SIMUMAT

DOMINÓ Project
AIRBUS-E / INTA / UAM / UPM

# Reunión Proyecto MATHEMATICA (Plataforma COMPUTING)

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# Diseño optimo aeronáutico

- C. Lozano, F. Monge y F. Palacios del INTA, C. Castro de la UPM y E. Zuazua de la UAM
- Descripción del Problema
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# Descripción del Problema y Dificultades



**Descripción del problema**: Diseño óptimo de aeronaves, en las cuales el aire se modeliza mediante las ecuaciones de Euler, Navier-Stokes o RANS.

**Métodos utilizados:** El método de optimización se realiza principalmente mediante técnicas de gradiente clásicas basadas en el cálculo de las ecuaciones adjuntas para la evaluación de los gradientes de funcionales de interés aeronáutico. A su vez, también se incorporan otras técnicas más sofisticadas, como el uso de level sets.

**Dificultades:**

a) Cálculo de gradientes en presencia de singularidades (choques).

b) Estudio de la adaptabilidad de la malla a cada nueva geometría

c) Estudio de la sensibilidad de la malla al cálculo de las soluciones

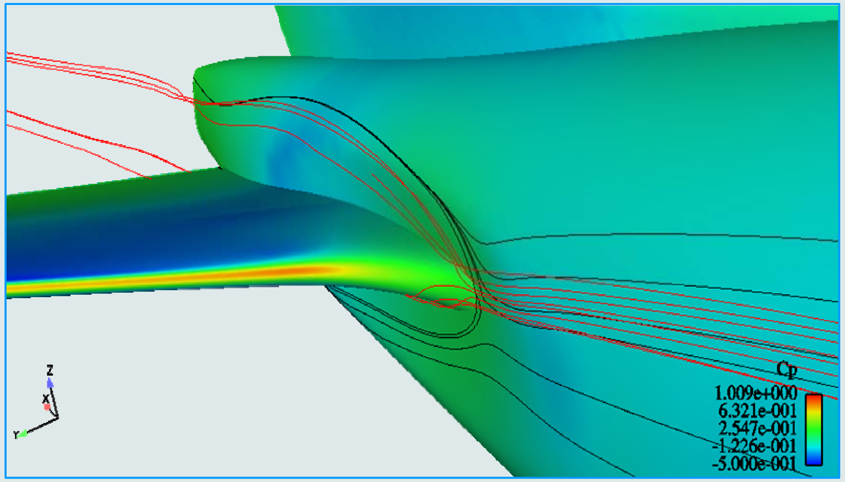
d) Falta de diferenciabilidad de los esquemas numéricos

e) Optimización del conjunto de variables de diseño para mejorar la eficacia.

f) Implementación de métodos de optimización multi-objetivo

g) Desarrollo de algoritmos numéricos robustos en condiciones reales de interés ingenieril.

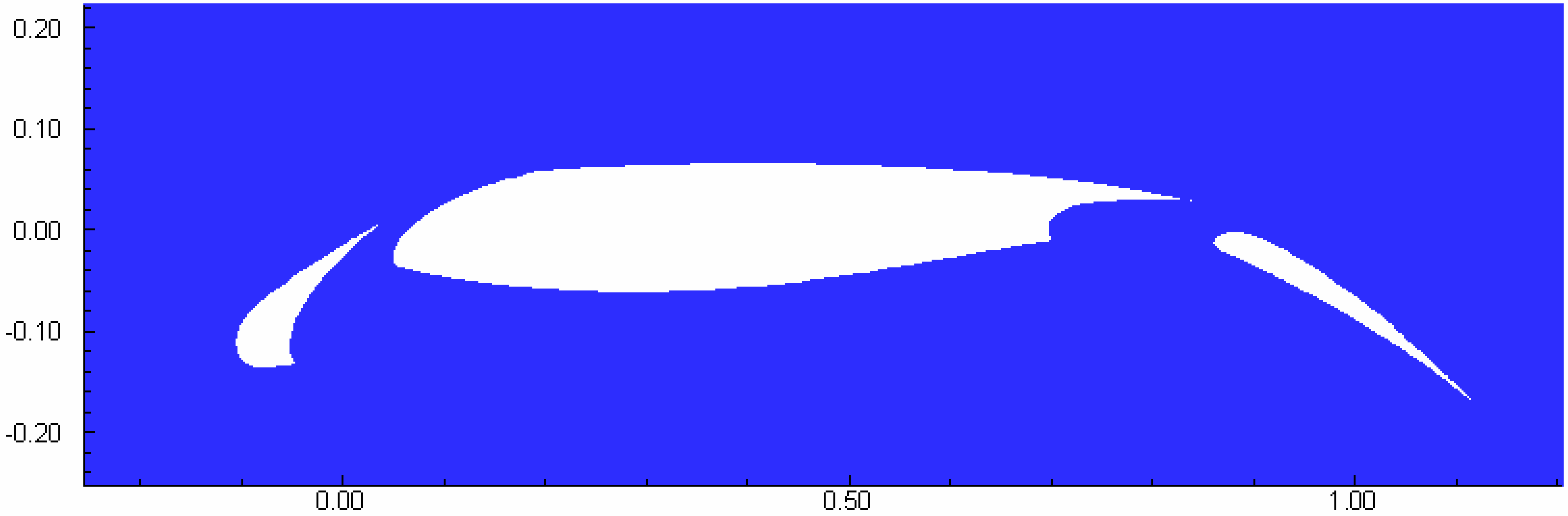
## Optimization is the goal of all practical design projects




The **decision-making process** is usually a **mixture of analysis, experiments, and intuition**.

When the variables in a problem become numerous, experiments are expensive, intuition breaks down, and **a systematic approach is necessary**.

Using the **modern theory of optimization**, one can often **model the relationships between the variables mathematically** and the, taking advantage of rapid computer, **seek the optimal solution of the model problem** numerically.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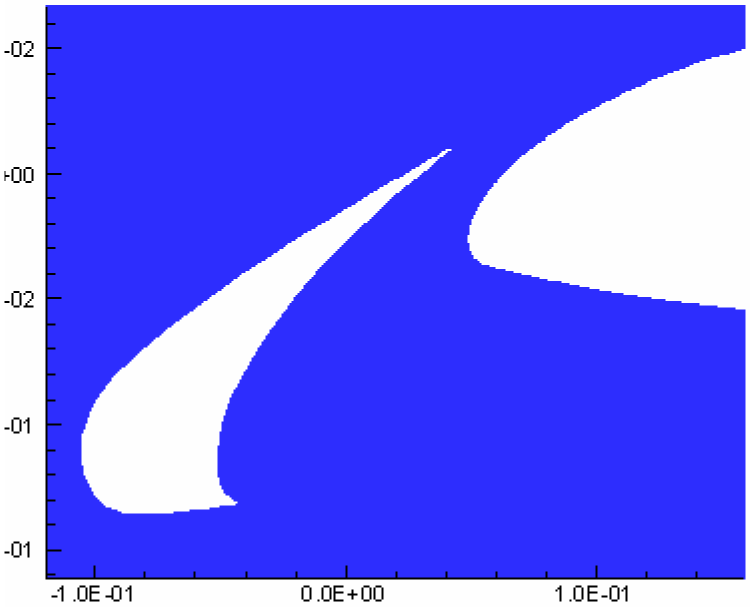
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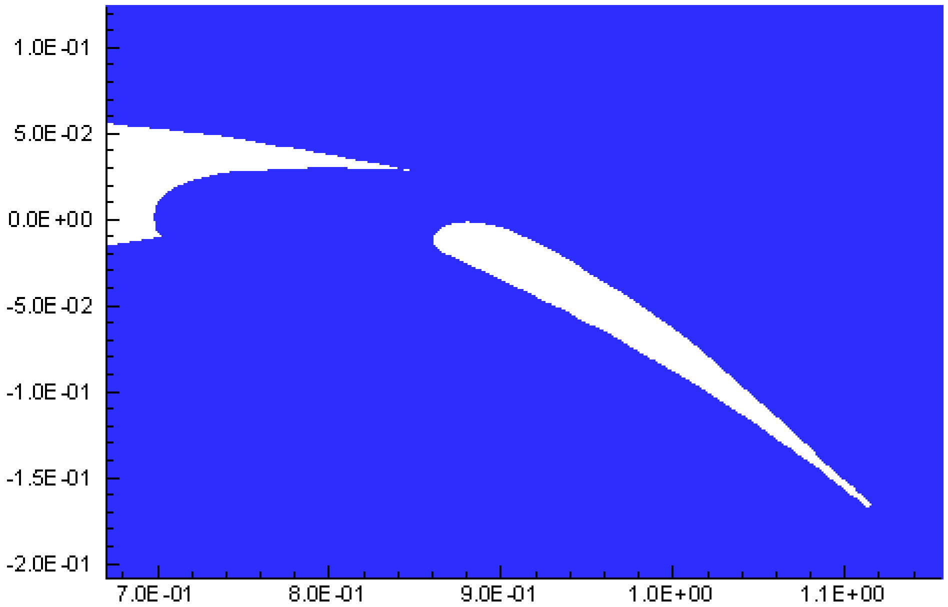
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-1.5E-01
-2.0E-01
7.0E-01
8.0E-01
9.0E-01
1.0E+00
1.1E+00

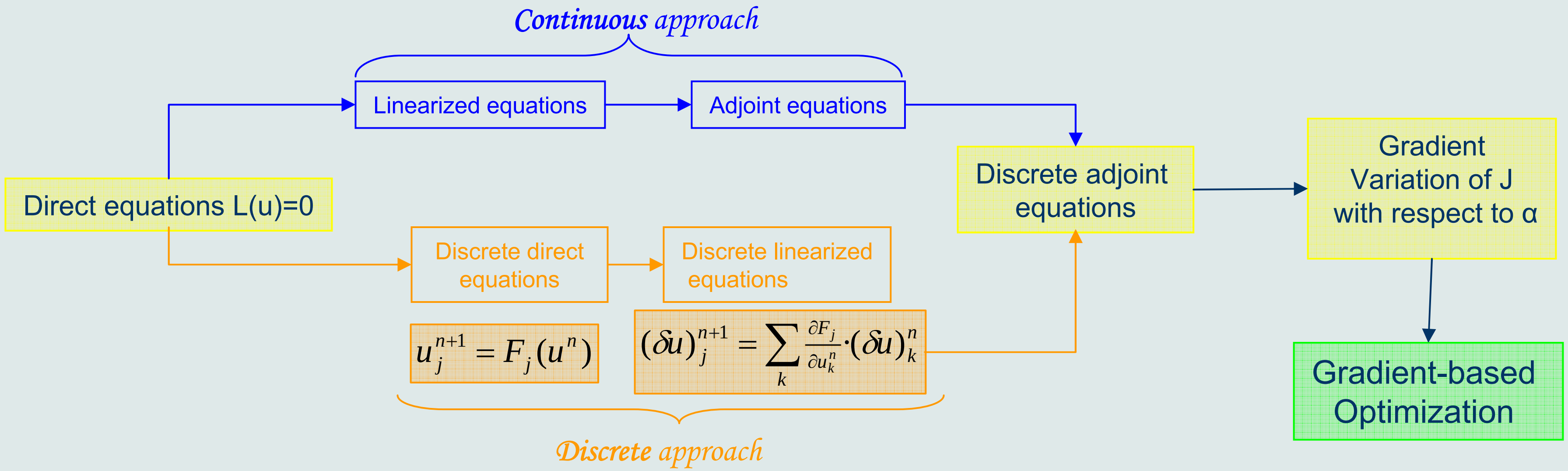
- The Adjoint Methodology is, presently, the only way to tackle design problems with a **great number of design variables**.
- The adjoint methods provide **Surface Functional Derivatives**.
- Finding new revolutionary airplane shapes requires the **combination of parametric and not parametric design.**


**Using a Gradient Based Method?**

**Maybe yes!**

## Adjoint Methodology

Given a field governed by a system of PDEs, the **Continuous and Discrete Adjoint Methods provide a efficient way to compute the gradient of a functional** which depends on the solution of the system for a set of design variables.




## Ideal Case: Regular Flow Solution Solved with a Differentiable Numerical Scheme

In simple problems such as Burgers' equation with control on the initial data, **it is possible to prove that the minima of the discrete functional converge to the minima of the continuous** one as the mesh-size tends to zero.

The **adjoint equations are linear equations**, so they can be solved by techniques which are easier than those used for the direct problem which is non-linear.

Classical aeronautical applications of optimal shape design in systems governed by PDEs consider a fluid domain Ω (usually air) delimited by a "far field" *Γ* and several solid wall boundaries *S*.

$$J(S^{\min}) = \min_{S \in \mathcal{S}_{ad}} J(S),$$

This kind of design problems is aimed at minimizing a functional *J* of the flow variables *U*

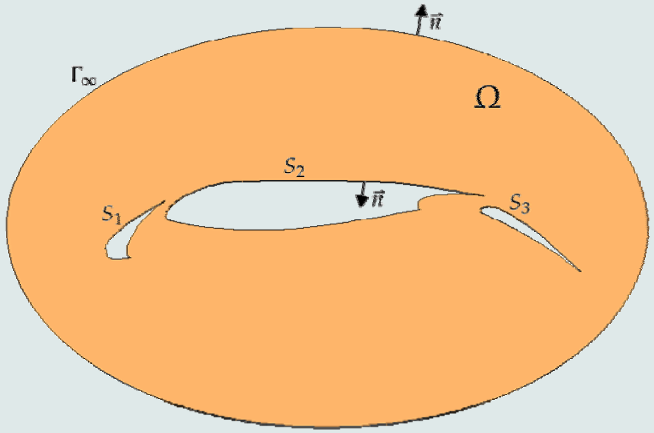
$$J(U) = \int_S j(U)\, ds,$$

In the continuous framework, assuming a regular flow solution *U*, the variation of the functional *J* can be evaluated as:

$$\delta J(U) = \int_{\delta S} j(U)\, ds + \int_S j'(U)\, \delta U\, ds,$$

where the first term comes from the boundary deformation and the second one corresponds to (infinitesimal) changes in the flow solution.

$$\int_{\delta S} j(U)\, ds = \int_S (\partial_n j - \kappa j) \delta S\, ds.$$




When the gradient of the objective function is known, classical line-search methods are used for finding a search direction. once such direction is found, the step length is multiplied by the search direction to advance the optimization to the following iteration.

$$f(x+\alpha p) = f(x) + \alpha p^T \vec{\nabla} f$$

The simplest optimization algorithm is obtained by fixing $p = -\vec{\nabla} f.$

The vector *x* is updated through the following expression:

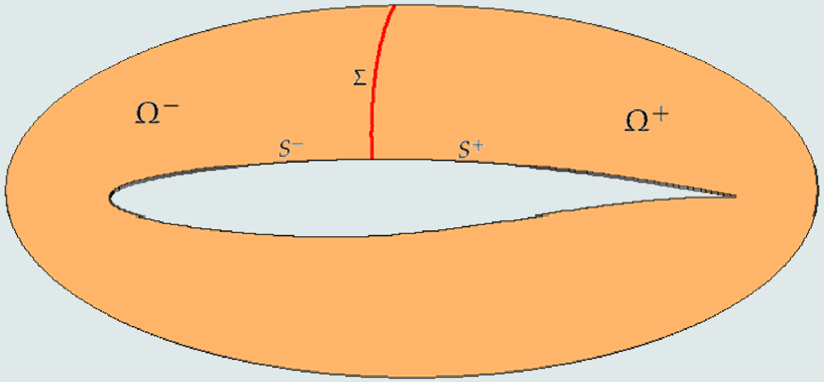
$$x^{n+1} = x^n - \alpha \vec{\nabla} f.$$

## Supposing Non-Regular Solutions of the Flow Variables (sonic shock wave)

A **discontinuity must be considered along a regular curve Σ** (a surface in three-dimensional problems). The curve Σ divides the fluid domain in two subdomains Ω- and Ω+ (to the left and right of Σ, respectively).

When taking flow discontinuities into account the **classical computation of the derivative** of the functional **fails** and has to be modified by **including the effect due to the sensitivity of the shock** location with respect to shape deformations.

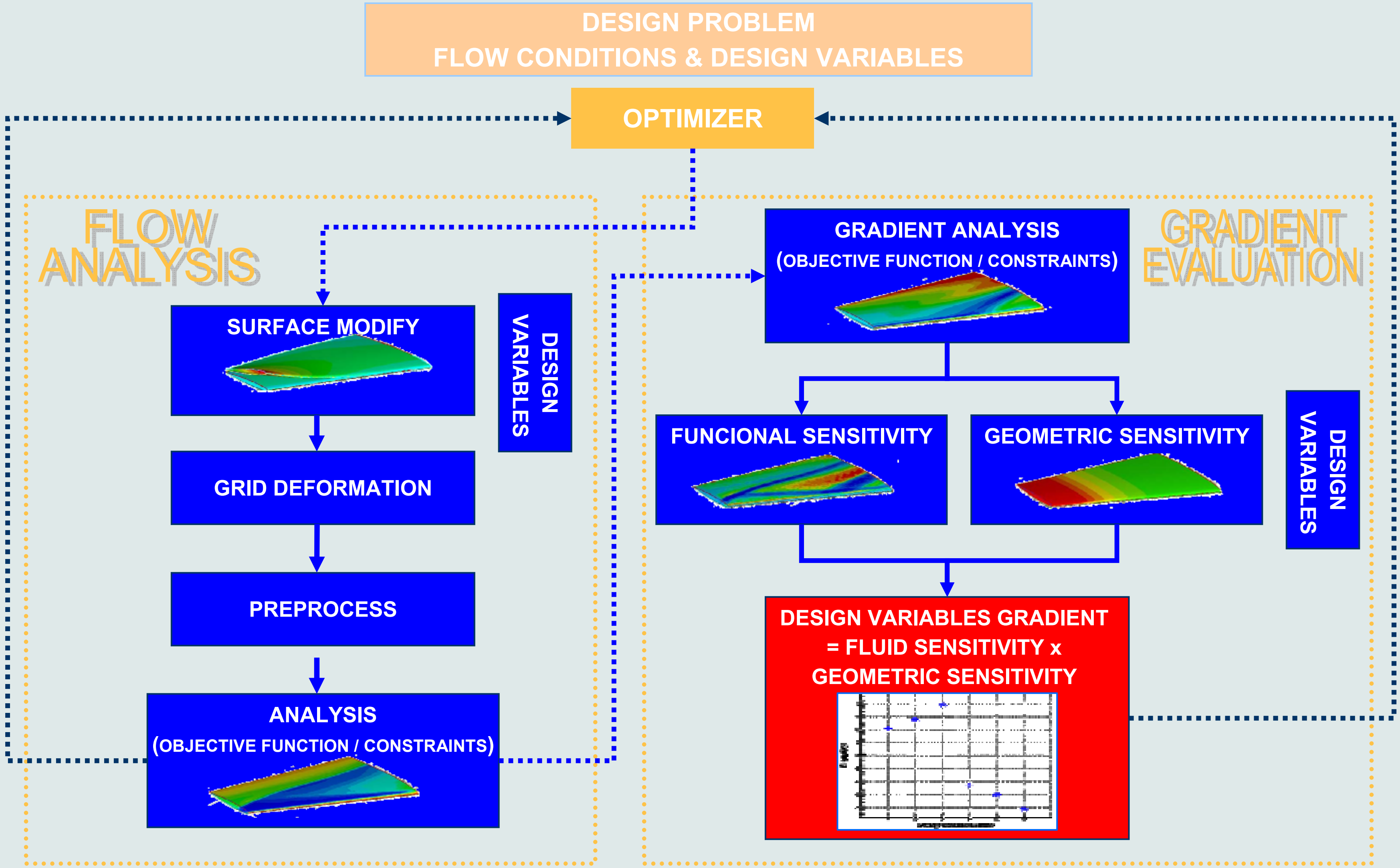
The expression for the functional variation must include a **new term due to the variation of the position of the discontinuity**.




$$\delta J = \int_{\delta S} j(U)\, ds + \int_{S^- \cup S^+} j'(U)\, \delta U\, ds + [j(U)]_\Sigma \delta\Sigma,$$

where the first term represents the contribution of a **boundary shape variation**, the second reflects the effect of a **change in the flow variables** and the last one gives the influence of a **variation in the position of the discontinuity** on the sensitivity calculation.

# GLOBAL OPTIMIZATION PROCESS



Ideal fluids are governed by the Euler equations.

$$\begin{cases} \partial_t U + \vec{\nabla} \cdot \vec{F} = 0, \\ \vec{v} \cdot \vec{n}]_S = 0, \end{cases}$$

where, at the "far field" boundary, boundary conditions are specified for incoming waves, while outgoing waves are determined by the solution inside the fluid domain.

$$U^T = (\rho, \rho u, \rho v, \rho E)$$

$$F_X = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uH \end{pmatrix}, \quad F_Y = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho vH \end{pmatrix},$$

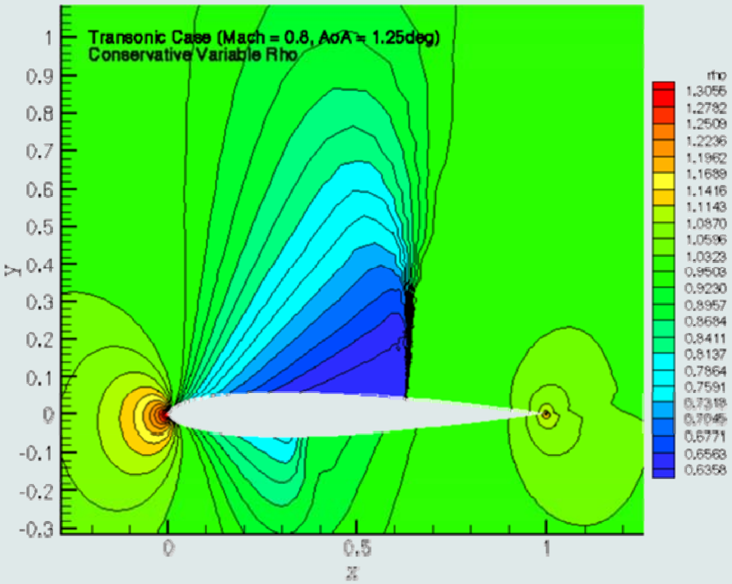
The system of equations must be completed by a state equation which defines the thermodynamic properties of the fluid. For a perfect gas:

$$P = (\gamma - 1)\rho \left[ E - \frac{1}{2}(u^2 + v^2) \right], \quad H = E + \frac{P}{\rho},$$

**Inviscid flows can develop discontinuities**.

The **Rankine.Hugoniot conditions**, for a discontinuity along a curve Σ moving with speed *s* with respect to the fluid, relate the flow variables on both sides of the discontinuity

$$\left[ \vec{F} \cdot \vec{n}_\Sigma \right]_\Sigma - s[U]_\Sigma = 0,$$



Let's introduce the notation

$$\begin{cases} \vec{n}_S \text{ and } \vec{n}_\Gamma \text{ are the inward-pointing unitary normal vector to } S \text{ and } \Gamma \text{ (respectively)}, \\ \vec{n}_\Sigma \text{ is the unitary normal in the shock speed direction}, \\ \vec{t}_S,\ \vec{t}_\Gamma \text{ and } \vec{t}_\Sigma \text{ are the 90 degree counter-clock-wise rotation of } \vec{n}_S,\ \vec{n}_\Gamma \text{ and } \vec{n}_\Sigma \text{ (respectively)}, \\ \partial_n = \vec{n}\cdot\vec{\nabla} \text{ is the normal derivative}, \\ \partial_s = \vec{t}\cdot\vec{\nabla} \text{ is the tangential derivative}. \end{cases}$$

Assuming a flow discontinuity located along a curve Σ that meets the boundary S at a point x=x_b, the variation of the functional δJ is written as

$$\delta J = \int_{\delta S} j(U)\,ds + \int_{S-\cup x_b} j'(U)\delta U\,ds - [j(U)]_{x_b}\,\delta\Sigma - [j(U)]_{x_b}\,(\vec{n}_S\cdot\vec{n}_\Sigma)\,\delta S,$$

And the flow variation solves the linearized equations

$$\begin{cases} \vec{\nabla}\cdot\left(\frac{\partial \vec{F}}{\partial U}\delta U\right) = 0, & \text{in } \Omega, \\ \delta\vec{v}\cdot\vec{n}_S = -\delta S\,\partial_n\vec{v}\cdot\vec{n}_S + \partial_s\delta S\,\vec{v}\cdot\vec{t}_S & \text{on } S, \\ (\delta W)_+ = 0, & \text{on } \Gamma_\infty, \end{cases}$$

The variation of S is the input of the design problem $S' = \{\vec{x} + \delta S(\vec{x})\vec{n}_S(\vec{x}),\ \vec{x}\in S\}$,

Using the linearized Rankine-Hugoniot condition on Σ $\left[\frac{\partial \vec{F}}{\partial U}(\delta\Sigma\,\partial_n U + \delta U)\right]_\Sigma\cdot\vec{n}_\Sigma + \left[\vec{F}\right]_\Sigma\cdot\delta\vec{n}_\Sigma,$

where the variation of Σ parametrizes infinitesimal normal deformations of the discontinuity due to a change in S, so the variation of Σ is not a design parameter, but rather its value being fixed by the linearized Euler equations and the linearized Rankine-Hugoniot conditions, and also depends on S.

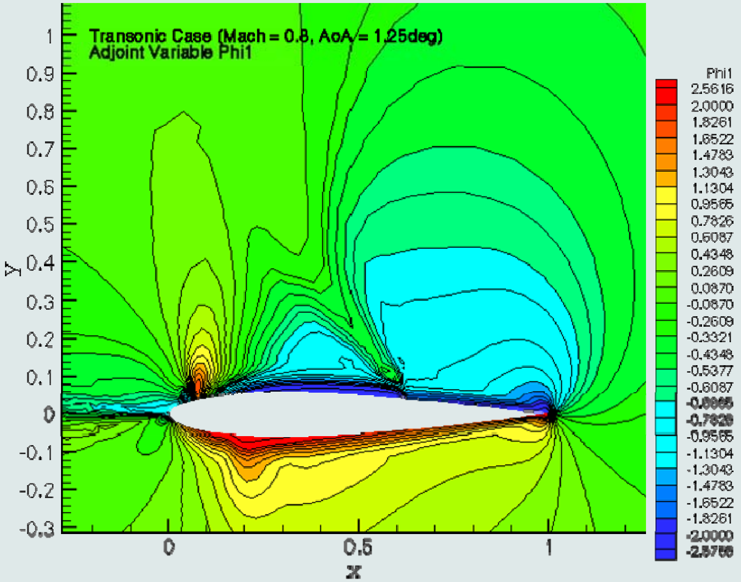
$$\Sigma' = \{\vec{x} + \delta\Sigma(\vec{x},\delta U,\delta S)\vec{n}_\Sigma(\vec{x}),\ \vec{x}\in\Sigma\},$$

Finally, it is possible to compute the variation of the functional J as:

$$\delta J = \int_{\delta S} j(U)\,dl - \int_{S^- \cup S^+} (\vec{n}_S \cdot \delta\vec{v})(\rho\,\psi_1 + \rho\vec{v}\cdot\vec{\varphi} + \rho H \psi_4)\,dl - [j(U)]_{x_b}(\vec{n}_S \cdot \vec{n}_\Sigma)\,\delta S(x_b),$$

where the adjoint variables are obtained from the solution of the adjoint Euler equations plus the adjoint Rankine-Hugoniot conditions, along with the following boundary conditions

$$\begin{cases} \left(\frac{\partial \vec{F}}{\partial U}\right)^T \cdot \vec{\nabla}\Psi = 0, & \text{in } Q^- \cup Q^+, \\ [\Psi]_\Sigma = 0, & \text{on } \Sigma, \\ ([\rho\vec{v}]_\Sigma \cdot \vec{t}_\Sigma)(\partial_{tg}\Psi_1 + H\partial_{tg}\Psi_4) & \\ +[\rho(\vec{v})^2 + 2P]_\Sigma \vec{t}_\Sigma \cdot \partial_{tg}\vec{\varphi} = 0, & \text{on } \Sigma, \\ \Psi\left(\vec{n}_{\Gamma_\infty} \cdot \frac{\partial \vec{F}}{\partial U}\right)\delta U = 0, & \text{on } \Gamma_\infty, \\ \vec{\varphi} \cdot \vec{n}_S = j'(P), & \text{on } S, \\ \Psi^T(x_b)\left[\vec{F} \cdot \vec{t}_\Sigma\right]_{x_b} = [j(P)]_{x_b} & \text{at } x_b, \\ \Psi^T(x_b)\left[\vec{F} \cdot \vec{t}_\Sigma\right]_{x_\infty} = 0, & \text{at } x_\infty. \end{cases}$$



# Navier-Stokes solution

The Navier-Stokes equations provide a complete description of viscous fluids. The complete system of Navier-Stokes equations (without source terms and assuming adiabatic boundary conditions on the solid walls) can be written in the following conservative form:

$$\begin{cases} \partial_t U + \vec{\nabla}\cdot\left(\vec{F} + \vec{F}^v\right) = 0, \\ \vec{v}|_S = 0, \\ \partial_n T|_S = 0, \end{cases}$$

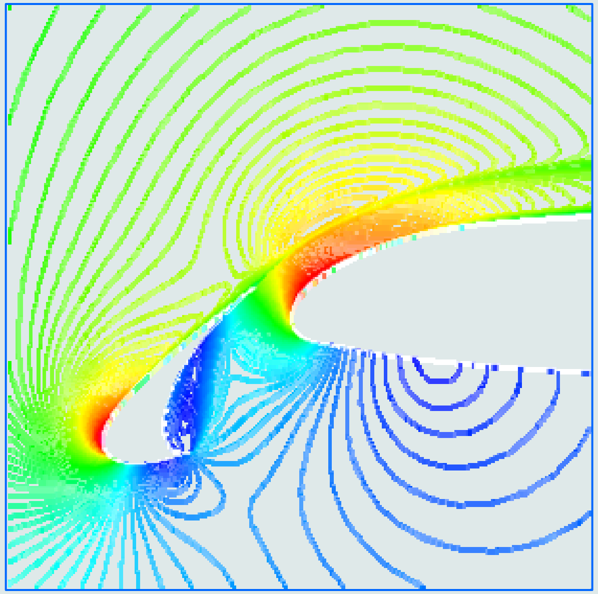
where, at the “far field” boundary, boundary conditions are specified for incoming waves, while outgoing waves are determined by the solution.

$$F_x^v = \begin{pmatrix} 0 \\ \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{xx}u + \sigma_{xy}v + k\partial_x T \end{pmatrix}, \quad F_y^v = \begin{pmatrix} 0 \\ \sigma_{yx} \\ \sigma_{yy} \\ \sigma_{yx}u + \sigma_{yy}v + k\partial_y T \end{pmatrix},$$

and

$$\sigma_{ij} = \mu\left(\partial_i v_j + \partial_j v_i\right) - (2/3)\mu(\vec{\nabla}\cdot\vec{v})\delta_{ij}$$

is the shear stress tensor, the dynamic viscosity and the thermal conductivity *k* being obtained from empirical relations.



Introducing the notation

$$\frac{\partial \vec{F}}{\partial U} = \vec{A}, \quad \frac{\partial \vec{F}^v}{\partial U} = \vec{A}^v, \quad \frac{\partial F_x^v}{\partial\left(\frac{\partial U}{\partial x}\right)} = D_{xx}, \quad \frac{\partial F_x^v}{\partial\left(\frac{\partial U}{\partial y}\right)} = D_{xy}, \quad \frac{\partial F_y^v}{\partial\left(\frac{\partial U}{\partial x}\right)} = D_{yx}, \quad \frac{\partial F_y^v}{\partial\left(\frac{\partial U}{\partial y}\right)} = D_{yy}.$$

The adjoint equation is

$$-\left(\vec{A}-\vec{A}^v\right)^T \cdot \vec{\nabla}\Psi + \vec{\nabla}\cdot\left(\begin{pmatrix} D_{xx}^T & D_{xy}^T \\ D_{yx}^T & D_{yy}^T \end{pmatrix}\cdot\begin{pmatrix} \partial_x\Psi \\ \partial_y\Psi \end{pmatrix}\right) = 0$$

No-slip (zero velocity) and adiabatic wall boundary conditions have been assumed on S.

From the above expression it is possible to determine which objective functions are permissible for the computation of $j = j(\vec{f},T)$ gradients with the adjoint method. $\vec{f} = P\vec{n}_S - \vec{n}_S\cdot\sigma,$ is an allowed functional, where ,

$$\Psi_2 = \frac{\partial j}{\partial f_x}, \quad \Psi_3 = \frac{\partial j}{\partial f_y}, \quad k\partial_n\Psi_4 = \frac{\partial j}{\partial T}.$$

which requires the following boundary conditions on the solid wall:

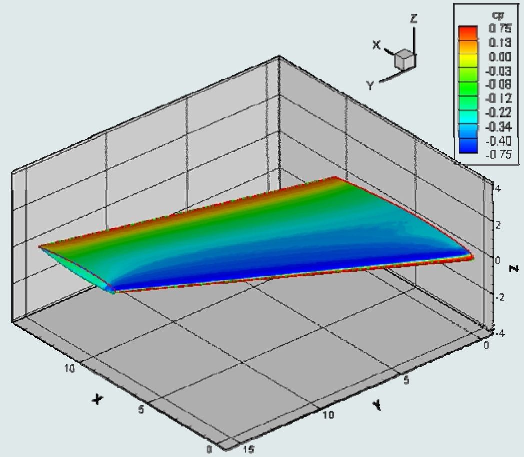
$$\delta J = \delta\int_S j\left(\vec{f},T\right)dS = \int_{\delta S} j\left(\vec{f},T\right)ds - I_{eq},$$

The corresponding variation of the functional is:

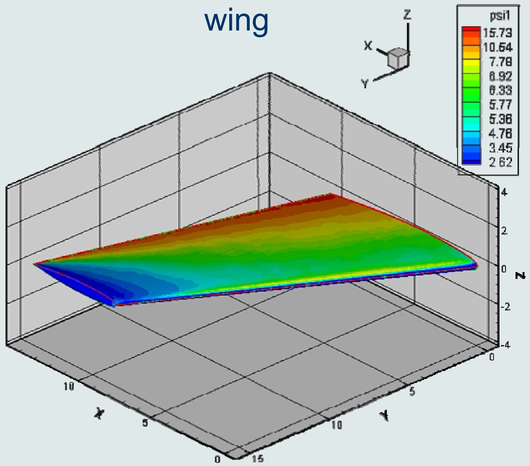
where

$$\begin{cases} I_{eq} = \int_S \vec{n}_S\cdot\delta\vec{v}\,(\rho\,\psi_1 + \rho H\,\psi_4) - \psi_4\vec{n}_S\cdot\sigma\cdot\delta\vec{v} + \vec{n}_S\cdot\Sigma\cdot\delta\vec{v}\,ds \\ \quad - \int_S k\,\psi_4\,\partial_n(\delta T)\,ds, \\ \delta u|_S = -\delta S\,\partial_n u, \\ \delta v|_S = -\delta S\,\partial_n v, \\ \vec{n}_S\cdot\vec{\nabla}\delta T|_S = -\delta S\,\partial_n\left(\vec{\nabla}T\right)\cdot\vec{n} + (\partial_\xi\delta S)\left(\vec{\nabla}T\right)\cdot\vec{t}_S. \end{cases}$$

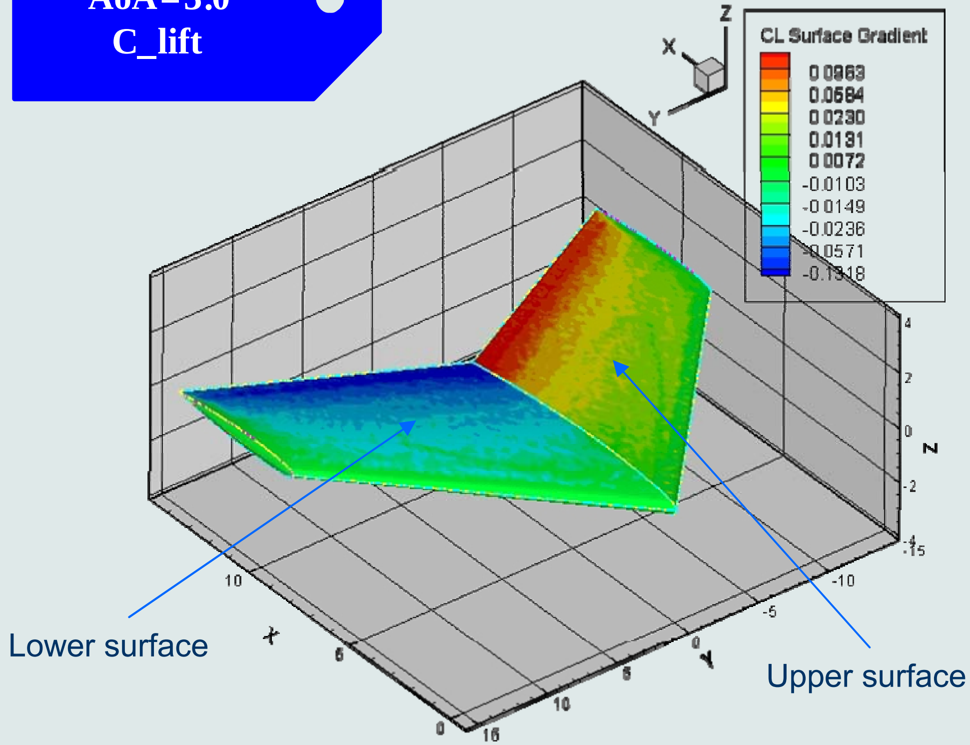
**Mach=0.5**
**AoA=3.0 º**
**C_lift**




Cp distribution around an ONERA M6 wing

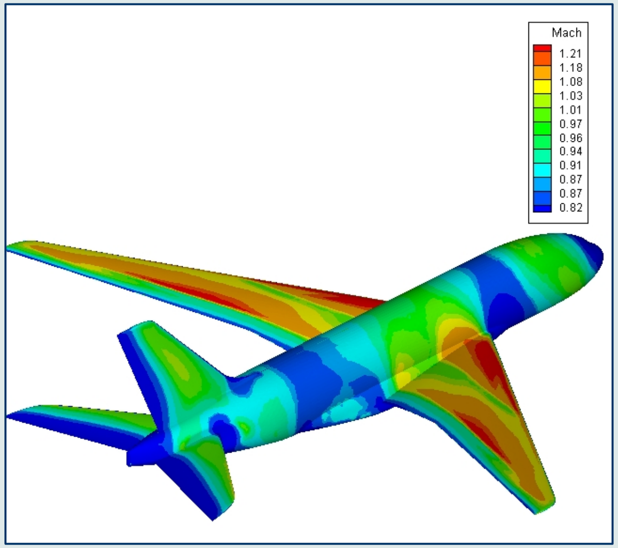



First adjoint variable distribution around an ONERA M6 wing

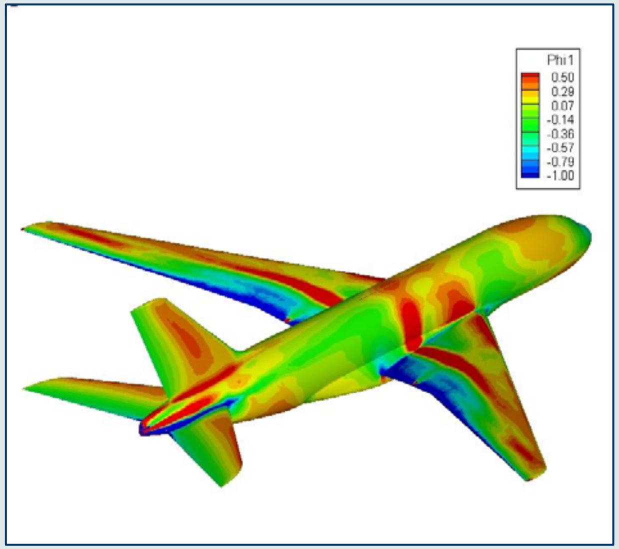



$C_L$ Surface gradient distribution around an ONERA M6

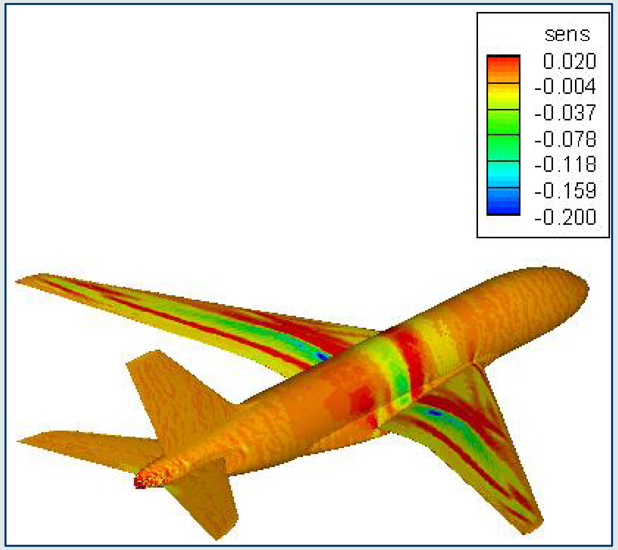
REMFI Euler computation, AoA =0.0º, Mach 0.85



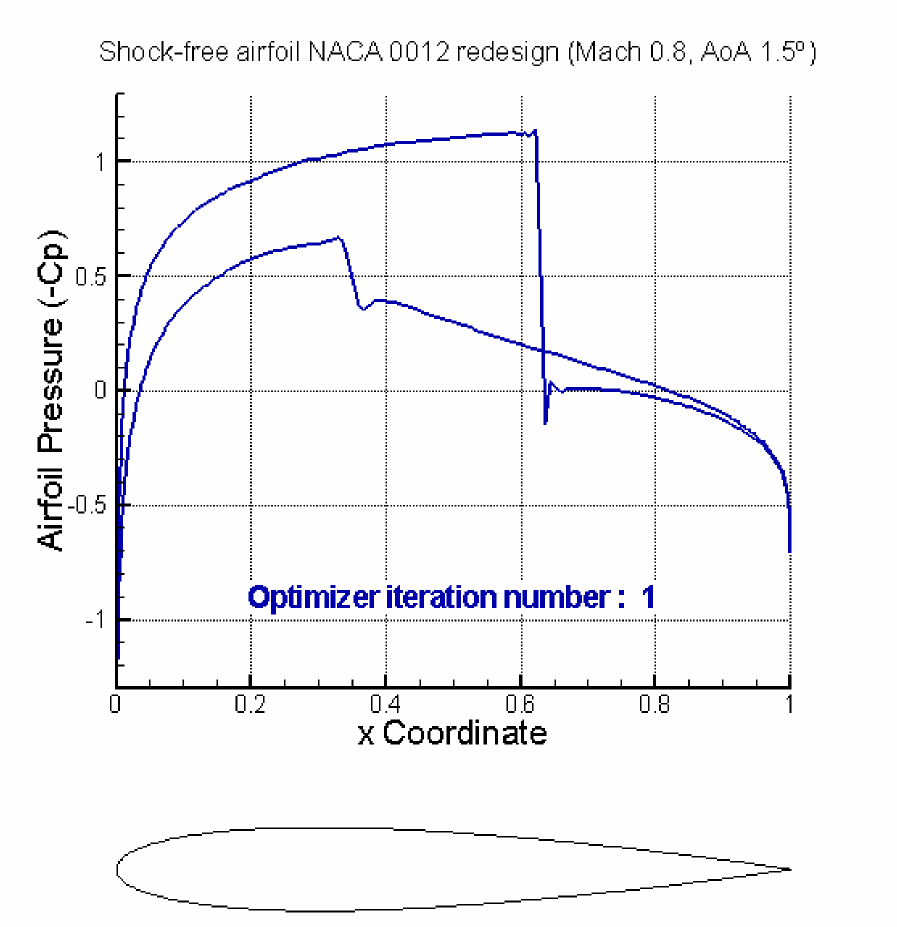

**Mach distribution**



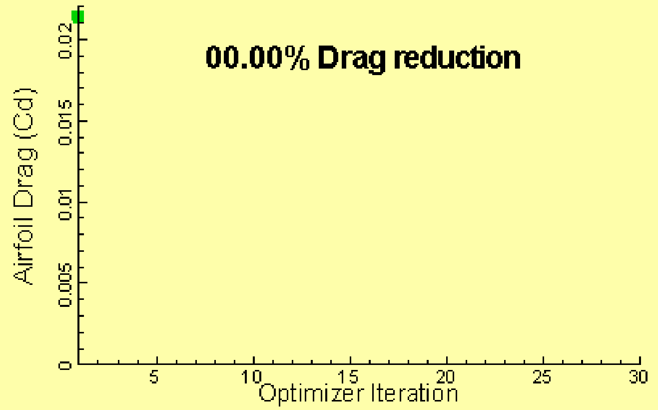

**First adjoint variable distribution**



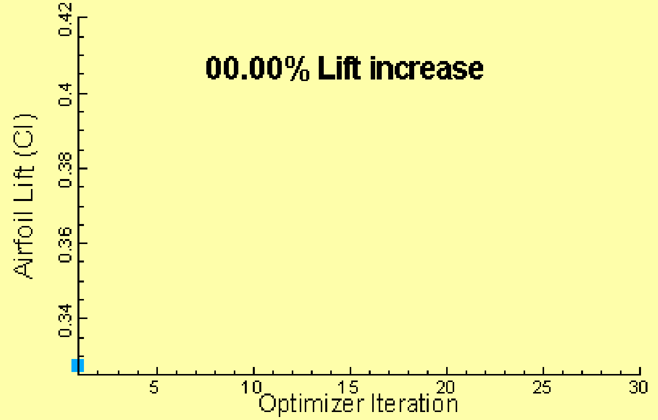

**$C_D$ Surface gradient distribution**



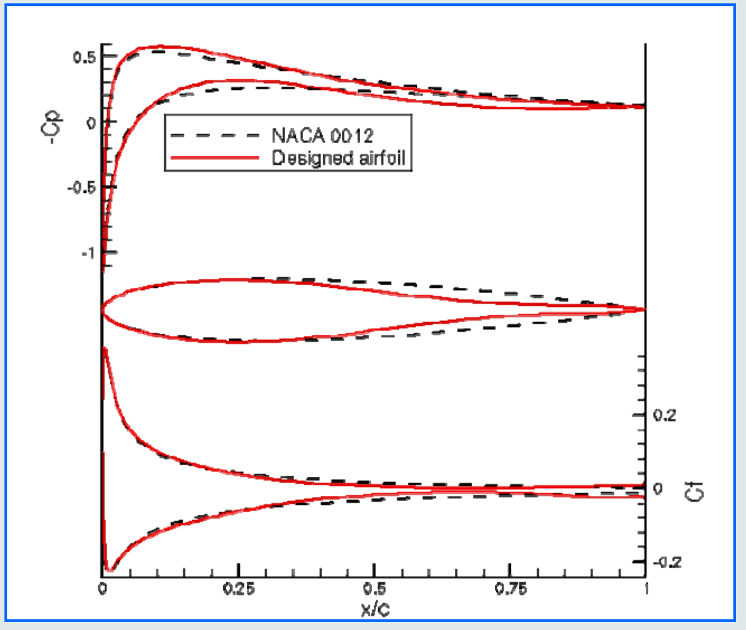
Shock-free airfoil NACA 0012 redesign (Mach 0.8, AoA 1.5º)
Airfoil Pressure (-Cp)
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1
x Coordinate
Optimizer iteration number : 1

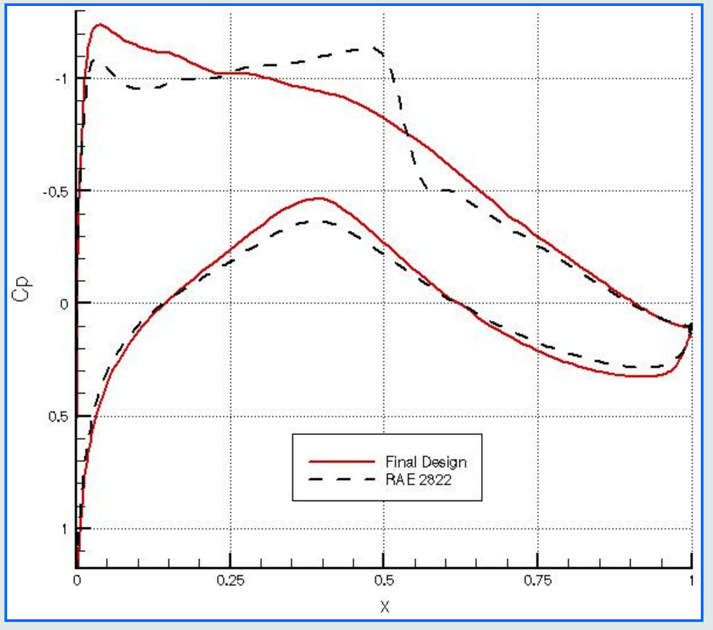
00.00% Drag reduction
Airfoil Drag (Cd)
0.02
0.015
0.01
0.005
0
5
10
15
20
25
30
Optimizer Iteration

00.00% Lift increase
Airfoil Lift (Cl)
0.42
0.4
0.38
0.36
0.34
5
10
15
20
25
30
Optimizer Iteration




Laminar Navier-Stokes Drag Reduction




Turbulent Navier-Stokes Drag Reduction

The flow conditions are:
Angle of attack = 2.50º, Mach Number = 0,3
Reynolds Number 1000, laminar Navier-Stokes
Constrained nose curvature, Constrained minimum greatest thickness
Minimum thickness at 75% of the chord
Constrained minimum lift to the original one
After few iterations the new airfoil based in a NACA 0012 has:
Final drag of 0.1225 that is a 97% of the original NACA 0012

The flow conditions are:
Angle of attack = 2.54º, Mach Number = 0,734
Reynolds Number 6.5e6, laminar Navier-Stokes
Constrained nose curvature, Constrained minimum greatest thickness
Minimum thickness at 75% of the chord
Constrained minimum lift to the original one

# Modelización y simulación determinista y estocástica de fenómenos y sistemas complejos en biología, sociología y economía

- A. Cuevas y J. Berrendero de la UAM
- Principales Problemas
- Métodos utilizados
- Dificultades

# Descripción del Problema y Dificultades

Introduction | Diseño Optimo | Mod. Sim. Det. | Alg. Lin. Num. | Conclusiones

**Principales problemas:**

a) Desarrollo de nuevos tests de hipótesis, válidos para datos funcionales y/o datos de alta dimensión.

b) Estudio de técnicas de clasificación aplicadas al reconocimiento de imágenes y a los datos funcionales. Aplicaciones a problemas médicos de diagnóstico basado en espectros de resonancia magnética.

c) Estudio de nuevos procedimientos para estimar las longitudes de frontera, con aplicaciones al análisis de imágenes.

d) Técnicas de estimación robusta en regresión.

En todos estos problemas surge de modo natural la necesidad de comparar diferentes procedimientos por medio de simulación. También el tratamiento de ejemplos con datos reales requiere el uso de computación intensiva.

**Métodos utilizados:**

Los métodos de computación utilizados se centran, cada vez más, en el uso del software "R". Se trata de un software libre que proporciona un entorno computacional sumamente flexible y potente, que permite cubrir la mayoría de nuestros requerimientos de programación y ofrece, además, una gran cantidad de "librerías" o "subrutinas" especializadas. Los actuales ordenadores personales ofrecen potencia de cálculo suficiente por el momento.

# Algebra Lineal Numérica

- F. Dopico de la UC3M
- Descripción
- Métodos utilizados
- Dificultades

# Descripción del Problema y Dificultades

**Principales problemas:**

a) Algoritmos de *alta precisión* para problemas espectrales. Incorporación a la librería LAPACK de algunos de estos algoritmos.

b) Algoritmos para calcular autovalores, autovectores y descomposiciones en valores singulares para matrices estructuradas (Cauchy, Vandermonde, Totalmente no negativas, Signo regulares, simplécticas....)

c) Algoritmos para factorizaciones tipo LU y QR de matrices generales y estructuradas.

d) Algoritmos para el cálculo de matrices de Jacobi de familias de polinomios ortogonales.

e) Análisis de estabilidad y de errores de redondeo de dichos algoritmos.

f) Teoría de Perturbaciones de Problemas Matriciales: factorizaciones matriciales, autovalores y autovectores, descomposición en valores singulares, formas canónicas espectrales de matrices y haces de matrices (Jordan, Weierstrass, Kronecker), y formas canónicas en control.

g) Problemas de Álgebra Lineal Numérica cerca de singularidades (autovalores múltiples y defectivos, polinomios matriciales singulares, altos números de condición....)

**Métodos utilizados:**

SOFTWARE: MATLAB, FORTRAN.

HARDWARE: Estaciones de trabajo LINUX, PCs. (No uso, ni desarrollo, cálculos en paralelo).