Optimal Shape Design: The Algorithmic Point of View

http://www.ann.jussieu.fr/pironneau

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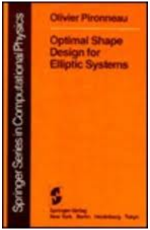
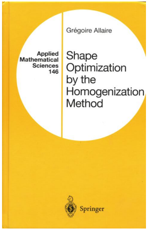
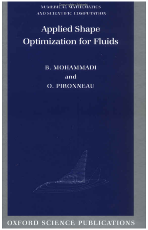
Lectures at MUSAF II

Courtesy of A. Jameson & Airbus.





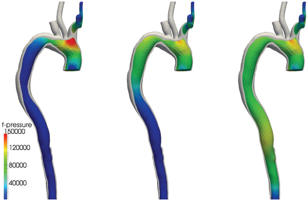


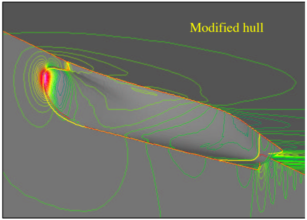
- **O. Pironneau** *Optimal Shape Design for Elliptic Systems.* Springer 1983.
- **G. Allaire**: *Shape Optimization by Homogenization* Springer 2001.
- **B. Mohammadi & O.P.** *Applied Optimal Shape Design*, Oxford U. Press 2000-2009.
- **J. Haslinger, R.A. Makinen** *Intro. to Shape Optimization*. SIAM series 2003.

- **C. Schillings** (UTrier) Optimal Aerodynamic Design under Uncertainties, 2010.
- **Andrea Mazoni**, Reduced Models for Optimal Control, Shape Optimization and Inverse Problems in Haemodynamics, PhD Thesis, EPFL, 2012.

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

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[1] A. MAZONI, (EPFL) Reduced Models for Optimal Control, Shape Optimization and Inverse Problems in Haemodynamics, PhD Thesis, 2012.

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

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

$\Omega_t = \mathcal{A}_t(\Omega_0)$ with $\mathcal{A}_t : x_0 \to x_t := \mathcal{A}_t(x_0)$. Let $u_\tau(x,t) = u(\mathcal{A}_t(\mathcal{A}_\tau^{-1}(x)),t), \quad \forall x \in \Omega_\tau$

Then, in Ω_t at $t=\tau$,

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

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

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

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

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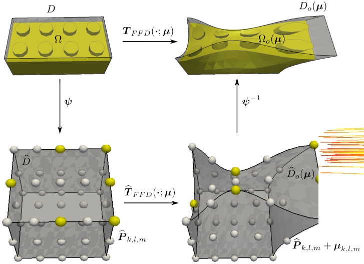
[1] Lassila T, Rozza G: Parametric free-form shape design with PDE models and reduced basis method. Comput. Meth. Appl. Mech. Engr. 2010, 199:1583-1592.

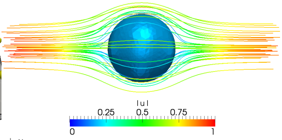
Free-Form Deformations

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

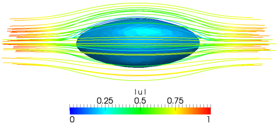
$$\hat{T}(x,\mu) = \sum_{k,l,m} C_k^K C_l^L C_m^M (1-x_1)^{K-k} x_1^k (1-x_2)^{L-l} x_2^l (1-x_3)^{M-m} x_3^m [P_{k,l,m} + \mu_{k,l,m}]$$

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





Flow in the reference shape



Flow in the optimal shape

[1] T.W. Sederberg & S.R. Parry. Free-Form Deformation of Solid Geometric Models. Computer Graphics, vol. 20, no. 4, p151-160,1986.

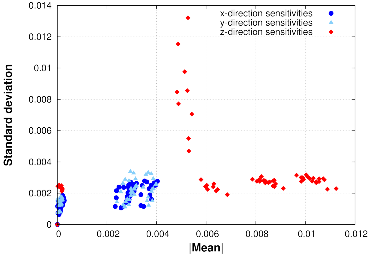
[2] R. Duvigneau, Conception Optimale en Mecanique des Fluides Numérique : Approches Hiérarchiques, Robustes et Isogéométriques; mémoire HdR, 2013

[3] Rozza et al Shape optimization by Free-Form Deformation JOMP 2014.

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:

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



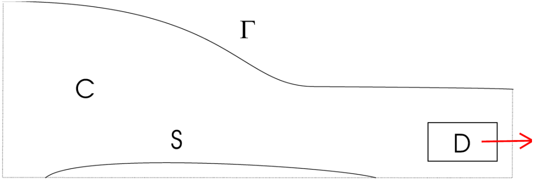
Select the dof with large deviation from (S,E) + uniform distribution (Ballarin et al [2]).
End result is a procedure that works for any shape, but it is expensive!

[1] M.D. Morris. Factorial sampling plans for preliminary computational experiments. Technometrics, 33(2):161-174, 1991.

[2] F. Ballarin, A. Manzoni, G. Rozza, S. SalsaShape optimization by Free-Form Deformation: existence results and numerical solution for Stokes flows. JOMP 2014.

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:

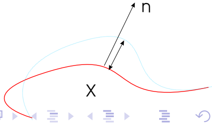
$$\min_{S\in\mathcal{S}_d}\left\{\int_D |\psi-\psi_d|^2+\epsilon|S|^2\ :\ -\Delta\psi=0,\ \text{in } C\backslash\dot{S},\quad \psi|_{\mathbf{S}}=0\ \ \psi|_{\partial C}=\psi_d\right\}$$

Sensitivity Analysis by Local Variations

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

Definition ψ *is n-differentiable in the direction* α *if*

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



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

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

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

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

with $\Delta\psi'_\alpha = 0,\ \ \psi'_\alpha|_S = -\alpha\frac{\partial\psi}{\partial n},\ \ \psi'_\alpha|_{\Gamma-S} = 0$

However if J is Frechet differentiable there must exists ξ s.t.

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

To find ξ we must use the adjoint trick : let p

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

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 (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 ψ^m and the adjoint p^m by solving

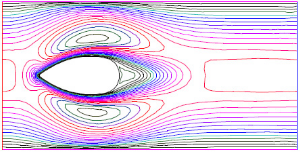
$$-\Delta\psi^m = 0,\quad \psi^m|_{S^m} = 0,\ \psi^m|_{\Gamma_d} = \psi_d$$
$$-\Delta p^m = (\psi^m - \psi_d)I_D,\quad p|_{\Gamma_d \cup S^m} = 0$$

- 2. Update the shape with the "Sobolev" gradient $\tilde\alpha$ with $\tilde\alpha = 0$ at both ends and

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

- 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])



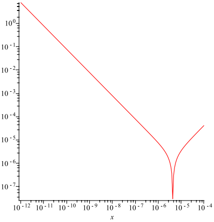
Extension to Navier-Stokes straightforward (zoom at Re=50, from Kawahara et al.)

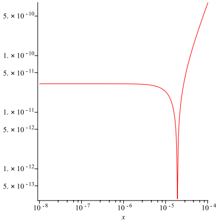
Discretization by Variational Methods

FEM does $H^1_0(\Omega) \approx V_{0h}$. Link inner vertices to boundary vertices

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

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





Complex FD, $\theta \in (0,1)$: $Re\dfrac{f(a+\mathbf{i}\delta a) - f(a)}{\mathbf{i}\delta a} = Im\dfrac{f(a+\mathbf{i}\delta a)}{\delta a} = f'(a) - f^{(3)}(a+\mathbf{i}\theta\delta a)\dfrac{\delta a^2}{6}$

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]):

. while $h > h_{min}$, {

. while $|\operatorname{grad}_{z_N} J^m| > \epsilon h^\gamma$, {

. try to find a step size ρ with $w = \operatorname{grad}_{z_N} J(z^m)$

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

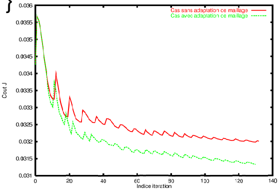
. if success then $\{z^{m+1} = z^m - \rho \operatorname{grad}_{z_N} J^m; \quad m := m+1;\}$

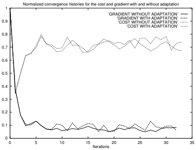
. else $N := N + K$;

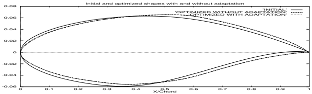
. }

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

. }







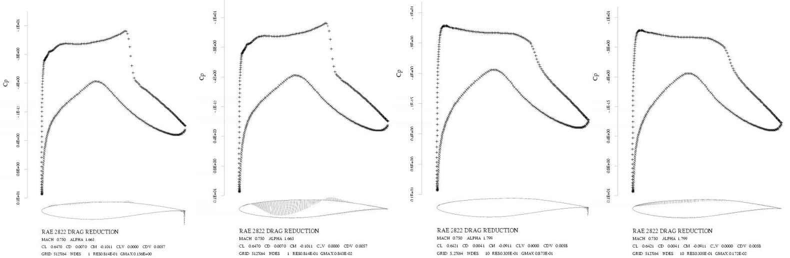
Compressible Flows

Euler or Navier-Stokes equations

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

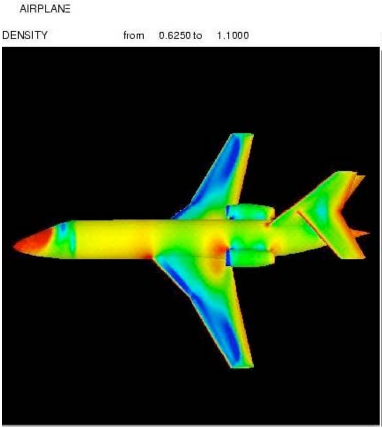
Involves an adjoint equation and complex formulae

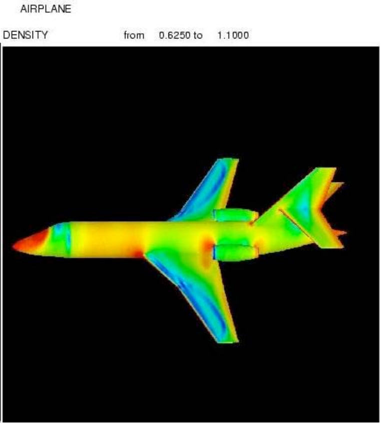
$$\partial_t P + (F'(W) - G'_{,1}(W, \nabla W))^T \nabla P - \nabla \cdot (G'_{,2}(W, \nabla W)^T \nabla P) = 0$$



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

Some Realizations (I) - 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

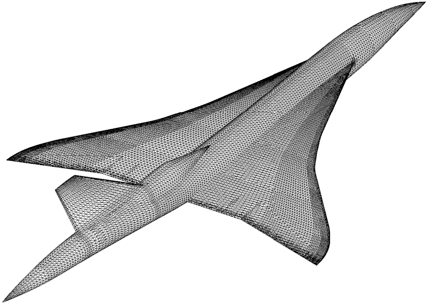
$$
\begin{aligned}
&\partial_t \rho + \nabla \cdot (\rho u) = 0 \\
&\partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla(p + \frac{2}{3}\rho k) = \nabla \cdot ((\mu + \mu_t) S) \\
&\partial_t(\rho E) + \nabla \cdot ((\rho E + p + \frac{5}{3}\rho k) u) = \nabla \cdot ((\mu + \mu_t) S u) + \nabla((\chi + \chi_t)\nabla T) \\
&\partial_t \rho k + \nabla.(\rho u k) - \nabla((\mu + \mu_t)\nabla k) = S_k \\
&\partial_t \rho \varepsilon + \nabla.(\rho u \varepsilon) - \nabla((\mu + c_\varepsilon \mu_t)\nabla \varepsilon) = S_\varepsilon .
\end{aligned}
$$

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)

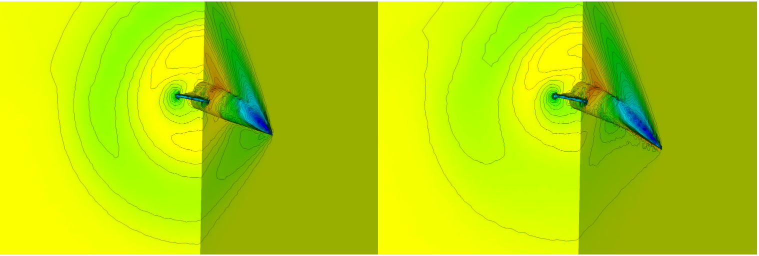
- A jet flying at Mach 1.8 over land also ⇒ Requires to optimize for the sonic boom.



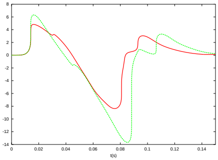
$$J(x) = I(p') + |C_l^0 - C_l| + |C_d^0 - C_d| + |V^0 - V| + \int_S |d - d_0| d\gamma$$

where $I(p') = a \int_{z=0} |p'|$, where C_l, 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 $\partial_t W + \nabla \cdot F(W) = 0$.

Results



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

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

for some vector $B \in R^4$ and a scalar b. The extended calculus of variation on J gives :

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

Turning to δW we know from above that it satisfies

$$\partial_t\delta W + \nabla\cdot(\overline{F'(W)}\delta W) = 0,\ \delta W(0) = 0$$

The adjoint equation :

$$\partial_t W^* + \overline{F'(W)}\nabla W^* = 0\,,\, W^*(T) = 0$$

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

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

F. ALAUZET & O. P. Continuous & discrete adjoints to Euler eq. Int. J. Num. Methods in Fluids 2012-70:135-157

Optimization of an Airfoil Σ with Euler equations

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

$$\partial_T W^* + \overline{F'(W)}^T \nabla W^* = 0,\ W^*(T) = 0,\ W^* \cdot n|_\Sigma = 0,\ W^*|_R = 0,\ W_3^*|_S = \overline{p - p_0}$$

Then, asymptotically in time,

$$\delta J = -\int_\Sigma (W_1^* + \vec{\bar{u}} \cdot \vec{W}_{2,3}^*)\delta \vec{W}_{2,3} \cdot \vec{n} = -\int_\Sigma (\rho^* + \vec{\bar{u}} \cdot (\rho\vec{u})^*)\delta(\rho\vec{u}) \cdot \vec{n}$$

Lemma

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

where t is the tangent vector, n the normal and κ the inverse of radius curvature.

Algorithm: Thus by choosing

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

for a small enough constant scalar λ, J will decrease because,

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

Numerical Tests

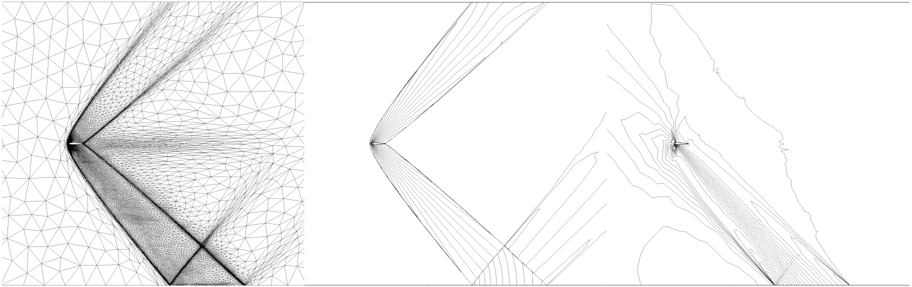
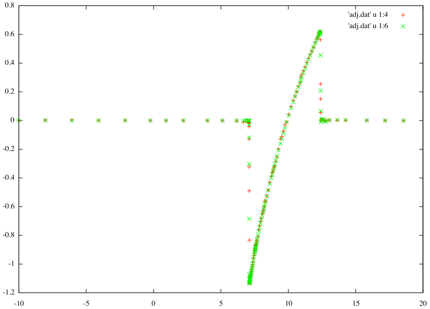


Figure: NACA0012 airfoil: the adapted mesh (left), the level lines of the density (middle) and the level lines of the adjoint density (right).

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.



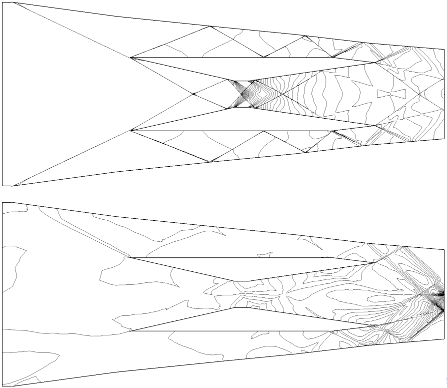


Figure: LEFT; comparison between W_3^*, the component of the adjoint in duality with ρv and $p - p_0$ on S for the NACA airfoil. RIGHT: density and adjoint density for a scramjet.

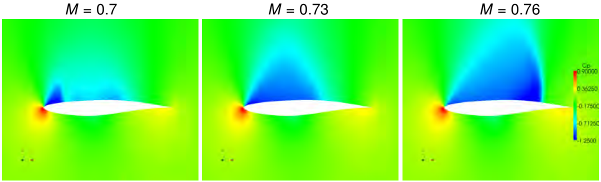
Uncertainty Quantification

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

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

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

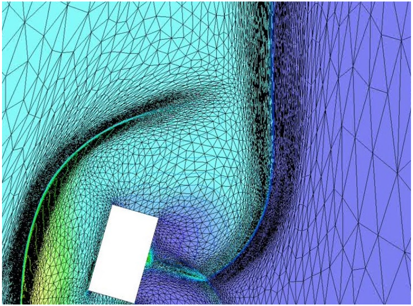
where $\{\Phi_i(x)\}_i^n$, are the Wiener orthogonal Polynomial Chaos given by the Karuhen-Loeve theorem and $u_i(s,x)$ are given by a Galerkin formulation of Euler equations on the Φ_i. Using that basis for the SPDE needs computations of nonlocal high dimension integrals (Monte-Carlo/Sparse Grids).



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

Perspectives

- Other approach to robust optimization: cf. R. Duvigneau
- Pareto front by gradient methods: cf. J-A. Desideri
- Uncertainty quantifications: still in the mill for calibration in finance
- OSD is expensive $\Rightarrow$ dedicated software fasterand better (Jameson, Lohner)
- Time dependent problems: no longer impossible.



Time dependent adapted mesh (courtesy of F. Alauzet)

Thank you for your attention