Optimal Shape Design: The Algorithmic Point of View

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Lectures at MUSAF II
Scope for Design

Aerodynamic Design
Aerodynamic Shape Optimization
Design Process
Applications of Aerodynamic Shape Optimization
Appendix
Appendix A - Biography of Antony Jameson
Appendix B - CFD Applications at Boeing and Airbus
Appendix C - FLO and SYN Codes and Their Usages
Appendix D - Mathematics of Adjoint Based Shape Optimization

CFD Contribution to A380
Antony Jameson

CFD and Airplane Design

Pironneau (LJLL)
Optimal Shape Design: The Algorithmic Point of View

Courtesy of A. Jameson & Airbus.

Important Applications ⇒ Learn from Other Fields

- **Aerodynamics**: Shape optimization to improve, cars, ventilators, turbines...
- **Hydrodynamics**: Wave drag of boats, pipes, harbours, buildings...
- **Hemodynamics**: Bypass, stents...

Cooler (B. Mohammadi & al)  Cardiac bypass (Deparis & al) & al.  Boat Hull (R. Lohner & al)

- Inverse problems in finance (calibration)
- Inverse problems in meteorology (data assimilation)
- Weight/Compliance (Topological) Optimization

Ideas from Hemodynamics

Cardiac flow are fluid-structure interactions with linear elasticity and Navier-Stokes eqs.

The domain of the fluid is mapped from a fixed domain: \( \min_{A(.)} J(u, p) \)

\[
\Omega_t = A_t(\Omega_0) \quad \text{with} \quad A_t : x_0 \rightarrow x_t := A_t(x_0).
\]

Let \( u_\tau(x, t) = u(A_t(A_\tau^{-1}(x)), t), \quad \forall x \in \Omega_\tau \)

Then, in \( \Omega_t \) at \( t = \tau \),

\[
\frac{\partial \vec{u}_\tau}{\partial t} + (\vec{u}_\tau - \vec{c}_\tau) \cdot \nabla \vec{u}_\tau + \nabla p - \nu \Delta \vec{u}_\tau = 0,
\]

\( \nabla \cdot \vec{u}_\tau = 0, \quad + \text{B.C. with } c_\tau(x) = -\frac{\partial A_t(A_\tau^{-1}(x))}{\partial t} \bigg|_{t=\tau} \)

The mapping is built from an extension of boundary displacement \( \vec{d} : x \rightarrow x + \vec{d}(x) \).

Use reduce basis methods on \( A \) and reduce the number of parameters. (Theory OK)

Free-Form Deformations

If $\psi$ maps $\Omega$ into the unit cube then the Free-Form Deformation [1][2][3] by $\mu$ is $\psi^{-1}(\hat{T}(\psi(x), \mu))$ with

$$\hat{T}(x, \mu) = \sum_{k,l,m} C^K_k C^L_l C^M_m (1 - x_1)^{K-k} x_1^k (1 - x_2)^{L-l} x_2^l (1 - x_3)^{M-m} x_3^m [P_{k,l,m} + \mu_{k,l,m}]$$

It is a 3D spline where the control points $P_{k,l,m}$ have moved to $P_{k,l,m} + \mu_{k,l,m}$

Reduce the Number of Parameters in Free-Form Deformations

Use Morris [1] randomize one-at-a-time sensitivity: keep the dof where $\frac{\partial J}{\partial \mu_{klm}}$ is large:

$$E = -\frac{1}{N} \sum_{n=[k,l,m]} \frac{\partial J}{\partial \mu_{klm}}, \quad S^2 = \frac{1}{N} \sum_{n=[k,l,m]} \left( \frac{\partial J}{\partial \mu_{klm}} + E \right)^2$$

Select the dof with large deviation from $(S,E) + \text{uniform distribution}$ (Ballarin et al [2]). End result is a procedure that works for any shape, but it is expensive!


An Academic Problem: Best Wind Tunnel

Adapt $S$ so that 2D irrotational flow is uniform in $D$.

**Theorem** (G. Allaire) The following problem has at least one solution:

$$
\min_{S \in S_d} \left\{ \int_D |\psi - \psi_d|^2 + \epsilon |S|^2 : -\Delta \psi = 0, \text{ in } C \setminus \hat{S}, \quad \psi|_S = 0 \quad \psi|_{\partial C} = \psi_d \right\}
$$

**Sensitivity Analysis by Local Variations**

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

**Definition** $\psi$ is $n$-differentiable in the direction $\alpha$ if

$$
\psi^{\epsilon \alpha} = \psi + \epsilon \psi'_{\alpha} + \frac{\epsilon^2}{2} \psi''_{\alpha} + \ldots + \frac{\epsilon^n}{n!} \psi^{(n)}_{\alpha} + o(\epsilon^n)
$$

By linearity, $-\Delta \psi'_\alpha = 0$, $-\Delta \psi''_\alpha = 0$, ...
Optimality Conditions

By Taylor expansion, \( x \in \Gamma \):

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

Therefore \( -\Delta \psi' = 0, \quad \psi' \mid _\Gamma = -\alpha \frac{\partial \psi}{\partial n} \), \( -\Delta \psi'' = 0, \quad \psi'' \mid _\Gamma = -\alpha \frac{\partial \psi'}{\partial n} - \frac{\alpha^2}{2} \frac{\partial^2 \psi}{\partial n^2} \)

For the Wind Tunnel Problem with \( S^\alpha = \{ x + \epsilon \alpha n : \ x \in S \} \)

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

with \( \Delta \psi' = 0, \quad \psi' \mid _S = -\alpha \frac{\partial \psi}{\partial n} \), \( \psi' \mid _\Gamma - S = 0 \)

However if \( J \) is Frechet differentiable there must exists \( \xi \) s.t.

\[
J(S^\alpha) = J(S) + \int_S \xi \alpha + o(\|\alpha\|)
\]

To find \( \xi \) we must use the adjoint trick : let \( p \)

\[
-\Delta p = (\psi^\epsilon - \psi_d) I_D, \quad p \mid _\Gamma = 0
\]

Then \( 2 \int_D (\psi^\epsilon - \psi_d) \psi' = -2 \int_\Omega \psi' \Delta p = -2 \int_\Omega \Delta \psi' p - \int_\Gamma (\frac{\partial p}{\partial n} \psi' - \frac{\partial \psi'}{\partial n} p) \)
Conceptual Algorithm: Gradient Descent in $H^1$

**Corollary** (O.P. 1972)

$$J(S^{\alpha}) = J(S) + 2\int_S \frac{\partial p}{\partial n} \frac{\partial \psi}{\partial n} \alpha + o(\|\alpha\|)$$

1. Compute the flow $\psi^m$ and the adjoint $p^m$ by solving

$$-\Delta \psi^m = 0, \quad \psi^m|_{S^m} = 0, \quad \psi^m|_{\Gamma_d} = \psi_d$$

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

2. Update the shape with the “Sobolev” gradient $\tilde{\alpha}$ with $\tilde{\alpha} = 0$ at both ends and

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

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

The $-\Delta_S$ avoids loss of regularity from $S^m$ to $S^{m+1}$! (B. Mohammadi - O.P.[2001-2009])

Extension to Navier-Stokes straightforward (zoom at Re=50, from Kawahara et al.)
Discretization by Variational Methods

FEM does $H_0^1(\Omega) \approx V_{0h}$. Link inner vertices to boundary vertices

$$\min_{S \in S_{dh}} \left\{ \int_D |\psi - \psi_d|^2 + \epsilon |S|^2 : \int_{\Omega} \nabla \psi \cdot \nabla \hat{\psi} = 0 \ \forall \hat{\psi} \in V_{0h}, \ \psi|_S = 0 \ \psi|_{\partial C} = \psi_d \right\}$$

- Re-derive the optimality conditions for the discretize problem manually or
- By using Automatics Differentiation in reverse mode
- By using complex finite differences
- By discretization of the continuous gradient

Complex FD, $\theta \in (0, 1)$:

$$\text{Re} \frac{f(a + i\delta a) - f(a)}{i\delta a} = \text{Im} \frac{f(a + i\delta a)}{\delta a} = f'(a) - f^{(3)}(a + i\theta \delta a) \frac{\delta a^2}{6}$$

Example with $f(a) = \sin(a)$, $a = 1$. (computed with Maple-14).
E. Polak et al: Gradient method with Armijo rule + mesh refinement & approx. gradients to solve \( \min_z J(z) \) can be shown to converge (B. Mohammadi - O.P.[2001]):

\[
\text{while } h > h_{\text{min}}, \{ \\
\text{while } |\text{grad}_{zN}J^m| > \epsilon h^\gamma, \{ \\
\text{try to find a step size } \rho \text{ with } w = \text{grad}_{zN}J(z^m) \\
\quad - \beta \rho \|w\|^2 < J(z^m - \rho w) - J(z^m) < -\alpha \rho \|w\|^2 \\
\text{if success then } \{ z^{m+1} = z^m - \rho \text{grad}_{zN}J^m; \ m := m + 1; \}
\text{else } N := N + K;\\n\} \\
h := h/2; \ N := N(h);\\n\}\]
Compressible Flows

Euler or Navier-Stokes equations

\[
W = \begin{pmatrix}
\rho \\
\rho u \\
\rho E
\end{pmatrix}
\]

\[
\partial_t W + \nabla \cdot F(W) - \nabla \cdot G(W, \nabla W) = 0, \quad W(0, x) = 0, \quad + \text{B.C.}
\]

Involves an adjoint equation and complex formulae

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

Before & after optimization. Plain vs Sobolev Gradients (A. Jameson)
Fluid Structure Optimization

Falcon jet: $C_D$ decreases from 234 to 216

Discretize the continuous optimality conditions and adjoints: use mesh refinement.
Some Realization (II) Airbus with Automatic Differentiation

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0 \]
\[ \partial_t (\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla (\rho + \frac{2}{3} \rho k) = \nabla \cdot ((\mu + \mu_t) S) \]
\[ \partial_t (\rho E) + \nabla \cdot ((\rho E + p + \frac{5}{3} \rho k) u) = \nabla \cdot ((\mu + \mu_t) Su) + \nabla ((\chi + \chi_t) \nabla T) \]
\[ \partial_t \rho k + \nabla \cdot (\rho u k) - \nabla ((\mu + \mu_t) \nabla k) = S_k \]
\[ \partial_t \rho \epsilon + \nabla \cdot (\rho u \epsilon) - \nabla ((\mu + c_{\epsilon} \mu_t) \nabla \epsilon) = S_{\epsilon}. \]

C++ operator overloading is OK up to 50 unknown else use Tapenade in reverse mode. Compute adjoint and gradients by Automatic Differentiation (Adol-C, Tapenade)

Courtesy of Airbus
Supersonic Business Jets (B. Mohammadi)

- A jet flying at Mach 1.8 over land also ⇒ Requires to optimize for the sonic boom.

\[ J(x) = I(p') + |C_i^0 - C_i| + |C_d^0 - C_d| + |V^0 - V| + \int_S |d - d_0| d\gamma \]

where \( I(p') = a \int_{z=0} |p'| \), where \( C_i, C_d \) are the components of the contribution to the drag coming from regions where the flow hits the plane \( \vec{n}.\vec{u}_\infty < 0 \)

\( V \) is the volume and \( d \) is the thickness and \( \partial_t W + \nabla \cdot F(W) = 0. \)
Mach lines before and after optimization
Validation and Extensions

- Discrete vs Continuous approach in case of shocks
- Robust optimization - Uncertainty Quantification
- Extension to Fluid Structure Systems
- Extension to multi-criteria Optimization
- Parallel Optimization, Parameter Reduction
- Stochastic Optimization
Sensitivity of Functionals of Euler Equations with Shocks

Let \( J = \frac{1}{2} \int_{S \times (0, T)} |B \cdot W - b|^2 \) with \( \partial_t W + \nabla \cdot F(W) = 0 + B.C. \)

for some vector \( B \in \mathbb{R}^4 \) and a scalar \( b \). The extended calculus of variation on \( J \) gives:

\[
\delta J = \int_{S \times (0, T)} (B \cdot \overline{W} - b)B \cdot \delta W \quad \text{with} \quad \overline{W} = \frac{1}{2}(W^+ + W^-)
\]

Turning to \( \delta W \) we know from above that it satisfies

\[
\partial_t \delta W + \nabla \cdot (F'(W)\delta W) = 0, \quad \delta W(0) = 0
\]

The adjoint equation:

\[
\partial_t W^* + F'(W)\nabla W^* = 0, \quad W^*(T) = 0
\]

\[
\Rightarrow \int_{\partial \Omega \times (0, T)} W^* \cdot (n \cdot (F'(W)\delta W)) = 0. \quad \text{So} \quad W^* \cdot (n \cdot (F'(W))) = (BW - b)B^T \Rightarrow
\]

\[
\delta J = - \int_{\partial \Omega \setminus S \times (0, T)} W^* \cdot (n \cdot (F'(W)\delta W))
\]

Optimization of an Airfoil $\Sigma$ with Euler equations

**Proposition:** Let $W^*$ be defined by ($\Sigma$ is the wing, $S$ is the ground, $R$ is outflow bdy)

$$\partial_T W^* + \nabla F(W)^T W^* = 0, \quad W^*(T) = 0, \quad W^* \cdot n|_{\Sigma} = 0, \quad W^*|_R = 0, \quad W^*_3|_S = \overline{p} - p_0$$

Then, asymptotically in time,

$$\delta J = - \int_{\Sigma} (W^*_1 + \vec{u} \cdot \vec{W}_{2,3}^*) \delta \vec{W}_{2,3} \cdot \vec{n} = - \int_{\Sigma} (\rho^* + \vec{u} \cdot (\rho \vec{u}^*)^*) \delta (\rho \vec{u}) \cdot \vec{n}$$

**Lemma**

Consider $\Sigma_{\alpha} = \{ x + \alpha(x)n(x) : x \in \Sigma \}$. Then $\delta W \cdot n|_{\Sigma} = -\alpha \left( \frac{\partial W_n}{\partial n} - \kappa W_t \right)$

where $t$ is the tangent vector, $n$ the normal and $\kappa$ the inverse of radius curvature.

**Algorithm:** Thus by choosing

$$\alpha = -\lambda (\rho^* + \vec{u} \cdot (\rho \vec{u}^*)^*) \left( \frac{\partial (\rho u_n)}{\partial n} - \kappa \rho u_t \right)$$

for a small enough constant scalar $\lambda$, $J$ will decrease because,

$$\delta J = -\lambda \int_{\Sigma} (\rho^* + \vec{u} \cdot (\rho \vec{u}^*)^*)^2 \left( \frac{\partial (\rho u_n)}{\partial n} - \kappa \rho u_t \right)^2 + o(\lambda)$$
Numerical Tests

Figure: NACA0012 airfoil: the adapted mesh (left), the level lines of the density (middle) and the level lines of the adjoint density (right).

The theory on the continuous systems tells that the adjoint is continuous across the shocks but maybe discontinuous elsewhere, including where $W$ has slip-discontinuities.
Numerical Tests: Analytic versus A.D.

Figure: LEFT; comparison between $W_3^*$, the component of the adjoint in duality with $\rho v$ and $p - p_0$ on $S$ for the NACA airfoil. RIGHT: density and adjoint density for a scramjet.
Uncertainty Quantification

The state equations $F$ involve random variables, function of a realization parameter $\omega$. Given $\theta > 0$ consider:

$$\min_{s \in S} \mathbb{E}[J(u, s, \omega)] + \theta \text{var}(J(u, s, \omega)) \mid \text{Euler}(u, x, s, \omega) = 0 \ \forall \omega$$

$$u(s, x, \omega) = \sum_{i=1}^{n} u_i(s, x) \Phi_i(\omega)$$

where $\{\Phi_i(x)\}_{i}^{n}$, are the Wiener orthogonal Polynomial Chaos given by the Karuhen-Loeve theorem and $u_i(s, x)$ are given by a Galerkin formulation of Euler equations on the $\Phi_i$. Using that basis for the SPDE needs computations of nonlocal high dimension integrals (Monte-Carlo/Sparse Grids).

Robust optimization of a wing profile with random Mach input (C. Schillings).
Perspectives

- Other approach to robust optimization: cf. R. Duvigneau
- Uncertainty quantifications: still in the mill for calibration in finance
- OSD is expensive $\Rightarrow$ dedicated software faster and better (Jameson, Lohner)
- Time dependent problems: no longer impossible.

Time dependent adapted mesh (courtesy of F. Alauzet)

Thank you for your attention