near-field predictions.

Superscript 0 denotes initial shape values. $(\cdot)_+ = \max_r(0, \cdot)$, where \max_r is a regularized max. U_∞ is the projection of the flight direction on the ground. The cost function prevents the volume and lift coefficient from decreasing.

In addition to the given lift constraint expressed in the cost function by penalty, we use the inflow incidence to enforce the given lift constraint. We know that in cruise condition (far from stall), the lift is linear with respect to the angle of incidence. During optimization the incidence is given by $(\theta^{n+1} = \theta^n - 0.5(C_l^n - C_l^0), \theta^0 = 0)$, where n is the optimization iteration.

However, a cost function involving pointwise values away from the shape is not suitable for incomplete sensitivity evaluation. As the boom is defined on the ground and not on the shape we propose reformulating the functional linking the pressure signature on the ground to wall-based quantities.

Bow shocks introduce less pressure jump than attached shocks. Bow shocks are usually associated with smooth geometries. Sharp leading edges lead to attached shocks leading to high boom levels. On the other hand, shape optimization based on drag reduction in supersonic regime leads to sharp leading edges. Therefore, it is important to keep the leading edges of the aircraft smooth while doing drag reduction. The requirements are as follows: (a) Specify that the wall has to remain smooth near leading edges, and (b) ask for the local drag force C_d^{loc} due to leading edges to remain unchanged or to increase while the drag decreases.

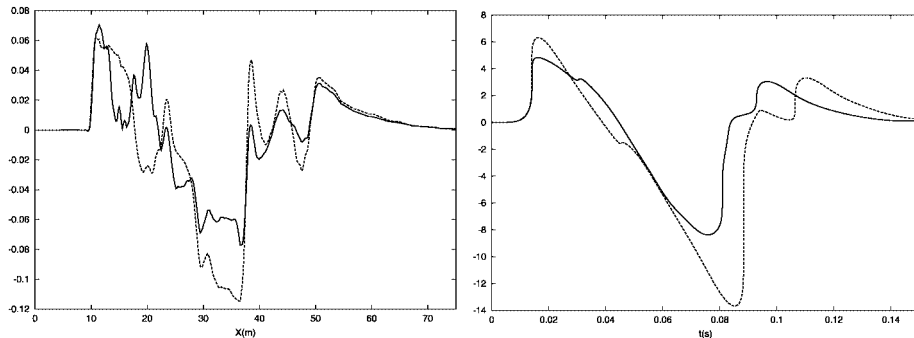


Figure 7 Cross-section of the near-field pressure variations ($\frac{p-p_\infty}{p_\infty}$) in the symmetry plane (*left*) and the corresponding ground pressure signatures (*right*) for the initial (*dashed curves*) and optimized (*continuous curves*) shapes. We observe a nontrivial impact of the modification of the near-field pressure distribution on the ground pressure: despite a rise in the initial shock intensity the boom is lower.

The cost function is

$$j(x) = C_d + (C_l^0 - C_l)_+ + (V^0 - V)_+ \\ + \int_S (d - d_0)^2 d\gamma + ((C_d^{loc})^0 - C_d^{loc})_+,$$

where C_d^{loc} is the drag force coming from regions where $\vec{n} \cdot \vec{u}_\infty < 0$ (\vec{n} being the local outward normal to the shape).

We consider a supersonic business jet geometry provided by Dassault Aviation company. The cruise speed is Mach 1.8 at no incidence and the flight altitude 55,000 feet. The results show the performance of the optimization method including the validity of the incomplete sensitivity approach and the reformulation of the functional we use for this configuration. After optimization, the drag has been reduced by 20%, the lift increased by 10%, C_d^{loc} is kept unchanged, and the geometric constraint is satisfied. More details on this simulation are available in (Mohammadi 2002). These results are compatible with those obtained in (Alonso et al. 2002) using a full adjoint approach (see Figures 7 and 8).

8. CONCLUSIONS AND PERSPECTIVES

OSD is still a difficult and computer-intensive task, especially in three dimensions. Even if the problem is well posed and the sensitivity is computed correctly (or approximately but intentionally), success is not guaranteed. Creeping convergence, local minima, and unphysical solutions can get in the way. Whenever possible, second-order optimization methods (Newton or quasi-Newton for instance) should be used because the problems are stiff. One should give great attention to the

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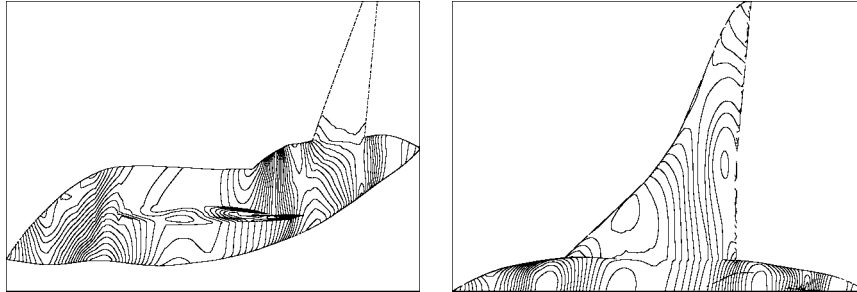


Figure 8 Iso-contours of normal deformation with respect to the original shape. Once this is known in the CAD-free parameterization, it is easy to express it in the original CAD parameters.

computing complexity and preferably use suboptimal approaches (for instance, with incomplete gradients) to avoid computing an adjoint state. In that sense, the industrial demand for cheap suboptimal methods (Anagnostou et al. 1992, Hirsh et al. 2001) is important.

There are still many unsolved problems; shock sensitivity and shape optimization for unsteady and turbulent flows are two examples. For unsteady flows, the shape could also be unsteady, given then a variant of what is known as active control. Hence, incomplete sensitivity has been successful for unsteady flow control by feedback (Mohammadi et al. 2001) applied for instance to drag reduction for a cylinder and to buffeting control by injection/suction for a transonic turbulent flow around an airfoil. Time dependent flows and optimized stationary shapes can be dealt with as in the sonic boom problem but with some time averaged incomplete gradient to define the shape deformation.

A simple time averaging has failed in an aerodynamic noise reduction problem (Marsden et al. 2001). The difference between the shape optimization case for unsteady flows and the control problems by feedback is that the control being active in time, its effect is seen by the incomplete sensitivity in time. In our opinion, for these unsteady problems, involving large eddy simulation, a full adjoint approach is out of reach and nongradient-based methods are only possible with a few design parameters (Marsden et al. 2002)]. There is therefore a clear need for low-complexity shape optimization approaches in this case.

Needs also exist in global optimization methods especially for multicriteria optimizations for which response surfaces or neural networks, genetic algorithms (Periaux et al. 1998, Hamda et al. 2000), and recursive optimization (Mohammadi et al. 2002) could be very useful. Often the flow solver is available in binary format only (such would be the case when using a commercial software) and differentiable optimization is then inefficient. However, genetic algorithms are slow and the future lies probably in the coupling of both classes of methods.

ACKNOWLEDGEMENTS

The optimization of the SSBJ has been supported by the French Committee for Scientific Orientation for Supersonic Transport and the Center for Turbulence Research at Stanford University.

The *Annual Review of Fluid Mechanics* is online at <http://fluid.annualreviews.org>

LITERATURE CITED

- Allaire G, Jouve F, Toader AM. 2002. A level-set method for shape optimization. *C. R. Acad. Sci. Paris* 334:1125–30
- Alonso JJ, Kroo IM, Jameson A. 2002. Advanced algorithms for design and optimization of QSP. AIAA Pap. 2002-0144. Reno, NV
- Anagnostou G, Ronquist E, Patera A. 1992. A computational procedure for part design. *Comp. Methods Appl. Mech. Eng.* 20:257–70
- Arian E, Ta'asan S. 1995. Shape optimization in one-shot. In *Optimal Design and Control*, ed. J Boggaard, J Burkardt, M Gunzburger, J Peterson, pp. 273–94. Boston: Birkhauser
- Bardos C, Pironneau O. 2002. A formalism for the differentiation of conservation laws. *C. R. Acad. Sci., Paris, Ser. I.* 335(10):839–45
- Baron F, O Pironneau 1993. Multidisciplinary optimal design of a wing prole, in *Structural optimization 93*, The World Congress on Optimal Design of Structural Systems, ed. J Herskovits, Vol. 2, pp. 61–68, Rio de Janeiro, Brazil: UFRJ Press
- Becache E, Chaigne A, Derveaux G, Joly P. 2001. Numerical simulation of a guitar. *Proc. Eur. Conf. Comput. Mech.* Krakow, Poland. In press
- Beux F, Dervieux A. 1993. A Hierarchical Approach for Shape Optimization, Inria Rapports de Recherche 1868.
- Bischof C, Carle A, Corliss G, Griewank A, Hovland P. 1992. ADIFOR: Generating derivative codes from Fortran programs. *Sci. Progr.* 1(1):11–29
- Borwall J, Petersson B. 2002. Topological optimization of fluids in stokes flow. *Int. J. Numer. Methods Fluids* 42(9):224–65
- Cea J. 1980. Numerical methods of shape optimal design. In *Optimization of Distributed Parameter Structures*, ed. EJ Haug, J Cea. Sijthoff & Noordholl Alphen dall den Rijn, Netherlands
- Chenais D. 1987. Shape optimization in shell theory. *Eng. Optim.* 11:289–303
- Delfour M, Zolezio JP. 2001. *Shapes and Geometries: Analysis, Differential Calculus and Optimization*. Advances in Design and Control 4. SIAM, Philadelphia
- Elliott J, Peraire J. 1996. Aerodynamic design using unstructured meshes. *AIAA* 96:1941
- Farin G. 1987. *Curves and Surfaces for Computer Aided Geometric Design*. 2001. 5th ed. Boston: Academic Press
- Faure C. 1996. Splitting of algebraic expressions for automatic differentiation. Proc. 2nd SIAM Workshop Comput. Differ. Santa Fe, NM
- Garreau S, Guillaume P, Masmoudi M. 2001. The topological asymptotic for PDE systems: the elasticity case. *SIAM J. Control Optim.* 39(6):1756–78
- George PL. 1991. *Automatic Mesh Generation. Applications to Finite Element Method*. New York: Wiley
- Gilbert JC, Le Vey G, Masse J. 1991. La différentiation automatique de fonctions représentées par des programmes. INRIA Rapport de Recherche 1557.
- Giles MA, Pierce NA. 2001. Analytic adjoint solutions for the quasi-one-dimensional euler equations. *J. Fluid Mech.* 426:327–45
- Giunta A. 1997. Aircraft multidisciplinary design optimization using design of experiments theory and response surface modeling. M.A.D. center rep. 97-05-01. Virginia Tech.
- Godlewski E, Olazabal M, Raviart PA. 1998.

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- On the linearization of hyperbolic systems of conservation laws. Application to stability. In *Equations aux Dérivées Partielles et Applications*, ed. D Cioranescu, JL Lions, pp. 549–70. Gauthier-Villars, Paris: Elsevier
- Gopalsamy S, Pironneau O. 1989. Interpolation C^1 de résultats C^0 . Rapport de Recherche INRIA 1000
- Griewank A. 2000. *Evaluating Derivatives, Principles and Techniques of Algorithmic Differentiation*. Number 19 in Frontiers in Appl. Math. SIAM, Philadelphia
- Hamda H, Schoenauer M. 2000. Adaptive Techniques for Evolutionary Topological Optimum Design. In *Evolutionary Design and Manufacture*, ed. IC Parmee, pp. 250–65. Springer-Verlag
- Hamalainen J, Malkamaki T, Toivanen J. 1999. Genetic algorithms in shape optimization of a paper machine headbox, in *Evolutionary Algorithms in Engineering and Computer Science*, ed. K Miettinen, M Makela, P Neittaanmaki, J Periaux, pp. 435–43. Wiley
- Haslinger J, Makinen R. 2003. *Introduction to Shape Optimization*. SIAM Ser. Adv. Des. Control, Vol. 7
- Hirsch C, Shun K. 2001. Numerical investigation of the 3D flow around NREL untwisted wind turbine blades. *Proc. 4th Conf. Turbomach*. Florence, Italy. In press
- Jameson A. 1988. Aerodynamics design via control theory. *J. Sci. Comp.* 3:233–60
- Jameson A. 2003. Aerodynamic Design and Optimization, Antony Jameson, 16th AIAA Comput. Fluid Dynamics Conf., *AIAA Pap. A-2003-3438*, Orlando, FL, June 23–26
- Jameson A, Martinelli L, Pierce NA. 1998. Optimum aerodynamic design using the Navier-Stokes equations. *Theoret. Comp. Fluid Dynamics* 10:213–37
- Kim SK, Alonso J, Jameson A. 1999. A Gradient Accuracy Study for the Adjoint-Based Navier-Stokes Design Method, 37th AIAA Aerospace Sciences Mtg. & Exhibit, AIAA Pap. 99-0299, Reno, NV, January
- Lemarchand G, Pironneau O, Polak E. 2002. Incomplete gradients. *Proc. Domain Decompos. Methods Sci. Eng.* Lyon, France. In press
- Lions JL. 1968. *Contrôle Optimal de systèmes gouvernés par des équations aux dérivées partielles*. Dunod-Gauthier Villars
- Lohner R. 2001. *Applied Computational Fluid Dynamics Techniques: An Introduction Based on Finite Element Methods*. Chichester: Wiley 376 pp.
- Lorenz E. 1963. Deterministic nonperiodic flow. *J. Atmos. Sci.* 20:130–41
- Makinen R, Periaux J, Toivanen J. 1999. Multidisciplinary shape optimization in aerodynamics and electromagnetics using genetic algorithms. *Int. J. Numer. Methods Fluids* 30:149–59
- Marrocco A, Pironneau O. 1978. Optimum design of a magnet with lagrangian finite elements. *Comp. Methods Appl. Mech. Eng.* 15(3):512–45
- Marsden AL, Wang M, Mohammadi B, Moin P. 2001. Shape optimization for aerodynamic noise control. *Annu. Res. Briefs, Cent. Turb. Res.*, pp. 241–47. NASA Ames/Stanford Univ.
- Marsden AL, Wang M, Koumoutsakos P, Moin P. 2002. Optimal aeroacoustic shape design using approximation modeling. *Cent. Turb. Res. Briefs* 201:213
- Mohammadi B. 1994. CFD with NSC2KE: user-guide. *Note Technique INRIA 164*
- Mohammadi B. 2002. Optimization of aerodynamic and acoustic performances of supersonic civil transports. *Proc. CTR Summer Program 2002*, Stanford, CA. In press
- Mohammadi B, Pironneau O. 2001. *Applied Shape Optimization for Fluids*. Oxford: Oxford Univ. Press
- Mohammadi B, Saiaç JH. 2002. *Pratique de la Simulation Numérique*. Dunod Publisher, Paris
- Mohammadi B, Santiago JG. 2001. Simulation and design of extraction and separation fluidic devices. *Esaim M2AN* 35(3):513–23
- Choi H, Moin P, Kim J. 1992. Turbulent drag reduction: studies of feedback control and flow over riblets. *CTR Rep. TF-55*. Stanford, CA
- Murat F, Simon J. 1976. *Etude de problèmes d'optimum design*. *Lect. Notes Comput. Sci.* 41:54–62

- Murat F, Tartar L. 1987. On the control of coefficients in partial differential equations. *Topics in the Mathematical Modelling of Composite Materials*, ed. A Cherkaev, R Kohn. pp. 1–8. Boston: Birkhauser
- Nadarajah S, Jameson A, Alonso J. 2002. Sonic boom reduction using an adjoint method for wing-body configurations in supersonic flow. AIAA-2002-5547, 9th AIAA/ISSMO Symp. Multidisciplinary Analysis and Optimization Conf., Atlanta, GA. September 4–6
- Neittaanmaki P. 1991. Computer aided optimal structural design. *Surv. Math. Ind.* 1:173–215
- Obayashi S. 1997. Pareto Genetic Algorithm for aerodynamic design using the Navier-Stokes equations. In *Genetic Algorithms and Evolution Strategies in Engineering and Computer Science*, ed. D Quagliarella et al., pp. 245–66. Chichester: Wiley
- Peri D, Campana EF. 2003. High fidelity models in the multi-disciplinary optimization of a frigate ship Second M.I.T. Conference on Computational Fluid and Solid Mechanics. Cambridge, MA, June
- Periaux J, Mantel B, Sefrioui M, Stoufflet B, Desideri J, et al. 1998. Evolutionary computational methods for complex design in aerodynamics. *AIAA Pap.* 98–222
- Pironneau O. 1973. On optimal shapes for Stokes flow. *J. Fluid Mech.* 70(2):331–40
- Pironneau O. 1984. *Optimal Shape Design for Elliptic Systems*. Springer Series in Computational Physics. New York: Springer-Verlag
- Quagliarella D, Vicini A. 1997. Coupling Genetic Algorithms and Gradient Based Optimization Techniques. In *Genetic Algorithms and Evolution Strategies in Engineering and Computer Science*, ed. D Quagliarella et al., pp. 289–309. Chichester: Wiley
- Reuther J, Jameson A, Farmer J, Martinelli L, Saunders D. 1996. Aerodynamic shape optimization of complex aircraft configurations via an adjoint formulation *AIAA Pap.* 96:94
- Rostaing N, Dalmas S, Galligo A. 1993. Automatic differentiation in Odyssee. *Tellus* 45a(5):558–68
- Sokolowski J, Zolezio JP. 1991. *Introduction to shape optimization. Shape sensitivity analysis*. Springer Ser. Comput. Math. Vol. 16
- Sverak A. 1992. On existence of solution for a class of optimal shape design problems. *C. R. Acad. Sci. Paris Ser. I.* 315(5):545–49
- Sverak V. 1993. On optimal design. *J. Maths. Pures Appl.* 72:537–51
- Tartar L. 1974. Control problems in the coefficients of PDE. In *Control Theory, Numerical Methods and Computer Systems Modelling (Internat. Sympos., IRIA LABORIA, Rocquencourt, 1974)*, pp. 420–426. Lecture Notes in Econom. and Math. Systems, 107. Berlin: Springer
- Thomas Ch L. 1972. Extrapolation of sonic boom pressure signatures by the waveform parameter method. *NASA TN.* D-6832
- Whitham GB. 1952. The flow pattern of a supersonic projectile. *Comm. Pure Appl. Math.* 5(3):301–48