Differentiable and quasi-differentiable methods for Optimal Shape Design

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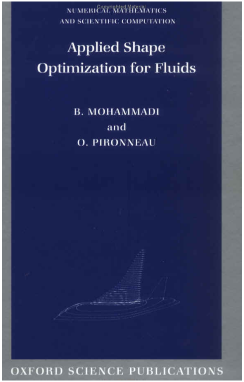
Machine Learning Conference

Outline

1. Conceptual Gradient Algorithm
2. Discretization
   - Summary
3. Topological Gradient-type Algorithms
4. Gradient Free Methods



More details in
B. Mohammadi & O.P. *Applied Optimal Shape Design*, Oxford U. Press (2001). Second edition 2009.
O.P. *Optimal shape design for elliptic systems*. Springer, (1984)

More Books

• **J. Haslinger and R. A. E. Makinen** Introduction to Shape Optimization, SIAM series 2003.

• **Jasbir S. Arora**: Introduction to Optimum Design. Elsevier 2004

• **E. Laporte, P. Letallec**: Numerical Methods in Sensitivity Analysis and Shape Optimization. Birkhauser, 2003.

• **M. Bendsoe and O. Sigmund.** *Topology Optimization,* . Springer 2003.

• **M. Delfour, J.P. Zolezio**: shape and geometries SIAM 2001.

• **G. Allaire**: *Shape Optimization by Homogenization* Springer 2001.

• **A. Cherkaev.** *Variational Methods for Structural Opt.* Springer 2000.

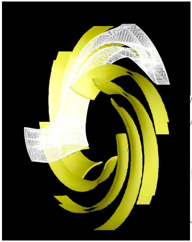
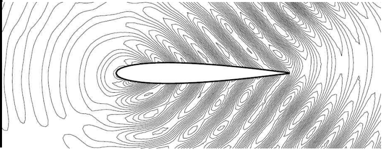
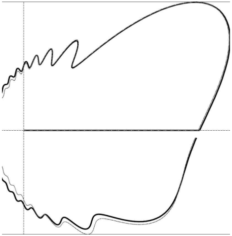
• **G.W. Litvinov.** *Optimization in elliptic problems*, vol 119 Operator Theory. Birkhauser, 2000.

• **J. Haslinger, P. Neittanmakki**: Finite Element Approximation for Optimal Shape. J. Wiley 1996.

• **M. Bendsoe** *Methods for optimization of structural topologyl*. Springer 1995.

Important Applications

- Aerodynamics: Shape optimization to improve airplanes, cars, ventilators, turbines...
- Hydrodynamics: wave drag of boats, pipes, by-pass, harbors...

- Electromagnetics: Stealth airplane, antenna, missiles...
- Combustion: Car and airplane engines, scramjets...
- Turbulence: delay the separation of boundary layers, reduce turbulent drag (active control, deformable airplane...)

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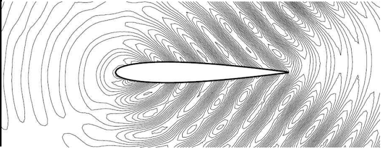
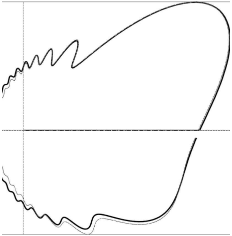

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Main Topics for Shape Optimization

$$\min_{v \in V \subset \mathcal{R}^d} E(v)$$

- Black Box Optimization: use only $v \to E(v)$
- Differentiable Optimization: use also $\text{grad}_v E(v)$

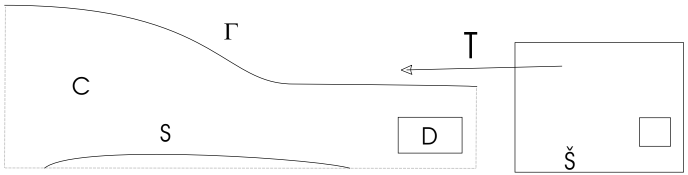
$$E(v+\delta v) = E(v) + < \text{grad} E(v), \delta v > + o(\|\delta v\|)$$
$$\delta v = -\rho \text{grad} E(v) \;\Rightarrow\; E(v+\delta v) - E(v) \approx -\rho \|\text{grad} E(v)\|^2$$

- Constrained Optimization: $V = \{v \in H \;:\; f(v) = 0, \;\; g(v) \leq 0\}$
- Multi-criteria and Pareto optimality:

$$E(v) = \sum_i \alpha_i E_i(v) \;\Leftrightarrow ?\; \nexists w : \; E_i(w) \leq E_i(v) \; \forall i$$

- Topological Optimization: Embed the problem into a larger class

An Academic Problem



$$\min_{\mathbf{S}\in\mathcal{S}_d}\{\int_D|\psi-\psi_d|^2\ :\ \ -\Delta\psi=0,\ \text{in } C-\dot{S},\quad \psi|_{\mathbf{S}}=0\ \ \psi|_{\partial C}=\psi_d\}$$

Wind tunnel Design by adapting S so that flow is uniform in D. Flow is irrotational inviscid and 2D.

Existence of Solution

Theorem

$$\min_{v \in V \subset \mathcal{R}^d} E(v)$$

has a solution if V is closed, E is bounded from below, l.s.c. and either V is bounded or $\lim_{||x|| \to \infty} E(x) = +\infty$

Thus if one can show that the criteria of the OSD problem is l.s.c. a solution will exist. It has been shown by Sverak that this is so if the number of connected component of Ω is bounded.

In Allaire, Bucur, Delfour et al, it is shown that a penalization of the perimeter of the unknown surface also induce existence in 2D.

Theorem The following problem has at least one solution:

$$\min_{\mathbf{S} \in \mathcal{S}_d} \{ \int_D |\psi - \psi_d|^2 + \epsilon |S|^2 \ : \ -\Delta\psi = 0, \text{ in } C - \dot{S}, \quad \psi|_{\mathbf{S}} = 0 \ \ \psi|_{\partial C} = \psi_d \}$$

Uniqueness is almost impossible to prove;

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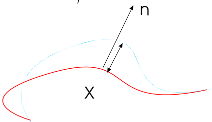
Sensitivity Analysis

$$-\Delta\psi^\epsilon = f \quad \text{in } \Omega^\epsilon \qquad \psi^\epsilon = 0 \text{ on } \Gamma^\epsilon := \{x + \epsilon\alpha n \ : \ x \in \Gamma\}$$

Definition *If $\psi'_\alpha := \lim \frac{1}{\epsilon}(\psi^\epsilon - \psi)$ exists then ψ is Gateau differentiable with respect to Γ in the direction α. If ψ'_α is linear in α then ψ is Frechet differentiable.* Similarly

$$\psi^{\epsilon\alpha} = \psi + \epsilon\psi'_\alpha + \frac{\epsilon^2}{2}\psi''_\alpha$$



To compute ψ' and ψ'' notice that, by linearity, they satisfy the same PDE but with $f = 0$. By Taylor expansion, $x \in \Gamma$:

$$0 = \psi^{\epsilon\alpha}(x + \epsilon\alpha n) = \psi^{\epsilon\alpha}(x) + \epsilon\alpha\frac{\partial\psi^{\epsilon\alpha}}{\partial n}(x) + \frac{\epsilon^2\alpha^2}{2}\frac{\partial^2\psi}{\partial n^2}(x) + \ldots$$

Therefore

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

Optimality Conditions

Consider the Wind Tunnel Problem with $S^\epsilon = \{x + \epsilon\alpha n : \ x \in S\}$. Think of the PDE as the implicit definition of $S \to \psi(S)$. Then $J()$ is a function of S only:

$$J(S^\epsilon) = \int_D |\psi^\epsilon - \psi_d|^2 = \int_D |\psi - \psi_d|^2 + 2\epsilon \int_D (\psi^\epsilon - \psi_d)\psi'_\alpha + o(\epsilon)$$

with $\Delta\psi'_\alpha = 0, \ \ \psi'_\alpha|_S = -\alpha\frac{\partial\psi}{\partial n}, \ \ \psi'_\alpha|_{\Gamma-S} = 0.$
If J is Frechet differentiable there exists ξ such that $J'_\alpha = \int_S \xi\alpha$. To find ξ we must use the adjoint trick and introduce

$$-\Delta p = (\psi^\epsilon - \psi_d)I_D, \ \ p|_\Gamma = 0$$

Then

$$2\int_D (\psi^\epsilon - \psi_d)\psi'_\alpha = -2\int_\Omega \psi'_\alpha \Delta p = -2\int_\Omega \Delta\psi'_\alpha p + \int_\Gamma (\frac{\partial p}{\partial n}\psi'_\alpha + \frac{\partial \psi'_\alpha}{\partial n} p)$$

Corollary $\quad J'_\alpha = 2\int_S \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n}\alpha$

Conceptual Algorithm

- 0. Choose a shape S^0, a small number $\rho > 0$ and set m=0.
- 1. Compute ψ^m and p^m by solving

$$-\Delta\psi^m = 0, \quad \psi^m|_{S^m} = 0, \quad \psi^m|_{\Gamma_d} = \psi_d$$
$$-\Delta p^m = (\psi^m - \psi_d) I_D, \quad p|_{\Gamma^m} = 0$$

- 2. Set

$$\alpha = -\rho \frac{\partial p^m}{\partial n} \frac{\partial \psi^m}{\partial n} \qquad \mathcal{S}^{m+1} = \{x + \alpha n : \ x \in S^m\}$$

- 3. Set $m \leftarrow m+1$ and go to 1.

It works because

$$J(S^{m+1}) = J(S^m) + \int_{S^m} \xi\alpha = J(S^m) - 2\rho \int_{S^m} (\frac{\partial p^m}{\partial n} \frac{\partial \psi^m}{\partial n})^2 + o(\alpha)$$

Notice that there is a loss of regularity from S^m to S^{m+1}!

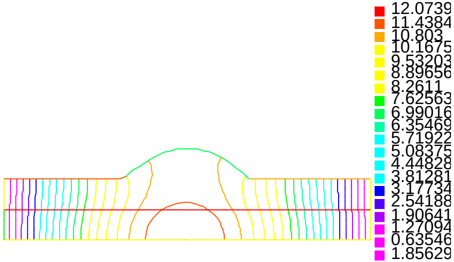
Implementation with freefem++

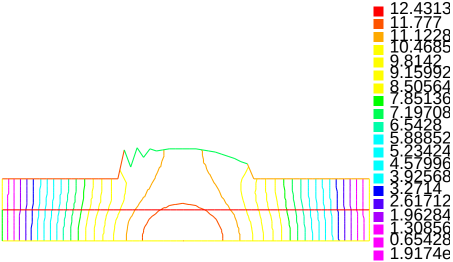
```
real xl = 5, L=0.3;
mesh th = square(30,30,[x,y*(0.2+x/xl)]);
func D=(x>0.4+L && x<0.6+L)*(y<0.1);
func psid = 0.8*y;
fespace Vh(th,P1);
Vh psi,p,w;
problem streamf(psi,w)=int2d(th)(dx(psi)*dx(w) + dy(psi)*dy(w))
   +on(1,4,psi = y/0.2)+on(2,psi=y/(0.2+1.0/xl)) + on(3,psi=1);

problem adjoint(p,w)=int2d(th)(dx(p)*dx(w) + dy(p)*dy(w))
   - int2d(th)(D*(psi-psid)*w)+ on(1,2,3,4,p=0);
Vh a=0.2+x/xl, gradE;
for(int i=0;i<100;i++){
      streamf; adjoint;
      real E = int2d(th)(D*(psi-psid)^2)/2;
      gradE = dx(psi)*dx(p) + dy(psi)*dy(p);
      a=a(x,0)-50*gradE(x,a(x,0))*x*(1-x);
      th = square(30,30,[x,y*a(x,0)]);
}
```

Execute

Oscillations





Regularity Preserving Algorithms: Sobolev Gradients

$$\alpha = -\rho \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n} \qquad \mathcal{S}^{m+1} = \{x + \alpha n : \ x \in S^m\}$$

can be replaced by

$$\frac{d^2\tilde\alpha}{ds^2} = \rho \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n} \quad \tilde\alpha(s_0) = \tilde\alpha(s_1) = 0. \qquad \mathcal{S}^{m+1} = \{x + \tilde\alpha n : \ x \in S^m\}$$

$$\Rightarrow \quad J(S^{m+1}) - J(S^m) = \frac{2}{\rho}\int_{S^m} \tilde\alpha \frac{d^2\tilde\alpha}{ds^2} = -\frac{2}{\rho}\int_{S^m} (\frac{d\tilde\alpha}{ds})^2 + o(\rho)$$

Alternatively one may use a smoothing operator like

$$\beta \to \gamma(\beta) = v \text{ where } v \text{ is solution of } -\Delta v = 0 \quad \frac{\partial v}{\partial n}|_\Gamma = \beta.$$

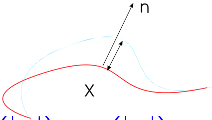
Let $\mathcal{S}^{m+1} = \{x + \gamma(\beta) n : \ x \in S^m\}$ with $\beta = \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n}$

$$J(S^{m+1}) - J(S^m) = 2\rho \int_\Gamma \gamma(\beta)\beta = 2\rho \int_\Gamma v \frac{\partial v}{\partial n} = -2\rho \int_\Omega |\nabla v|^2$$

Geometric Constraints

- Projected Gradient: the case $\int_\Omega = 1$.

$$\Gamma' = \{x + \alpha n(x) : \ x \in \Gamma\} \Rightarrow \quad \delta J = \int_\Gamma \chi \alpha ds + o(|\alpha|)$$



$$\Gamma' = \{x + (\alpha - \frac{1}{|\Gamma|}\int_\Gamma \alpha) n(x) : \ x \in \Gamma\}$$

$$\Rightarrow \quad \delta \int_\Omega = \int_\Gamma (\alpha - \frac{1}{|\Gamma|}\int_\Gamma \alpha) + o(|\alpha|) = o(|\alpha|)$$

$$\delta J = \int_\Gamma (\chi - \frac{1}{|\Gamma|}\int_\Gamma \chi)(\alpha - \frac{1}{|\Gamma|}\int_\Gamma \alpha) ds + o(|\alpha|)$$

- Penalization: replace J by

$$J + \frac{1}{\epsilon}|F(\Omega)^+|^2 + \frac{1}{\omega}|G(\Omega)|^2$$

to maintain $F(\Omega \le 0), \ G(\Omega) = 0$

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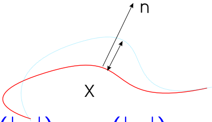

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State Constraints

$$\min_v \{J(u,v) : \; Au = g(v), \;\; F(u,v) \le 0\}$$

where A is a linear invertible operator.

$\delta J = J'_u \delta u + J'_v \delta v$ with $A\delta u = g'_v \delta v, \;\; F'_u \delta u + F'_v \delta v \le 0$ if $F(u,v) = 0$

Introducing $A^T p = J'_u, \;\; A^T q = F'_u$ leads to

$$J'_u \delta u = \delta u \cdot A^T p = p \cdot A\delta u = p \cdot g'_v \delta v \qquad F'_u \delta u = \delta u \cdot A^T p = q \cdot A\delta u = q \cdot g'_v \delta v$$

$$\delta J = (p \cdot g'_v + J'_v)\delta v \text{ with } (q \cdot g'_v + F'_v)\delta v \le 0 \text{ if } F(u,v) = 0$$

A direction of descent is built from this.
Notice that two adjoint vectors are needed

Example

Build a stealth airfoil with "good" aerodynamic properties

$$\min_S J := \int_D |u|^2 \ : \ \int_S \frac{\partial\psi}{\partial n} = a$$

$$\omega^2 u + \Delta u = 0, \text{ in } \Omega \quad u|_\Gamma = g$$
$$-\Delta\psi = 0, \text{ in } \Omega \quad \psi|_\Gamma = \psi_d$$

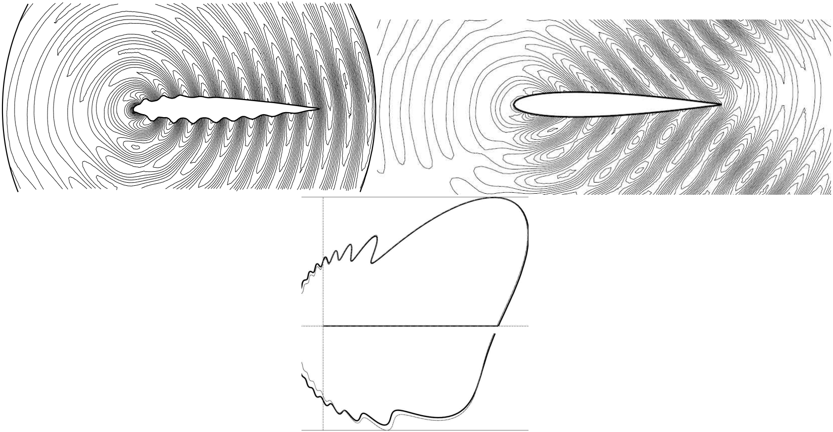
Requires the following

Lemma

$$\Gamma' = \{x + \alpha n : \ x \in \Gamma\} \Rightarrow \delta \int_\Gamma f = \int_\Gamma \alpha(\frac{\partial f}{\partial n} - \frac{f}{R})$$

where R is the mean radius of curvature.

Example



Computed by A. Baron

The Minimum Drag Problem

$$J(\Omega) \equiv \min_{\Omega\in C, vol(C)=1} \int_\Omega \frac{1}{2}||\nabla u||^2 dx \ : \qquad u|_{\partial\Omega} = g$$
$$u\nabla u + \nabla p - \nu\Delta u = 0, \quad \nabla\cdot u = 0,$$

The solution exists in 2D if the nb of connected component is bounded. In 3D ? but probably yes because the criteria is the energy of the system. For safety regularize by adding $\epsilon call(C)$.

Proposition

$$\partial\Omega' = \{x + \alpha n(x) : \ x \in \partial\Omega\} \Rightarrow ? \ \delta J = \int_{\partial\Omega} \chi\alpha ds + o(|\alpha|)$$

$$\delta J = \int_{\partial\Omega} \alpha \frac{\partial u}{\partial n}\cdot(\frac{1}{2}\frac{\partial u}{\partial n} + \frac{\partial w}{\partial n}) + o(|\alpha|)$$

where $-u\nabla w + w\nabla u^T + \nabla q - \nu\Delta w = \nu\Delta u, \quad \nabla\cdot w = 0, \ w|_{\partial\Omega} = 0$

From JFM 73. See also, Modi, Gunzberger, Tasan, Jameson... Q? What minimal norm on α?

The Minimum Drag Problem

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Proof

Recall that $\delta \int_\Omega f = \int_\Gamma \alpha f$. Then

$$\delta J = \int_\Omega \nabla u \cdot \nabla \delta u + \frac{1}{2}\int_{\partial\Omega} \alpha |\nabla u|^2 + o(|\alpha|)$$

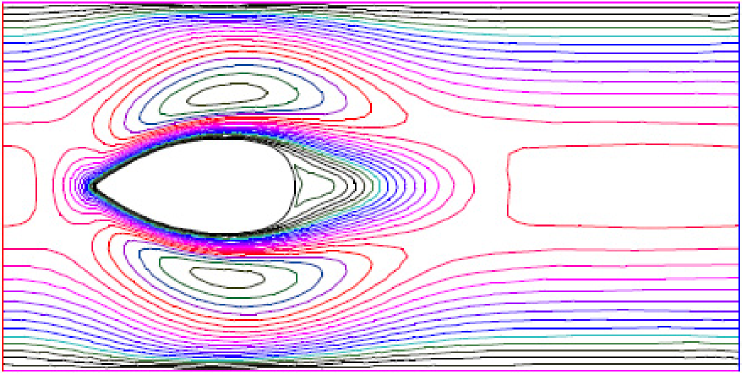
and $\delta u \nabla u + u \nabla \delta u + \nabla \delta p - \nu \Delta \delta u = 0, \;\; \nabla \cdot \delta u = 0, \;\; \delta u|_\Gamma = -\alpha \dfrac{\partial u}{\partial n}$

So $\displaystyle\int_\Omega \nabla u \cdot \nabla \delta u = -\int_\Omega \delta u \Delta u$

$$= -\frac{1}{\nu}\int_\Omega (-u\nabla w + w \nabla u^T + \nabla q - \nu \Delta w)\delta u$$

$$= -\frac{1}{\nu}\int_\Omega (\nabla \cdot (u \otimes \delta u + \delta u \otimes u) - \nu \Delta \delta u) w - \int_\Gamma \nu \frac{\partial w}{\partial n} \delta u + o(|\alpha|)$$

Example



Minimum drag object of given area at Reynold 50 (Courtesy of Kawahara et al.).

Compressible Flows

Euler or Navier-Stokes equations

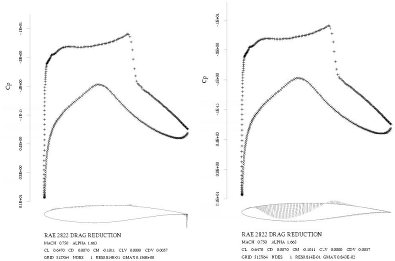
$$W = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} \qquad \partial_t W + \nabla \cdot F(W) - \nabla \cdot G(W, \nabla W) = 0$$

$$W(0, x) = 0, \quad + \text{B.C.}$$

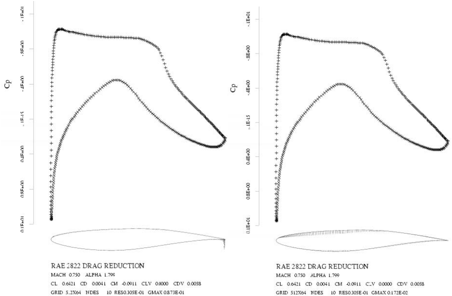
Involves an adjoint equation

$$\partial_t P + (F'(W) - G'_{,1}(W, \nabla W)^T \nabla P - \nabla \cdot (G'_{,2}(W, \nabla W)^T \nabla P) = 0$$

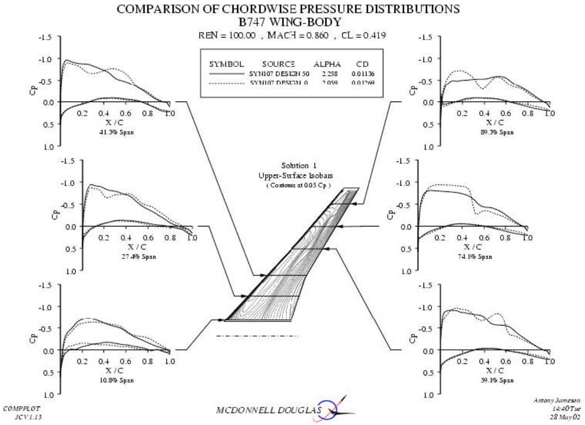
Some Realizations - A. Jameson (I)



Plain vs Sobolev Gradients

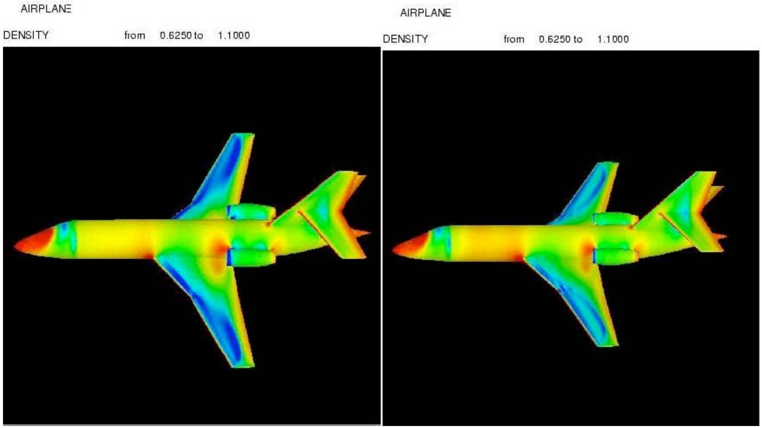


Before & after optimization



Optimization of the Boeing 747: 10% wing drag saving (5% aircraft drag)

Some Realizations - A. Jameson (III)



Falcon jet: C_D decreases from 234 to 216

Outline

Summary

- Optimal Shape Design of S relies on Optimization

$$\min_S J(u,S) \ : \ A(S)u = f$$

- The Continuous problem is well posed after regularization

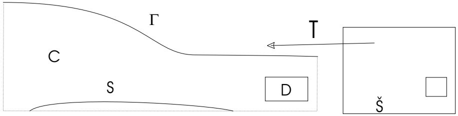
$$\min_S J(u,S) + \epsilon|S|^2 \ : \ A(S)u = f$$

- The L^2 local gradient χ is computable by calculus of variation:

$$\delta J = \int_S \chi\alpha + o(|\alpha|), \quad S(\alpha) = \{x + \alpha(x)n(x) \ : \ x \in S\}$$

- The Sobolev gradient is the right tool for gradient methods:

$$-\Delta_S \beta = \chi, \quad S^{n+1} = \{x - \rho\beta(x)n(x) \ : \ x \in S^n\}$$



$$\min_{\mathbf{S}\in\mathcal{S}_d} J(S) := \{\int_D |\psi-\psi_d|^2 \ : \ -\Delta\psi = 0, \text{ in } C-\dot{S}, \quad \psi|_{\mathbf{S}} = 0 \ \ \psi|_{\partial C} = \psi_d\}$$

Discretization of gradients $J'_\alpha = \nabla\psi\nabla p$ where $-\Delta p = 2I_D(\psi-\psi_d)$, $p|_\Gamma = 0$ or derivation of gradient for the discrete problem?

Optimization of the Discrete Problem

- The Finite Element Method,
- Discrete Gradients
- Finite Volume Methods

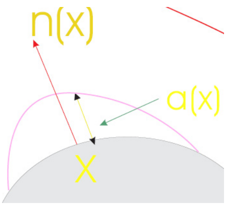
The Finite Element Method

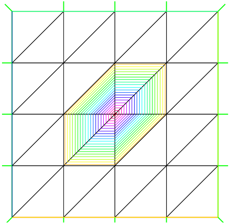
Ω is covered with triangles T_k and q^i are the vertices. The PDE of the wind tunnel problem is approximated by

$$\int_\Omega \nabla\psi_h \nabla w_h = 0, \quad \psi_h|_S = 0, \quad \psi_h|_\Gamma = \psi_d$$

for all w_h continuous and affine on each T_k and zero on $\partial\Omega$.

$$J = \int_D ||\psi_h - \psi_d||^2 + \epsilon \int_S |\frac{d^2\alpha}{dn^2}|^2$$





Let $\delta q_h(x) = \sum_i \delta q_i w(x)$, the basis $\{w^j\}$, the hat function of q_j.

Summary: Continuous versus Discrete Gradient

$$\min_{\mathbf{S}\in\mathcal{S}_d} J(S) := \{\int_D |\psi-\psi_d|^2 \ : \ -\Delta\psi = 0, \text{ in } C-\dot{S}, \quad \psi|_{\mathbf{S}} = 0 \ \ \psi|_{\partial C} = \psi_d\}$$

$$\delta J = \int_S \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n} \text{ with } -\Delta p = 2(\psi-\psi_d)I_D$$

use normal displacement $\approx v \ : \ -\Delta v = 0, \ \ \frac{\partial v}{\partial n}|_\Gamma = \frac{\partial p}{\partial n}\frac{\partial \psi}{\partial n}$

For the discrete system

$$\min_{\mathbf{q^i}\in\mathcal{Q}_d} J(S_h) = \{\int_D |\psi_h-\psi_d|^2 : \int_\Omega \nabla\psi_h\cdot\nabla w^j = 0, \ \forall j \ \psi_h|_{\mathbf{S}} = 0 \ \ \psi_h|_{\partial C} = \psi_d\}$$

$$\delta J = \int_\Omega (\nabla\psi_h(\nabla\delta q_h + \nabla\delta q_h^T)\nabla p_h - \nabla\psi_h\cdot\nabla p_h \nabla\cdot\delta q_h) = \sum \chi_j \delta q^j$$

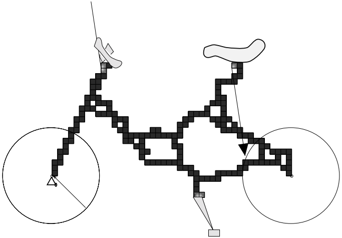
$$\textit{with} \int_\Omega \nabla p_h \nabla w^j = 2\int_D (\psi_h-\psi_d)w^j, \ \ p_h \in V_{0h}$$

And use a smoothed version of χ_j to move the vertices and find the new shape (and triangulation).

Topological Optimization

- Applies when the topology is not known
- Black-box favors Genetic algorithm (yet slow)
- Combine topological and geometrical shape design?

From T. Borrval and J. Petterson



From Schoenauer et al

Topological Derivatives

Following the work of L. Tartar and N. Kikuchi, J. Sokolowski came with the following idea (f has zero mean, $B(0,1)$ the unit ball)

$$-\Delta u = f \text{ in } \Omega, \qquad u|_\Gamma = 0,$$
$$-\Delta u^\epsilon = f \text{ in } \Omega \backslash B(x_0,\epsilon), \qquad u^\epsilon|_\Gamma = 0,$$
$$\text{Neumann or Dirichlet on } \partial B(x_0,\epsilon) = 0,$$
$$u'_{x_0}(x) = \lim_{\epsilon\to 0} \frac{1}{\epsilon^\gamma}(u^\epsilon - u)$$

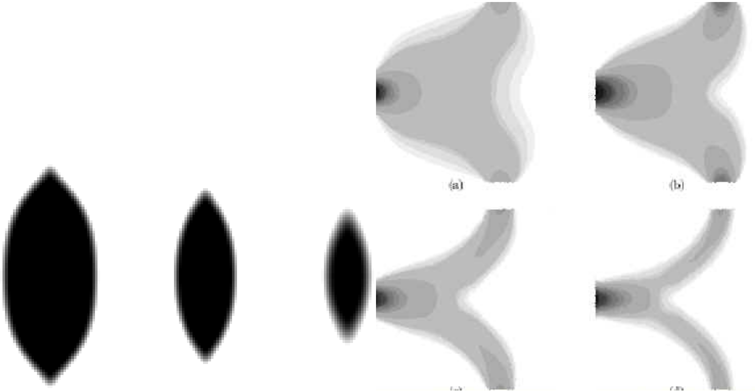
exists and is not identically 0 or $+\infty$ for some value of γ.

Theorem For the Neumann (resp Dirichlet) problem $\gamma = 2$ (resp $log\epsilon$) in 2D and u' solves

$$\int_\Omega \nabla u \cdot \nabla w = c \nabla u \nabla w|_{x_0}$$

This is sufficient for gradient type algorithm, but convergence is usually a problem.

Applications of Topological Optimization



Stokes flow drag optimization (courtesy of M. Masmoudi)

Micro Channel flow (Borrval and Petterson)

Optimization of a micro channel flow averaged vertically gives

$$\min_{z(x)\in Z} j(u) := \int_D (u-u_d)^2 \ : \ \frac{5}{2z^2}u - \Delta u + \nabla p = 0, \quad \nabla\cdot u = 0, \quad u|_\Gamma = g$$

where the pointwise values of functions of Z are equal to ϵ or h. Let $\rho = 2.5z^{-2}$; notice that

$$[\rho u] = \bar\rho[u] + [\rho]\bar u \qquad \bar a = \frac{a_1 + a_2}{2} \qquad [a] = a_1 - a_2$$

Therefore if u' exists, the derivative w/r "ρ_2 becoming ρ_1" at x_0, it must be

$$\bar\rho u' + \rho'\bar u - \Delta u' + \nabla p' = 0 \quad \nabla\cdot u' = 0 \text{ with } \rho' = [\rho]\delta(x-x_0), \quad u'|\,\Gamma = 0$$

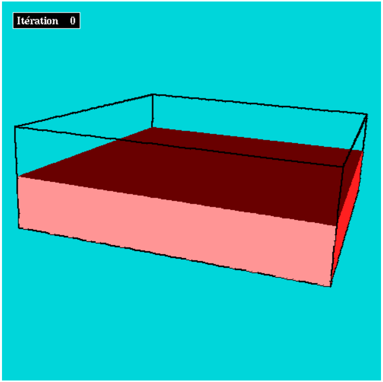
But u is continuous so $\bar u = u$. Introduce the adjoint state v, q

$$\bar\rho v - \Delta v + \nabla q = 0 \quad \nabla\cdot q = 2(u-u_d)\chi_D, \quad v|\,\Gamma = 0$$
$$\Rightarrow \quad j' = -[\rho]u(x_0)p(x_0)$$

Replace : ρ_2 by ρ_1 at x_0 when $[\rho]u(x_0)p(x_0) > 0$

Important Applications

Solid mechanics: Weight optimization of airplanes, cars, parts...



Topological optimization of the weight of a stool for a given strength (courtesy of F. Jouve et al)

Steepest Descent with Mesh Refinement

Now consider the same algorithm with parameter refinement

Algorithm

(Steepest descent with refinement)

while $h > h_{min}$ do

{

while $\| grad_z J_h(z^m) \| > \epsilon h^\gamma$ do

{

$z^{m+1} = z^m - \rho\, grad_z J_h(z^m)$ where ρ such that,

$$-\beta\rho\|w\|^2 < J_h(z^m - \rho w) - J_h(z^m) < -\alpha\rho\|w\|^2$$

with $w = grad_z J_h(z^m)$ Set $m := m + 1;$

}

$h := h/2;$

}

Steepest Descent and Inexact Gradients

• Convergence obvious : it is either S.Descent or $\text{grad} J_h \to 0$ because $h \to h/2$.

• Gain in speed : we do not need the exact gradient $\text{grad}_z J_h$!

• Let N be an iteration parameter and $J_{h,N} \approx J_h$ and $\text{grad}_z J_{h,N} \approx \text{grad}_z J_h$ in the sense that

$$\lim_{N\to\infty} J_{h,N}(z) = J_h(z) \qquad \lim_{N\to\infty} \text{grad}_{zN} J_{h,N}(z) = \text{grad}_z J_h(z)$$

Add K and $N(h)$ with $N(h) \to \infty$ when $h \to 0$:

Inexact Gradient (II)

Algorithm

(E. Polak et al)(Steepest descent with Goldstein's rule mesh refinement and approximate gradients)

while $h > h_{min}\{$

while $|\, grad_{z^N} J^m| > \epsilon h^\gamma \{$

try to find a step size ρ with $w = \; grad_{z^N} J(z^m)$

$$-\beta\rho\|w\|^2 < J(z^m - \rho w) - J(z^m) < -\alpha\rho\|w\|^2$$

if success *then*

$\{z^{m+1} = z^m - \rho \, grad_{z^N} J^m; \;\; m := m+1;\}$

else $N := N + K;$

$\}$

$h := h/2; \;\; N := N(h);$

$\}$

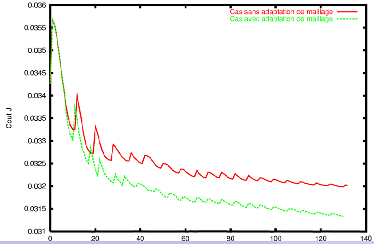
algorithm

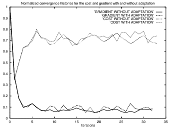
The convergence could be established from the observation that Goldstein's rule gives a bound on the step size:

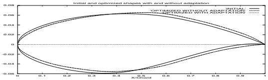
$$-\beta\rho\ \mathrm{grad}_z J\cdot h < J(z+\rho h) - J(z) = \rho\ \mathrm{grad}_z J\cdot h + \frac{\rho^2}{2}J''hh$$

$$\Rightarrow\quad \rho > 2(\beta-1)\frac{\mathrm{grad}_z J\cdot h}{J''(\xi)hh}\quad \text{so } J^{m+1}-J^m < -2\frac{\alpha(1-\beta)}{\|J''\|}|\ \mathrm{grad}_z J|^2$$

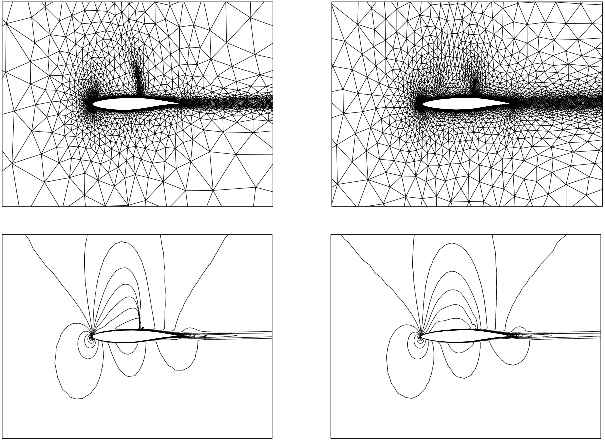
Thus at each grid level the number of gradient iterations is bounded by $O(h^{-2\gamma})$. Therefore the algorithm does not jam hence convergence.







Mesh Refinements



Finite Difference Gradient

$$\frac{f(x+h)-f(x)}{h} = f'(x) + f^{(2)}\frac{h}{2} - f^{(3)}\frac{h^2}{6} + \ldots$$

$$\mathcal{R}e\frac{f(x+\mathbf{i}h)-f(x)}{\mathbf{i}h} = f'(x) + O(h^2)$$

$$\frac{f(x+h)-f(x-h)}{2h} = f'(x) + f^{(3)}\frac{h^2}{6} + f^{(5)}\frac{h^4}{60} + \ldots$$

$$\frac{f(x+h)-f(x-h)}{4h} + \mathcal{R}e\frac{f(x+\mathbf{i}h)-f(x-\mathbf{i}h)}{4\mathbf{i}h} = f'(x) + O(h^6)$$

Principle of Automatic Differentiation

Let $J(u) = |u - u_d|^2$, then its differential is

$$\delta J = 2(u - u_d)(\delta u - \delta u_d) \quad \frac{\partial J}{\partial u} = 2(u - u_d)(1.0 - 0.0)$$

Obviously the derivative of J with respect to u is obtained by putting $\delta u = 1, \ \ \delta u_d = 0$. Now suppose that J is programmed in C/C++ by

```
double J(double u, double u_d){
    double z = u-u_d;
    z = z*(u-u_d);
    return z;
 }
int main(){  double u=2,u_d = 0.1;
    cout << J(u,u_d) << endl;
 }
```

A program which computes J and its differential can be obtained by writing above each differentiable line its differentiated form:

A simple example (cont)

```
class ddouble  {public: double v,d;
ddouble(double a, double b=0){ v = a; d=b;}
};

ddouble JandDJ(ddouble u, ddouble u_d)
{   ddouble z;
        z.d = u.d - u_d.d;
        z.v = u.v-u_d.v;
        z.d= z.d*(u.v-u_d.v) + z.v*(u.d - u_d.d);
        z = z*(u-u_d);
        return z;
}
int main()
 {
      ddouble u(2.,1.),   u_d= 0.1, J = JandDJ(u,u_d);
       cout << J << "  dJ="<<dJ<<endl;
 }
```

The class ddouble

```
class ddouble{ public: double v[2];
ddouble(double a, double b=0){ v[0] = a; v[1]=b;}
ddouble operator=(const ddouble& a)
  { val[1] = a.v[1]; val[0]=a.v[0];
    return *this;
  }
friend ddouble operator-(const ddouble& a,const ddouble& b)
       {    ddouble c;
            c.v[1] = a.v[1] - b.v[1];    // (a-b)'=a'-b'
            c.v[0] = a.v[0] - b.v[0];
            return c;
        }
friend ddouble operator*(const ddouble& a,const ddouble& b)
       {    ddouble c;
            c.v[1] = a.v[1]*b.v[0] + a.v[0]* b.v[1];
            c.v[0] = a.v[0] * b.v[0];
            return c;}
};
```

A Simple Example (final)

```
#include "ddouble.hpp"

ddouble J(ddouble u, ddouble u_d){
    ddouble z = u-u_d;
    z = z*(u-u_d);
    return z;
 }
int main(){
   ddouble u=2, u_d = 0.1;
   u.v[1]=1;
    cout << J(u,u_d).v[1] << endl;
 }
```

Simply replace all double by ddouble and link with the class lib.
A few pitfalls: e.g.

```
ddouble sqrt(ddouble x){    ddouble y;
 y.v[1]=x.v[1]/sqrt(fabs{x.v[0])+eps); y.v[0]=sqrt(x.v[0]);
 return y;  }
```

Limitations

```
program newtontest
x=0.0;
al=0.5
call newton(x,10,al)
write(*,*) x
end
```

```
subroutine newton(x,n,al)
do i=1,n
   f = x-alpha*cos(x)
   fp= 1+alpha*sin(x)
   x=x-f/fp
 enddo
 return
 end
```

2n adjoint variables are needed! while the theory is

$$f(x,\alpha)=0 \quad\Rightarrow\quad x'f'_x+f'_\alpha=0 \quad\Rightarrow\quad x'=-\frac{f'_\alpha}{f'_x}$$

So it is better to understand the output of AD-reverse and clean it. see www.autodiff.org

Tapenade

```
program newtontest
x=0.0
xb=2
al=0.5
call newton_b(x,xb,5,al,alb)
write(*,*) x,xb
end
SUBROUTINE NEWTON_B(x,xb,n,al,alb)
   DO i=1,n
     CALL PUSHREAL4(f)
     f = x - al*COS(x)
     CALL PUSHREAL4(fp)
     fp = 1 + al*SIN(x)
     CALL PUSHREAL4(x)
     x = x - f/fp
   ENDDO
```

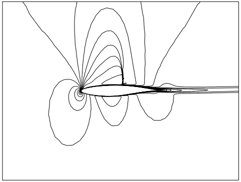
```
   CALL PUSHINTEGER4(i-1)
   alb = 0.0
   CALL POPINTEGER4(nb)
   DO i=nb,1,-1
       CALL POPREAL4(x)
       fb = -(xb/fp)
       fpb = f*xb/fp**2
       CALL POPREAL4(fp)
       alb = alb+SIN(x)*fpb-COS(x)*fb
       xb = xb + al*COS(x)*fpb
&      + (al*SIN(x)+1.0)*fb
       CALL POPREAL4(f)
   ENDDO
   END
```

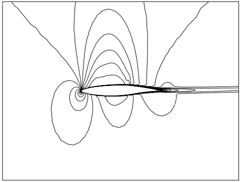
Optimization of a wing profile

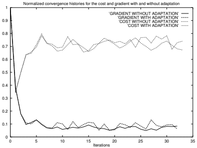
Drag is mostly pressure by the shock. The lift & area are imposed

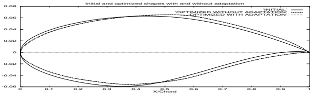
$$J(u,p,\theta) = F\cdot u_\infty + \frac{1}{\epsilon}|F\times u_\infty - C_l|^2 + \frac{1}{\beta}(\int_S dx - a)^2$$

with $F = \int_S (p\mathbf{n} + (\mu\nabla u + \nabla u^T))$ and Navier-Stokes + $k-\epsilon$ + wall laws

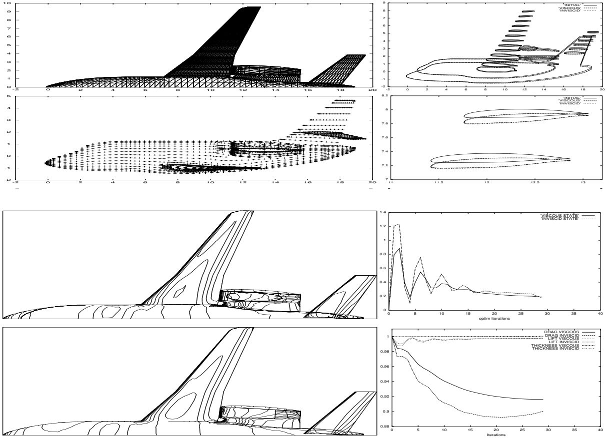








Optimization of a 3D Business Jet



Done by B. Mohammadi in a few hours on a workstation

Gradient Free Methods

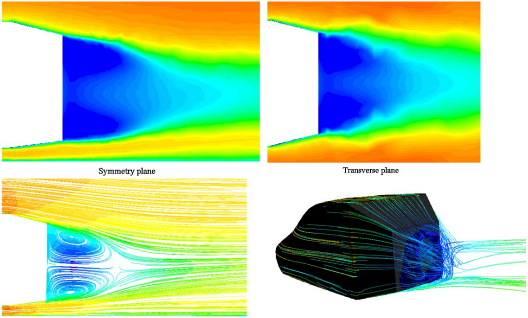
The main motivation is the non access to the source and the prototyping speed

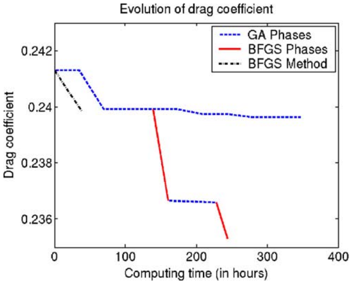
- Powells' **NEWUOA**
- Evolutionary algorithms
- Hybrid methods

[width=5cm]rastrigin Rastrigin's test with 20 param

Proposed by L. Dumas

- Random initialization of a population
- *Until convergence do:*
  - GA evolution (selection, crossover and mutation)
  - If stagnation during three generations then three iterations of BFGS on the current best individual
- *Repeat*





Optimization of a mockup car with 4 param. (Dumas-Muyr)

Perspectives

- Parallel and Stream Computing (MPI and CUDA)
- Enormous systems: automatic Differentiations ?
- Link with CAD
- Progresses of G.A. algorithms

Bis petit obscurum et condit se Luna tenebris (Nostradamus)

"For Optimal Shape Design the future lies in mixing Gradient Free methods with Differentiable Optimization".

The End