Flow control in the presence of shocks

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Le modèle et l'algorithme, INRIA, Rocquencourt, May 2008

Outline

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1. Introduction: Motivation, examples and problem formulation
2. Optimal shape design in aeronautics
3. Shocks: Some remedies
4. Conclusions

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Flow control, as many other fields of applied mathematics involves:

- Partial Differential Equations: Models describing motion in the various fields of Mechanics: Elasticity, Fluids,...
- Numerical Analysis: Allowing to discretize these models so that solutions may be approximated algorithmically.
- Optimal Design: Design of shapes to enhance the desired properties (bridges, dams, aeroplanes,..)
- Control: Automatic and active control of processes to guarantee their best possible behavior and dynamics.

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These topics meet together in many relevant applications.

- Noise reduction in cavities and vehicles.
- Laser control in quantum mechanical and molecular systems.
- Seismic waves, earthquakes.
- Flexible structures.
- Environment: the Thames barrier.
- Optimal shape design in aeronautics.
- Human cardiovascular system.
- Oil prospection and recovery.
- Irrigation systems.

Complexity arises in many ways:

- Geometry;
- Oscillations.

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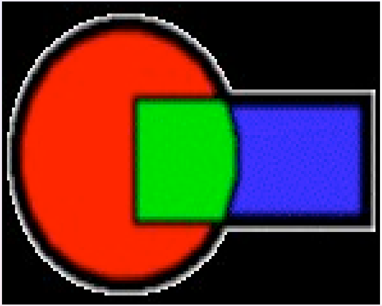
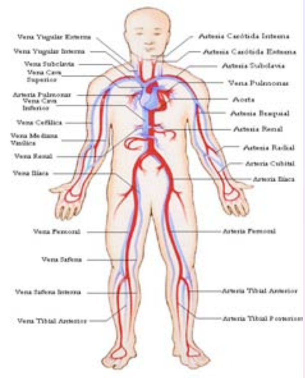
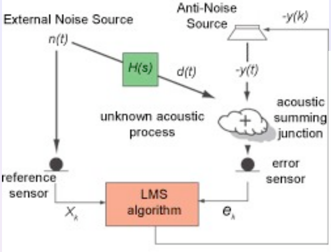




The logo of the web page “Domain decomposition”, one of the most widely used computational techniques for solving PDE in domains (“divide y vencerás”), and a drawing of the human cardiovascular system illustrating the graph along which blood circulates.


External Noise Source
Anti-Noise Source
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n(t)
H(s)
d(t)
-y(t)
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+
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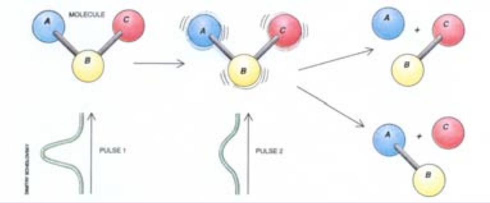
error sensor
LMS algorithm
X_k
e_k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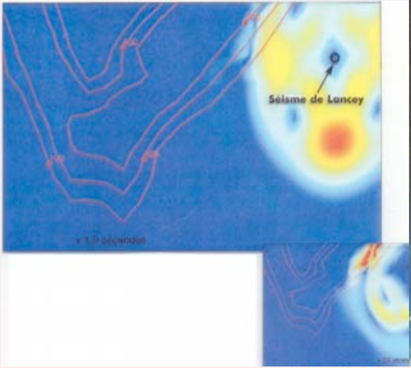
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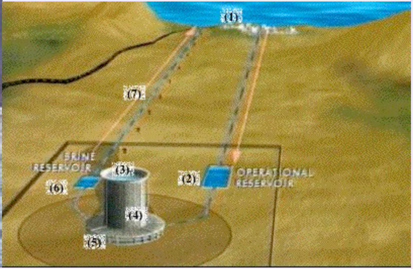
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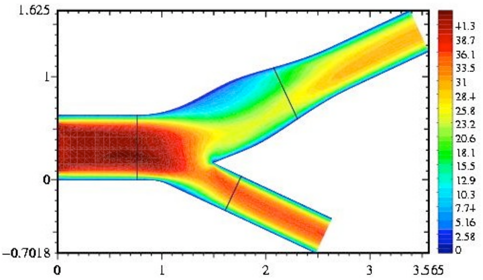
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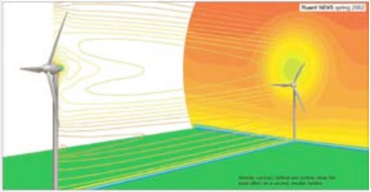
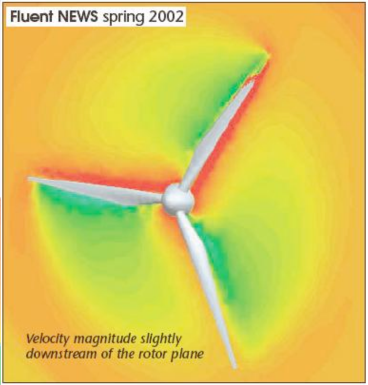
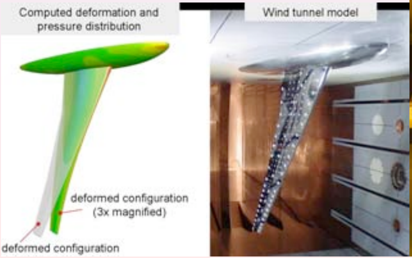
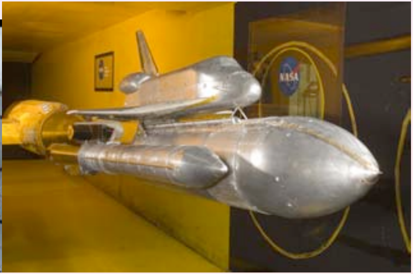


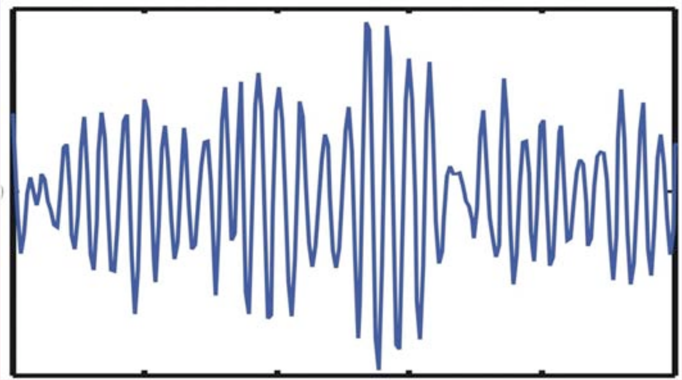

Fluent NEWS spring 2002
Velocity magnitude slightly
downstream of the rotor plane


Computed deformation and
pressure distribution
Wind tunnel model
deformed configuration
(3x magnified)
deformed configuration



Computer simulation → far beyond the fields in which its use is justified (consistency + stability ≡ convergence).

The risk: To end up getting numerical data whose validity....



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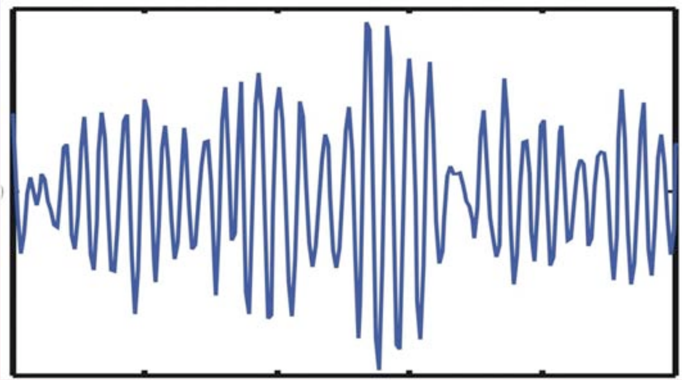
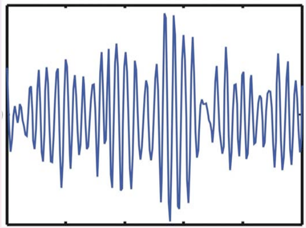


Is this difficulty solvable in practice?

- Solvable for problems with well known data.
- Much harder for inverse, design and control problems,,,,

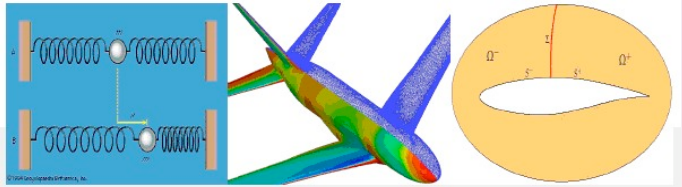
In those cases the obtained final numerical results and simulations may simply mean nothing.



Shape design in aeronautics

Optimal shape design in aeronautics. Two aspects:

- Shocks.
- Oscillations.



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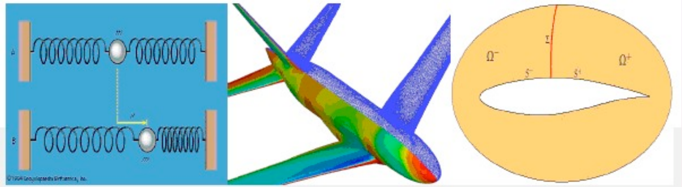

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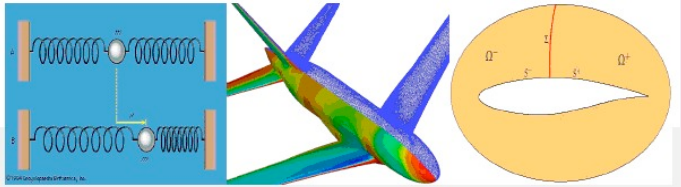

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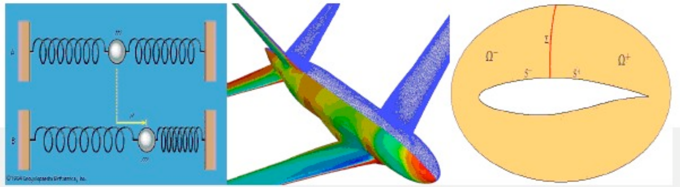

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Optimal shape design in aeronautics

- Aeronautics: to simulate and optimize complex processes is indispensable.
- Long tradition: J. L. Lions, A. Jameson,...
- However, this needs an immense computational effort.

For practical optimization problems, in which at least 100 design variables are to be considered, current methodological approaches applied in industry will need more than a year to obtain an optimized aircraft.

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Mathematical problem formulation

Minimize

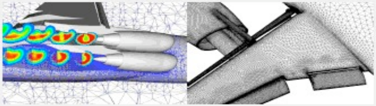
$$J(\Omega^*) = \min_{\Omega \in \mathcal{C}_{ad}} J(\Omega)$$

$\mathcal{C}_{ad}$ = class of admissible domains.

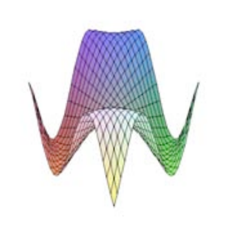
J = cost functional (drag reduction, lift maximization, exploitation cost, overall cost over the life cycle of the aircraft, benefit maximization, etc).

J depends on Ω through $u(\Omega)$, solution of the PDE (elasticity, Fluid Mechanics,...).

The domains under consideration are often complex. Geometric and parametrization issues play a key role.



The dependence of the functional on the domain, through the solution of the PDE is complex as well. J it is far from being a nice convex function.



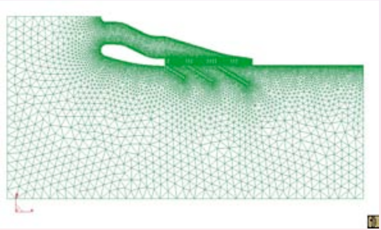
Analytical difficulties:

- Lack of good existence, uniqueness, and continuous dependence theory for the PDE.
- Lack of convexity of the functional.
- Lack of compactness within the class of relevant domains...

In practice

Descent algorithm (gradient based method) on a discrete version of the problem:

- The domains Ω have been discretized (finite element mesh)
- The PDE has been replaced by a numerical scheme,
- The functional J has been replaced by a discrete version.



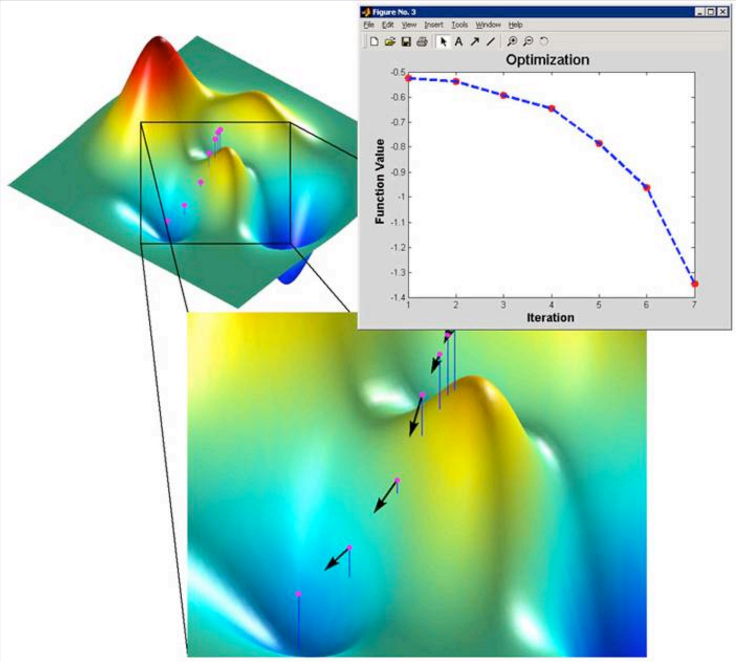


Figure No. 3
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Optimization
Function Value
Iteration
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-1.1
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-1.3
-1.4
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2
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4
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7

Classical steepest descent:

$J : H \to \mathbf{R}$. Two main assumptions:

$$< \nabla J(u) - \nabla J(v), u - v > \geq \alpha |u - v|^2, \quad |\nabla J(u) - \nabla J(v)|^2 \leq M |u - v|^2.$$

Then, for

$$u_{k+1} = u_k - \rho \nabla J(u_k),$$

we have

$$|u_k - u^*| \leq (1 - 2\rho\alpha + \rho^2 M)^{k/2} |u_1 - u^*|.$$

Convergence is guaranteed for $0 < \rho <$ 1 small enough.

Compare with the continuous marching gradient system

$$u'(\tau) = -\nabla J(u(\tau)).$$

We end up with:

- A discrete optimization problem of huge dimensions,
- No idea of whether discrete optima, if they exist, will converge or not to the optimal continuous one.
  - Analytical difficulties.
  - Divergence of algorithms.

The worst scenario: When using results provided by divergent algorithms, for which divergence is hard to detect.

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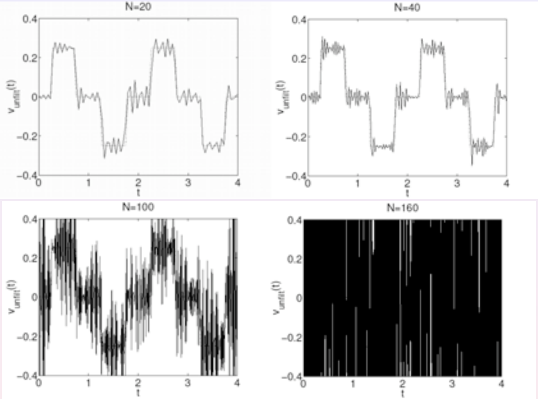
An example: boundary control of vibrations.



Can we guarantee this kind of pathologies do not arise in realistic problems of optimal shape design in aeronautics?

How to detect them? How to avoid them?

Two approaches:

Discrete: Discretization + gradient

- Advantages: Discrete clouds of values. No shocks. Automatic differentiation, ...
- Drawbacks:
  - "Invisible" geometry.

  - Scheme dependent.

Continuous: Continuous gradient + discretization.

- Advantages: Simpler computations. Solver independent. Shock detection.
- Drawbacks:
  - Yields approximate gradients.
  - Subtle if shocks.

The relevant models in aeronautics (Fluid Mechanics):

- Navier-Stokes equations;
- Euler equations;
- Turbulent models: Reynolds-Averaged Navier-Stokes (RANS), Spalart-Allmaras Turbulence Model, $k - \varepsilon$ model;

  ....
- Burgers equation (as a $1 - d$ theoretical laboratory).

Euler equations

$$\begin{cases} \partial_t U + \vec{\nabla} \cdot \vec{F} = 0, & \text{in } \Omega, \\ \vec{v} \cdot \vec{n}_S = 0, & \text{on } S, \end{cases}$$

with suitable boundary conditions at infinity,
$U = (\rho, \rho v_x, \rho v_y, \rho E) =$ conservative variables, $\vec{F} = (F_x, F_y)$=flux

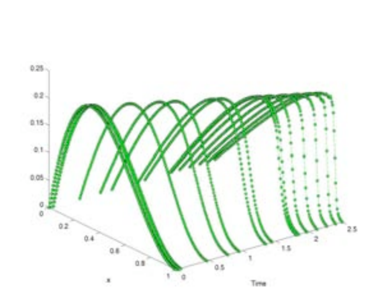
$$F_x = \begin{pmatrix} \rho v_x \\ \rho v_x^2 + P \\ \rho v_x v_y \\ \rho v_x H \end{pmatrix}, \; F_y = \begin{pmatrix} \rho v_y \\ \rho v_x v_y \\ \rho v_y^2 + P \\ \rho v_y H \end{pmatrix}, \tag{1}$$

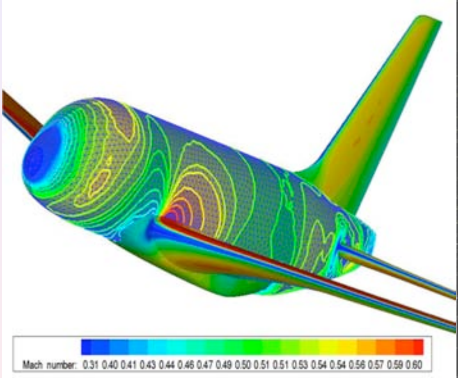
$\rho =$ density , $\vec{v} = (v_x, v_y) =$ velocity, $E =$ total energy, $P =$ pressure, $H =$ enthalpy, where

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

Solutions may develop shocks or quasi-shock configurations.

- For shock solutions, classical calculus fails;
- For quasi-shock solutions the sensitivity is so large that classical sensitivity clalculus is meaningless.

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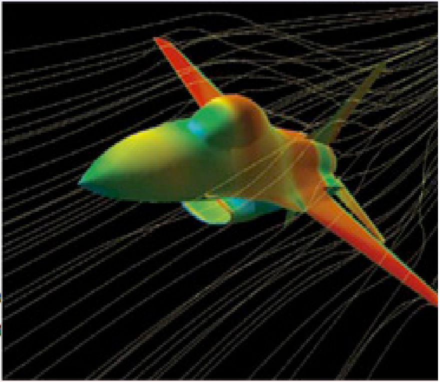


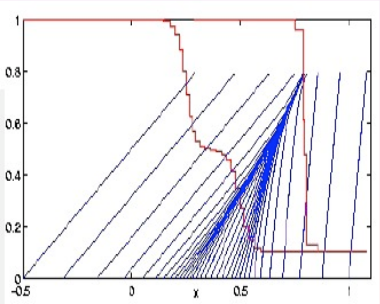
Burgers equation

- Viscous version:

$$\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} + u \frac{\partial u}{\partial x} = 0.$$

- Inviscid one:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0.$$



In the inviscid case, the simple and “natural” rule

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \rightarrow \frac{\partial \delta u}{\partial t} + \delta u\frac{\partial u}{\partial x} + u\frac{\partial \delta u}{\partial x} = 0$$

breaks down in the presence of shocks

$\delta u =$ discontinuous, $\frac{\partial u}{\partial x} =$ Dirac delta $\Rightarrow \delta u \frac{\partial u}{\partial x}$????

The difficulty may be overcame with a suitable notion of measure valued weak solution using Volpert's definition of conservative products and duality theory (Bouchut-James, Godlewski-Raviart,...)

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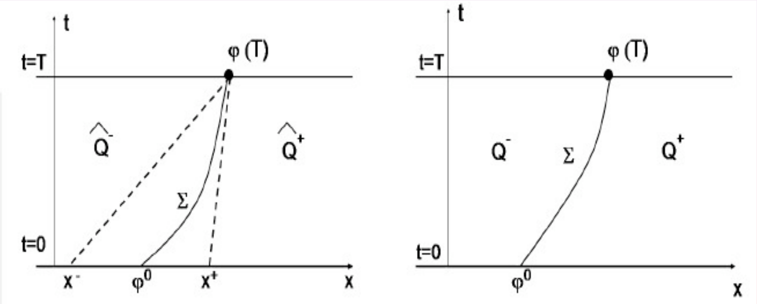
A new viewpoint: Solution = Solution + shock location. Then the pair (u, φ) solves:

$$\begin{cases} \partial_t u + \partial_x(\frac{u^2}{2}) = 0, & \text{in } Q^- \cup Q^+, \\ \varphi'(t)[u]_{\varphi(t)} = \left[u^2/2\right]_{\varphi(t)}, & t \in (0, T), \\ \varphi(0) = \varphi^0, & \\ u(x,0) = u^0(x), & \text{in } \{x < \varphi^0\} \cup \{ x > \varphi^0\}. \end{cases}$$



The corresponding linearized system is:

$$\begin{cases} \partial_t \delta u + \partial_x (u \delta u) = 0, \quad \text{in } Q^- \cup Q^+, \\ \\ \delta\varphi'(t)[u]_{\varphi(t)} + \delta\varphi(t)\left(\varphi'(t)[u_x]_{\varphi(t)} - [u_x u]_{\varphi(t)}\right) \\ \quad +\varphi'(t)[\delta u]_{\varphi(t)} - [u\delta u]_{\varphi(t)} = 0, \quad \text{in } (0,T), \\ \\ \delta u(x,0) = \delta u^0, \quad \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}, \\ \delta\varphi(0) = \delta\varphi^0, \end{cases}$$

Majda (1983), Bressan-Marson (1995), Godlewski-Raviart (1999), Bouchut-James (1998), Giles-Pierce (2001), Bardos-Pironneau (2002), Ulbrich (2003), ...

None seems to provide a clear-cut recipe about how to proceed within an optimization loop.

A new method

A new method: Splitting + alternating descent algorithm.
C. Castro, F. Palacios, E. Z., M3AS, to appear.
Ingredients:

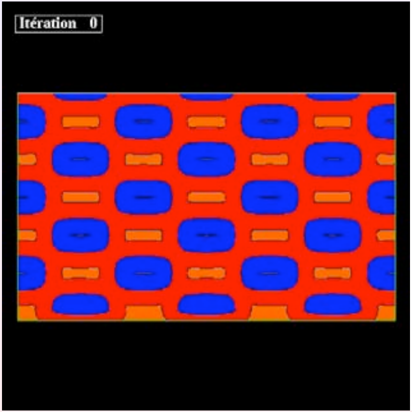
- The shock location is part of the state.

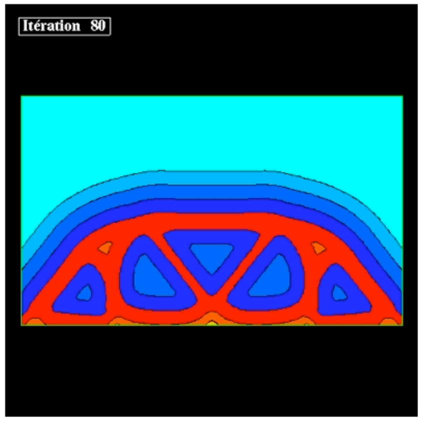
  State = Solution as a function + Geometric location of shocks.

- Alternate within the descent algorithm:
  - Shock location and smooth pieces of solutions should be treated differently;
  - When dealing with smooth pieces most methods provide similar results;
  - Shocks should be handeled by geometric tools, not only those based on the analytical solving of equations.

Lots to be done: Pattern detection, image processing, computational geometry,... to locate, deform shock locations,....

Compare with the use of shape and topological derivatives in elasticity:





An example: Inverse design of initial data

Consider

$$J(u^0) = \frac{1}{2}\int_{-\infty}^{\infty} |u(x,T) - u^d(x)|^2 dx.$$

u^d = step function.

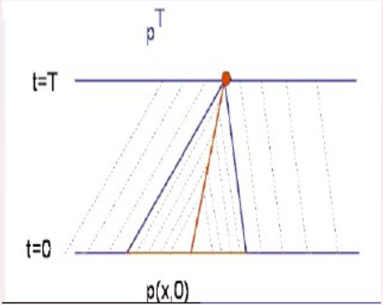
Gateaux derivative:

$$\delta J = \int_{\{x<\varphi^0\}\cup\{x>\varphi^0\}} p(x,0)\delta u^0(x)\, dx + q(0)[u]_{\varphi^0}\delta\varphi^0,$$

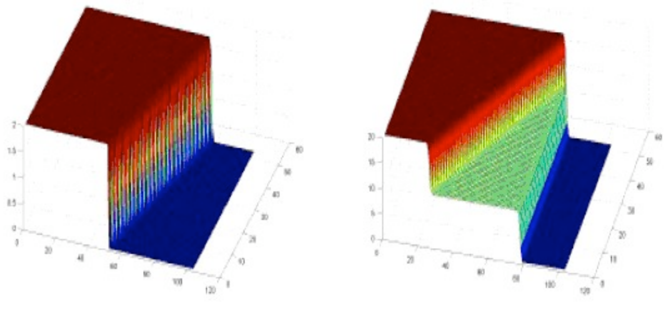
(p,q) = adjoint state

$$\begin{cases} -\partial_t p - u\partial_x p = 0, \quad \text{in } Q^- \cup Q^+, \\ [p]_\Sigma = 0, \\ q(t) = p(\varphi(t),t), \text{ in } t\in(0,T) \\ q'(t) = 0, \text{ in } t\in(0,T) \\ p(x,T) = u(x,T) - u^d, \quad \text{in } \{x<\varphi(T)\}\cup\{x>\varphi(T)\} \\ q(T) = \frac{\frac{1}{2}\left[(u(x,T)-u^d)^2\right]_{\varphi(T)}}{[u]_{\varphi(T)}}. \end{cases}$$

- The gradient is twofold= variation of the profile + shock location.
- The adjoint system is the superposition of two systems = Linearized adjoint transport equation on both sides of the shock + Dirichlet boundary condition along the shock that propagates along characteristics and fills all the region not covered by the adjoint equations.



State u and adjoint state p when u develops a shock:



solution u adjoint p

The discrete aproach

Recall the continuous functional

$$J(u^0) = \frac{1}{2} \int_{-\infty}^{\infty} |u(x, T) - u^d(x)|^2 dx.$$

The discrete version:

$$J^{\Delta}(u^0_{\Delta}) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2,$$

where $u_{\Delta} = \{u_j^k\}$ solves the 3-point conservative numerical approximation scheme:

$$u_j^{n+1} = u_j^n - \lambda \left(g_{j+1/2}^n - g_{j-1/2}^n \right) = 0, \quad \lambda = \frac{\Delta t}{\Delta x},$$

where, g is the numerical flux

$$g_{j+1/2}^n = g(u_j^n, u_{j+1}^n), \; g(u, u) = u^2/2.$$

Examples of numerical fluxes

$$
\begin{aligned}
g^{LF}(u,v) &= \frac{u^2+v^2}{4} - \frac{v-u}{2\lambda}, \\
g^{EO}(u,v) &= \frac{u(u+|u|)}{4} + \frac{v(v-|v|)}{4}, \\
g^{G}(u,v) &= \begin{cases} \min_{w\in[u,v]} w^2/2, & \text{if } u \le v, \\ \max_{w\in[u,v]} w^2/2, & \text{if } u \ge v, \end{cases}
\end{aligned}
$$

The Γ-convergence of discrete minimizers towards continuous ones is guaranteed for the schemes satisfying the so called one-sided Lipschitz condition (OSLC):

$$\frac{u_{j+1}^n - u_j^n}{\Delta x} \leq \frac{1}{n\Delta t},$$

which is the discrete version of the Oleinick condition for the solutions of the continuous Burgers equations

$$u_x \leq \frac{1}{t},$$

which excludes non-admissible shocks and provides the needed compactness of families of bounded solutions.

As proved by Brenier-Osher, [1] Godunov's, Lax-Friedfrichs and Engquits-Osher schemes fulfil the OSLC condition.

[1] Brenier, Y. and Osher, S. The Discrete One-Sided Lipschitz Condition for Convex Scalar Conservation Laws, SIAM Journal on Numerical Analysis, **25** (1) (1988), 8-23.

A new method: splitting+alternating descent

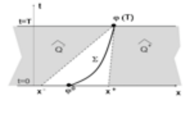
- Generalized tangent vectors $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ s. t.

$$\delta\varphi^0 = \left(\int_{x^-}^{\varphi^0} \delta u^0 + \int_{\varphi^0}^{x^+} \delta u^0 \right) \Big/ [u]_{\varphi^0}.$$

do not move the shock $\delta\varphi(T) = 0$ and

$$\delta J = \int_{\{x<x^-\}\cup\{x>x^+\}} p(x,0)\delta u^0(x)\, dx,$$

$$\begin{cases} -\partial_t p - u\partial_x p = 0, & \text{in } \hat{Q}^- \cup \hat{Q}^+, \\ p(x,T) = u(x,T) - u^d, & \text{in } \{x < \varphi(T)\} \cup \{ x > \varphi(T)\}. \end{cases}$$



For those descent directions the adjoint state can be computed by "any numerical scheme"!

- Analogously, if $\delta u^0 = 0$, the profile of the solution does not change, $\delta u(x, T) = 0$ and

$$\delta J = -\left[\frac{(u(x,T) - u^d(x))^2}{2}\right]_{\varphi(T)} \frac{[u^0]_{\varphi^0}}{[u(\cdot,T)]_{\varphi(T)}}\delta\varphi^0.$$

This formula indicates whether the descent shock variation is left or right!

WE PROPOSE AN ALTERNATING STRATEGY FOR DESCENT

In each iteration of the descent algorithm do two steps:

- Step 1: Use variations that only care about the shock location
- Step 2: Use variations that do not move the shock and only affect the shape away from it.

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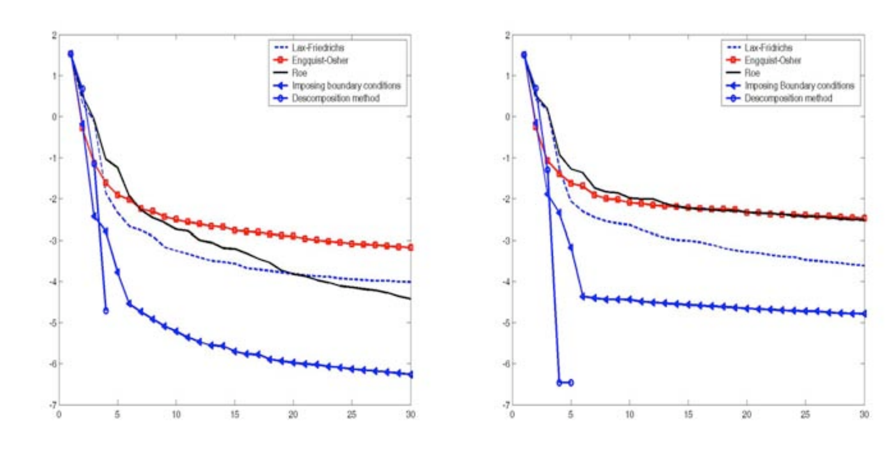
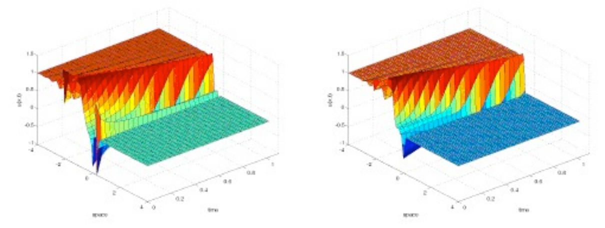
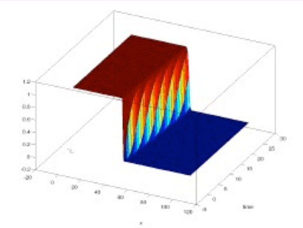


Splitting+Alternating wins!

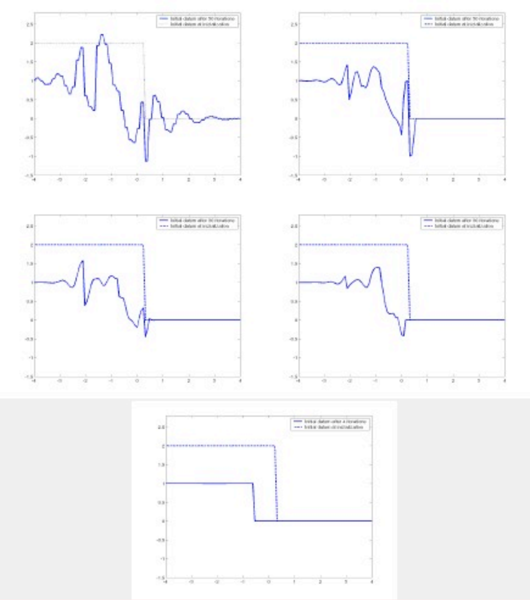


Results obtained applying Engquist-Osher's scheme and the one based on the complete adjoint system



Splitting+Alternating method.

After 30 iterations:

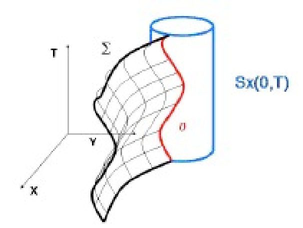


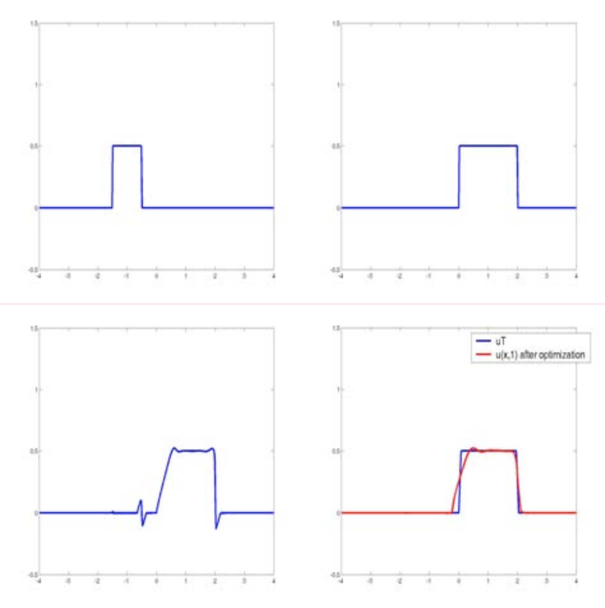
Splitting+alternating is more efficient:

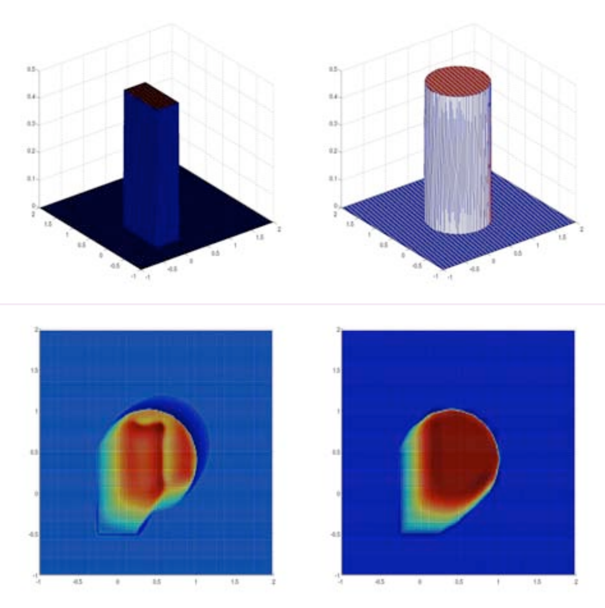
- It is faster.
- It does not increase the complexity.
- Rather independent of the numerical scheme.

Extending these ideas and methods to more realistic multi-dimensional problems is a work in progress and much remains to be done.

Numerical schemes for PDE + shock detection + shape, shock deformation + mesh adaptation,...




uT
u(x,1) after optimization



Conclusions: Inner + outer boundaries

- Much remains to be done in the interfaces between PDE, numerical analysis and optimal design:
    - Well-posedness of relevant models;
    - New approximation schemes for linearized and adjoint equations;
    - Rigorous proof of convergence of new descent algorithms (shock handeling, regularization,...)
- An important effort has to be done to bring all this mathematical understanding and theory to real applications: Make all this to become algorithmic and insert it into the relevant software to be used in (in particular) aeronautical engineering.

Thanks to: E. Andrés, T. Baeza, C. Castro, M. Cea, L. Ignat, C. Lozano, A. Marica, F. Palacios, ...

Thank you!