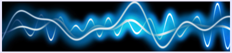

# Flow control in the presence of shocks: theory, numerics and applications

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bcam courses on applied and computational mathematics,
November 2009

# Outline

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1. Introduction: Motivation and examples
2. Divide and conquer
3. Computing: How far?
4. Optimal shape design in aeronautics
5. The models in aeronautics
6. Continuous versus discrete
7. Shocks: Some remedies
8. OTHER APPLICATIONS
9. Conclusions

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- 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.

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- Geometry;
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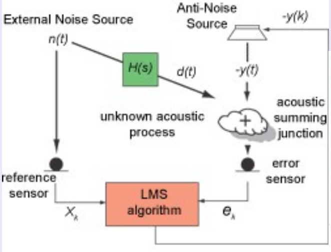
External Noise Source
n(t)
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Anti-Noise Source
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error sensor
LMS algorithm
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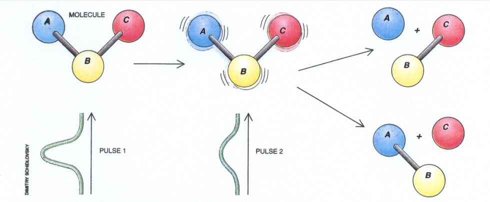
$e_k$


MOLECULE
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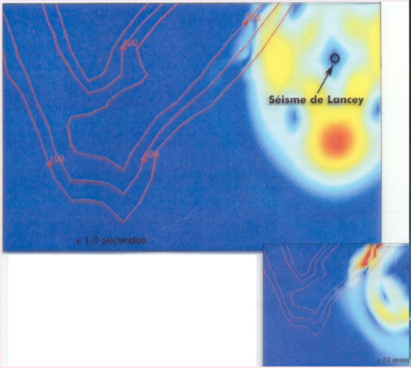
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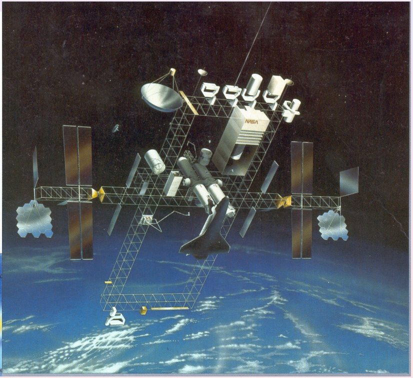

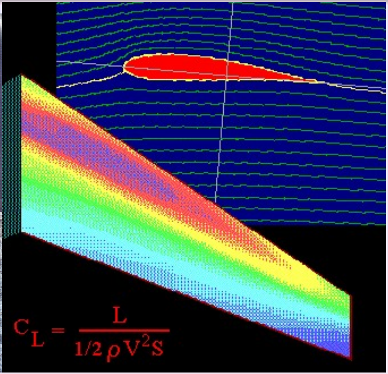
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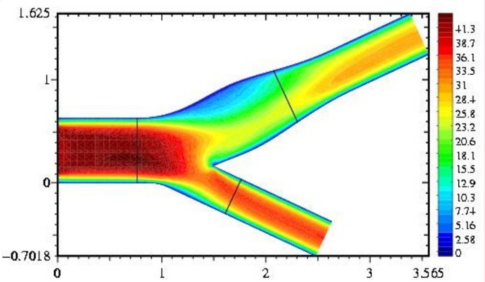
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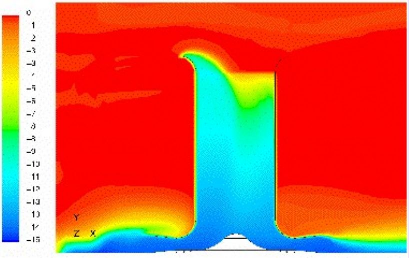
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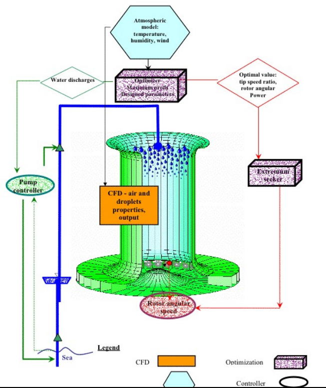
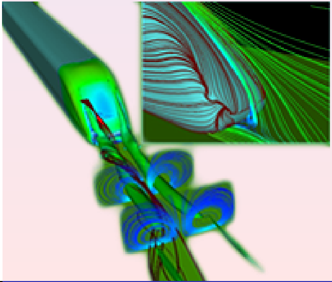
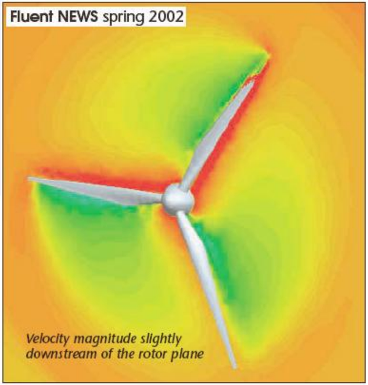
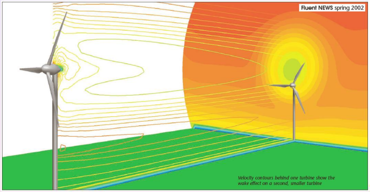
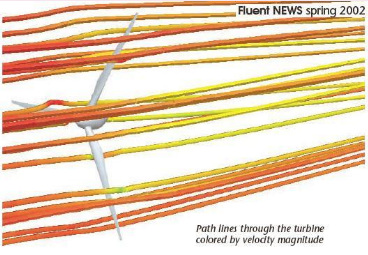
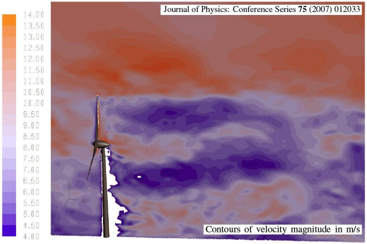

Atmospheric model: temperature, humidity, wind
Water discharges
Optimizer – Maximum profit – Designed parameters
Optimal value: tip speed ratio, rotor angular Power
Pump controller
CFD - air and droplets properties, output
Extremum seeker
Rotor angular speed
Sea
Legend
CFD
Optimization
Controller




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


Fluent NEWS spring 2002
Velocity contours behind one turbine show the wake effect on a second, smaller turbine


Fluent NEWS spring 2002
Path lines through the turbine colored by velocity magnitude


Journal of Physics: Conference Series 75 (2007) 012033
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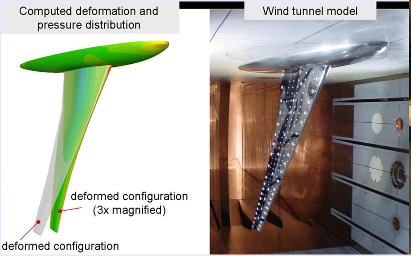
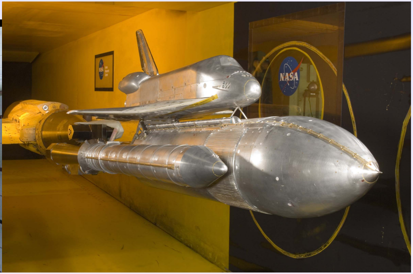
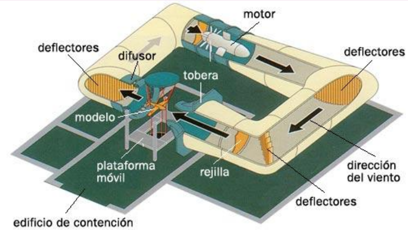
Contours of velocity magnitude in m/s


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




motor
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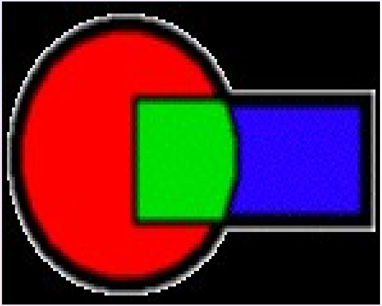
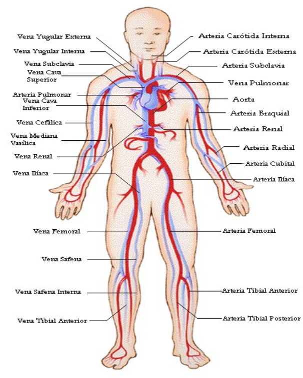
deflectores
tobera
modelo
plataforma móvil
rejilla
dirección del viento
deflectores
edificio de contención






The logo of the web page “Domain decomposition”, one of the most widely used computational techniques for solving PDE in domains (“zatitu eta irabazi”), and a drawing of the human cardiovascular system illustrating the graph along which blood circulates taken from the web page of A. Quarteroni.

Karl Hermann Amandus Schwarz (25 January 1843 – 30 November 1921)

The Schwarz alternating method is an iterative method to find the solution of a partial differential equations on a domain which is the union of two overlapping subdomains, by solving the equation on each of the two subdomains in turn, taking always the latest values of the approximate solution as the boundary conditions. It was first formulated by H. A. Schwarz and served as a theoretical tool. Nowadays is systematically used in most computational challenges

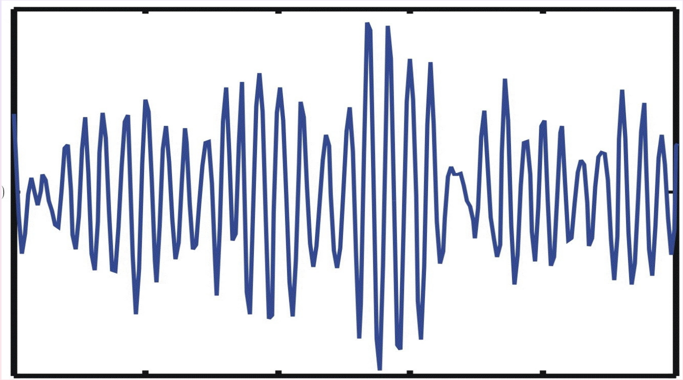
Marius Sophus Lie (17 December 1842 – 18 February 1899)

$$\exp(A+B) = \lim_{n\to\infty} \left[ \exp(A/n) \exp(B/n) \right]^n.$$

$$\exp(A+B) \sim \exp(A/n) \exp(B/n) .... \exp(A/n) \exp(B/n).$$

Computer simulation $\longrightarrow$ far beyond the fields in which its use is justified (consistency + stability $\equiv$ convergence).

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



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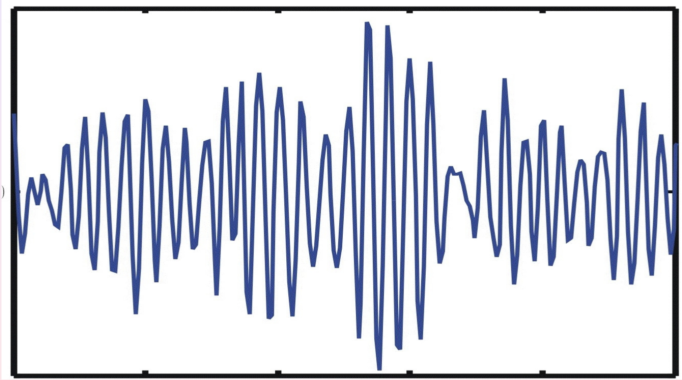
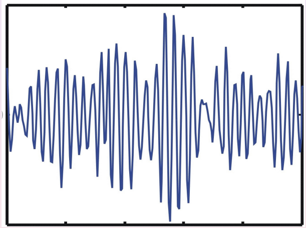


## Is this difficulty solvable in practice?

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

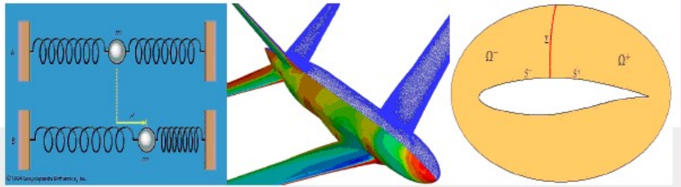
In those cases the obtained final numerical results and simulations may simply mean nothing.



## Shape design in aeronautics

Optimal shape design in aeronautics. Two aspects:

- Shocks.
- Oscillations.



Optimal shape ∼ Active control. The shape of the cavity or airfoil controls the surrounding flow of air.

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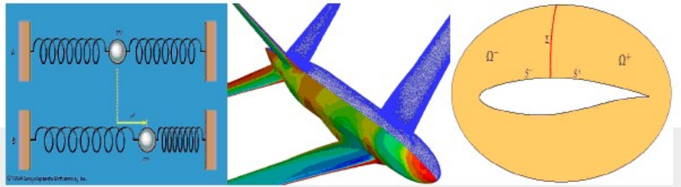

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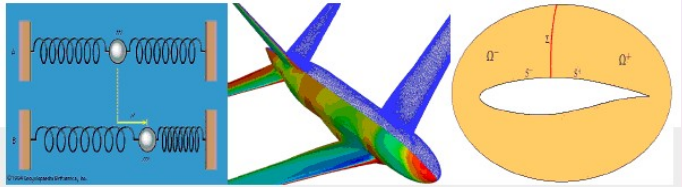

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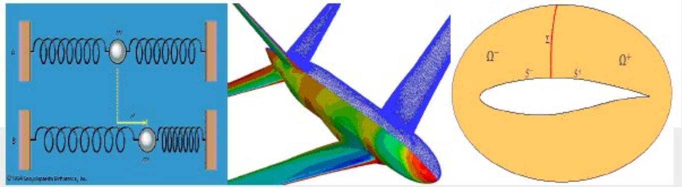


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## Optimal shape design in aeronautics

- 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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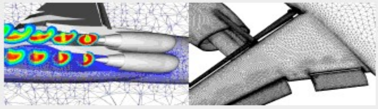
## Mathematical problem formulation

Minimize

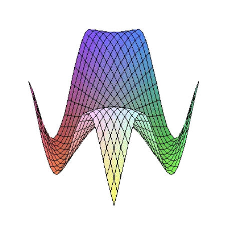
$$J(\Omega^*) = \min_{\Omega \in \mathcal{C}_{ad}} J(\Omega)$$

$\mathcal{C}_{ad}$ = 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 $\Omega$ 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.



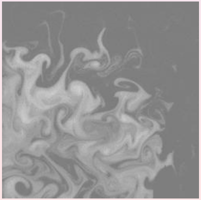
The dependence of the functional on the domain, through the solution of the PDE is complex as well. $J$ it is far from being a nice convex function.



Analytical difficulties:

- Lack of good existence, uniqueness, and continuous dependence theory for the PDE.

http://www.claymath.org/millennium/Navier-Stokes_Equati

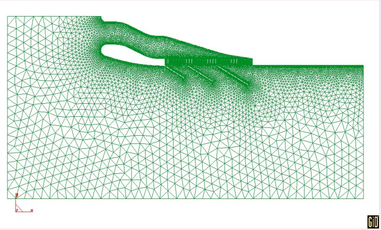


- Lack of convexity of the functional.
- Lack of compactness within the class of relevant domains...

# 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.



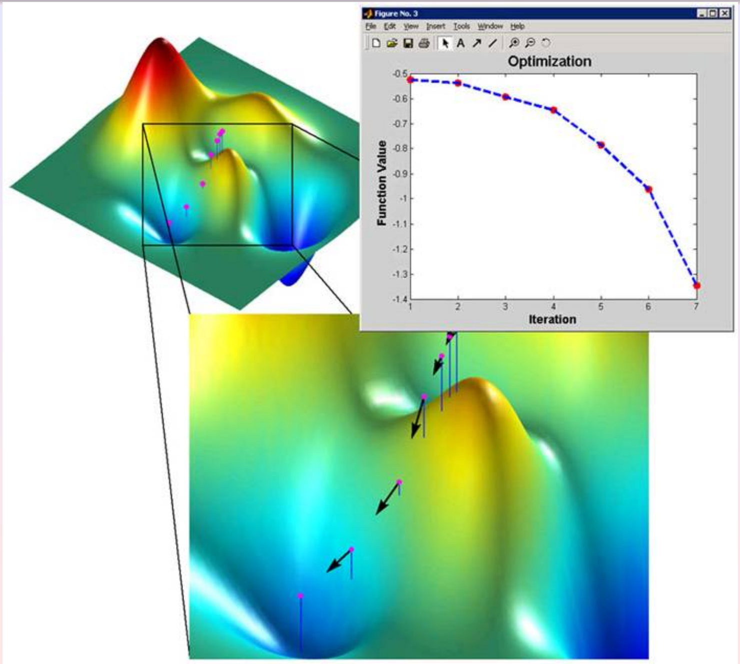


Figure No. 3
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Optimization
Function Value
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-0.8
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-1.1
-1.2
-1.3
-1.4
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7

## 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

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

# LaSalle's invariance principle

Taking the scalar product in equation $u'(t) = -\nabla J(u(t))$ with $\nabla J(u(t))$ we deduce that

$$dJ(u(t)/dt = -|\nabla J(u(t))|^2.$$

Thus, for the gradient system, $J(u(t))$ constitutes a Lyapunov function whose value diminishes along trajectories.
Assume that $J$ is bounded below. This is typically the case when searching the minimizers of $J$ under the standard coercivity and continuity assumptions.
Then, necessarily, $J(u(t))$ has a limit $I$ as $t \to \infty$.
Furthermore, when $J$ is coercive, this necessarily means that the trajectory $\{u(t)\}_{t \geq 0}$ is bounded. In the finite-dimensional context this means that the trajectory is precompact. In the infinite-dimensional case this requires further analysis of the dynamical properties of the evolution system under consideration.

Let us then define the $\omega$-limit set. Given the initial datum $u_0$ of the solution of the gradient system, $\omega(u_0)$ is the set of accumulation points of the trajectory as $t \to \infty$. Obviously $J(z) = I$ for all $z \in \omega(u_0)$. On the other hand, if we denote by $z(t)$ the trajectory of the same gradient system starting at $z$ at time $t = 0$, by the semigroup property, we also deduce that $J(z(t)) = I$ for all $t \geq 0$. This implies, in particular, that $z$ is a critical point of $J$: $J(z) = 0$. In case $J$ has an unique minimizer, as it happens when $J$ is strictly convex, then $z$ is this minimizer. Taking into account that the accumulation point is unique, we deduce that $\omega(u_0) = \{z\}$. This implies that the whole trajectory $u(t)$ converges to $z$.

As we mentioned above, in the infinite-dimensional case, the boundedness of trajectories does not necessarily imply that they are relatively compact. The compactness of trajectories is normally achieved by imposing further monotonicity properties.
Indeed, when $J$ is convex, distances diminish along trajectories. Indeed, if $u$ and $v$ are two trajectories of the same system then $|u(t) - v(t)|$ diminishes as time evolves.
According to this it is sufficient to prove convergence towards equilibrium for a dense set of initial data. This dense set is chosen normally to ensure compactness through the compactness of the embedding into the phase space, and the boundedness of the trajectories in that subspace.

## The Direct Method of the Calculus of Variations (DMCV)

Consider a continuous, convex and coercive functional $J : H \to \mathbb{R}$ in a Hilbert space $H$. Then, the functional achieves its minimum in at least one point:

$$\exists h \in H : \; J(h) = \min_{g \in H} J(g). \tag{1}$$

This can be easily proved in a systematic manner by means of the DMCV:

**Step 1.** Define the infimimum

$$I = \inf_{g \in H} J(g)$$

that, by the coercivity of $J$, necessarily satisfies $I > -\infty$.

**Step 2.** Consider the minimizing sequence

$$(g_n)_{n\in\mathbb{N}} \subset H : \; J(g_n) \searrow I. \tag{2}$$

By the coercivity of the functional $J$ we deduce that $(g_n)_{n\in\mathbb{N}}$ is bounded in $H$.

**Step 3.** $H$ being a Hilbert space, there exists a weakly convergent subsequence $(g_n)_{n\in\mathbb{N}}$

$$g_n \rightharpoonup g \text{ en } H. \tag{3}$$

**Step 4.** $J$ being continuous in $H$ and convex it is lowe semicontinuous with respect to the weak topology. Therefore,

$$J(g) \leqslant \varliminf_{n\to\infty} J(g_n). \tag{4}$$

We deduce that $J(g) \leqslant I$ which, by the definition of infimum, implies that $J(g) = I$, which shows that the minimum is achieved.

Going back, to the shape optimization problem, 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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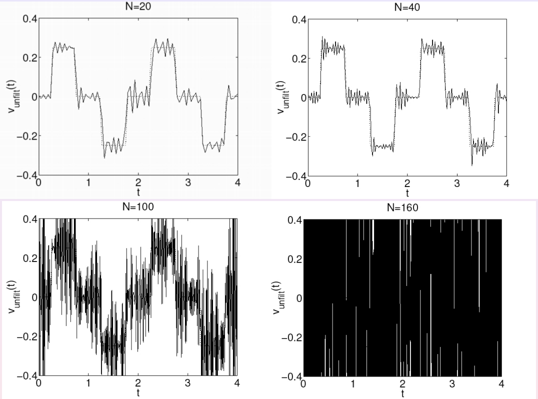
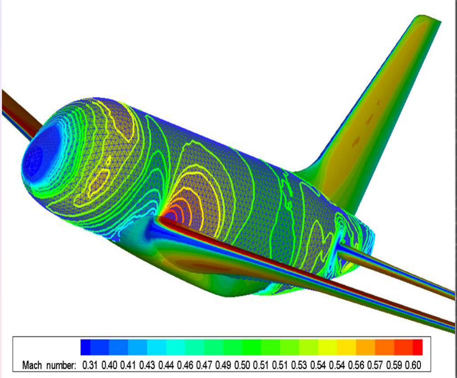
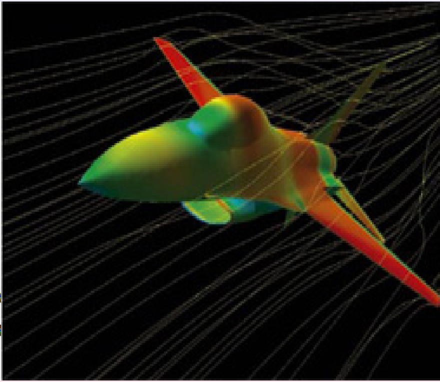
An example: boundary control of vibrations.




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?


Mach number: 0.31 0.40 0.41 0.43 0.44 0.46 0.47 0.49 0.50 0.51 0.51 0.53 0.54 0.54 0.56 0.57 0.59 0.60



## 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

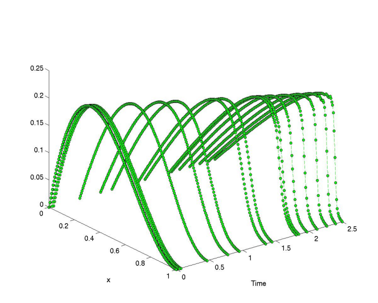
$$F_x = \begin{pmatrix} \rho v_x \\ \rho v_x^2 + P \\ \rho v_x v_y \\ \rho v_x H \end{pmatrix}, \; F_y = \begin{pmatrix} \rho v_y \\ \rho v_x v_y \\ \rho v_y^2 + P \\ \rho v_y H \end{pmatrix}, \tag{5}$$

$\rho =$ 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: The derivative of a discontinuous function is a Dirac delta;
- For quasi-shock solutions the sensitivity (gradient) is so large that classical sensitivity calculus is meaningless.



## Computational fluid dynamics: Overview

- **Incompressible Flows:** At slow motion of a fluid or gas (low Mach numbers) the density and temperature changes can be neglected. The flow equations can be simplified into incompressible Navier- Stokes equations.
- **Compressible Flows:** Density and temperature changes are not anymore neglectable due to higher Mach numbers. An important characteristic of compressible flows is the occurrence of shocks which leads to discontinuities.

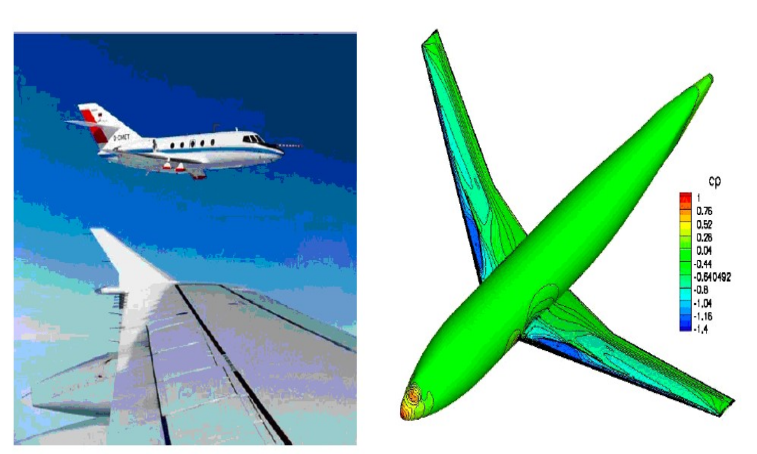
## Example for incompressible flow

ONERA: $M < 0.3$

## Example for incompressible flow

Soaring plane

## Example for compressible flow



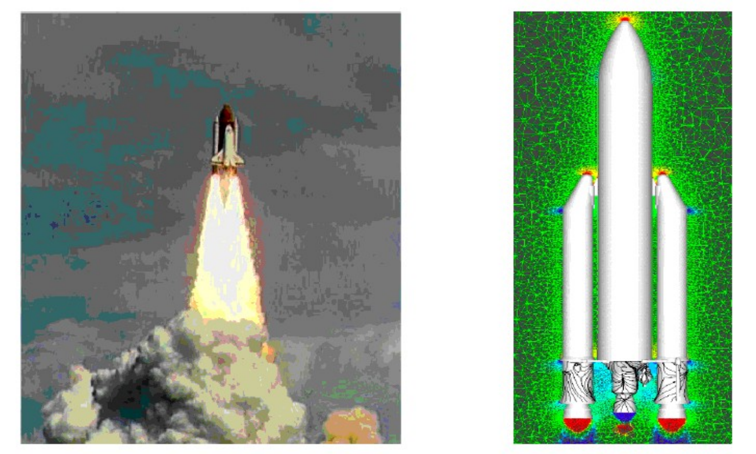

Passenger and transport aircraft with transonic flow

**Transonic** refers to a range of velocities just below and above the speed of sound (about mach 0.8 – 1.2). It is defined as the range of speeds between the critical mach number, when some parts of the airflow over an aircraft become supersonic, and a higher speed, typically near Mach 1.2, when all of the airflow is supersonic. Between these speeds some of the airflow is supersonic, and some is not.

**Severe instability can occur at transonic speeds. Shock waves move through the air at the speed of sound.** When an object such as an aircraft also moves at the speed of sound, these shock waves build up in front of it to form a single, very large shock wave. During transonic flight, the plane must pass through this large shock wave, as well as contending with the instability caused by air moving faster than sound over parts of the wing and slower in other parts. The difference in speed is due to Bernoulli's principle.

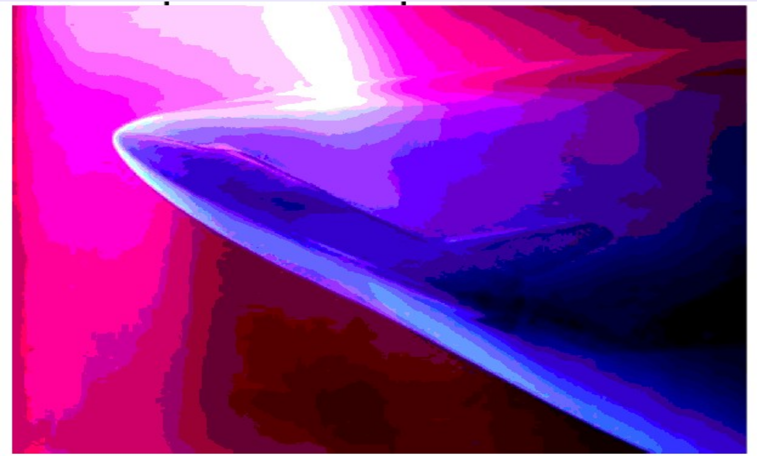
Transonic speeds can also occur at the tips of rotor blades of helicopters and aircraft.

## Example for compressible flow



NASA: Hypersonic flow with shocks at the nose

## Example for compressible flow



NASA: Visible shocks at the nose in the windtunnel test

## The $1-d$ model: Burgers equation

- J. M. Burgers, Application of a model system to illustrate some points of the statistical theory of free turbulence, Proc. Konink. Nederl. Akad. Wetensch. 43, 2Ð12 (1940).
- E. Hopf, The partial dfferential equation $u_t + uu_x = u_{xx}$, Comm. Pure Appl. Math. 3, 20–230 (1950).
- J. D. Cole, On a quasi-linear parabolic equation occurring in aerodynamics, Quart. Appl. Math. 9, 225 – 236 (1951).

Celebrated because:

- It has the same scales as the Navier-Stokes equations

$$u_t - \mu\Delta u + u \cdot \nabla u = \nabla p.$$

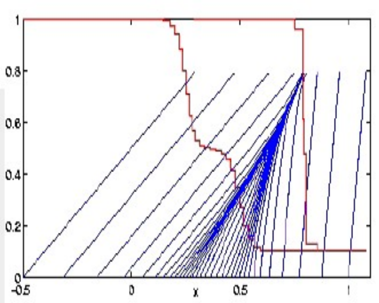
- There is a change of variable reducing the problem to the linear heat equation. This leads to explicit solutions.
- One can show explicitly the presence of shocks.
  G.B. Whitham, Linear and nonlinear waves, New York, Wiley-Interscience, 1974.

- Viscous version:

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

- Inviscid one:

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



## The Hopf-Cole transform

Let $u = u(x, t)$ be a solution of

$$u_t - \nu u_{xx} + (u^2)_x = 0.$$

such that $| u(x, t) | + | u_x(x, t) | \to 0$ as $| x | \to \infty$.
Then

$$v = v(x, t) = \int_{-\infty}^{x} u(s, t) ds \tag{6}$$

solves

$$v_t - \nu v_{xx} + | v_x |^2 = 0. \tag{7}$$

Define then

$$w = v(x, t/\nu)$$

that satisfies

$$w_t - w_{xx} + \frac{1}{\nu} | w_x |^2 = 0. \tag{8}$$

On the other hand,

$$z = 2/\nu \tag{9}$$

satisfies

$$z_t - z_{xx} + \mid z_x \mid^2 = 0. \tag{10}$$

Introduce, at last,

$$\eta(x, t) = e^{-z} \tag{11}$$

that solves the heat equation

$$\eta_t - \eta_{xx} = 0. \tag{12}$$

Undoing the change of variables

$$u = v_x$$
$$v(\cdot, t/\nu) = w(\cdot, t) = \nu z(\cdot, t) = -\nu \log(\eta).$$

Then

$$u(x, t) = -\nu \frac{\eta_x(x, \nu t)}{\eta(x, \nu t)}. \tag{13}$$

The solution$\eta$ of this heat equation can be obtained by convolution with the heat kernel:

On the other hand,

$$G_x(x,\ t) = -\frac{x}{4\sqrt{\pi}t^{3/2}} \exp\left(- \mid x \mid^2 \Big/ 4t\right). \tag{16}$$

In this way we get

$$u(x,\ t) = \frac{\int_{\mathbb{R}}(x-y)e^{-|x-y|^2/4\nu t}\eta_0(y)dy}{2t\int_{\mathbb{R}} e^{-|x-y|^2/4\nu t}\eta_0(t)dy}. \tag{17}$$

But

$$\eta_0(x) = e^{-\int_{-\infty}^{x} u_0(\sigma)d\sigma/\nu}. \tag{18}$$

So that

$$u_\nu(x,\ t) = \frac{\int_{\mathbb{R}}(x-y)e^{-H(x,y,t)/\nu}dy}{2t\int_{\mathbb{R}} e^{-H(x,y,t)/\nu}dy} \tag{19}$$

where

$$H(x,\ y,\ t) = \frac{\mid x-y \mid^2}{4t} + \int_{-\infty}^{y} u_0(\sigma)d\sigma. \tag{20}$$

## Shocks

We write the inviscid Burgers equation in the form

$$u_t + 2uu_x = 0. \tag{21}$$

Solutions, while smooth, are constant along characetristics

$$u(x(t),\, t) = C,$$

where $x = x(t)$ is given by the equation

$$x'(t) = 2u(x(t),\, t). \tag{22}$$

Since $u$ is constant along characteristics, $u(x(t),\, t)$ has to coincide with its value at $t = 0$, so that

$$u(x(t),\, t) = u_0(x_0), \tag{23}$$

where $x_0$ is the starting point of the characteristic line.

The equation of the characteristic line then reads

$$x(t) = 2u_0(x_0)t + x_0 \tag{24}$$

and therefore

$$u(x(t),\, t) = u_0(x_0). \tag{25}$$

Thus $u$ is constant along lines with slope $1/2u_0$in the $(x,\, t)$-plane. This implies that, if $u_0$ is decreasing, $u$ has to generate discontinuities in finite-time. Indeed, the existence of $x_0 < x_1$ such that $u(x_0) > u(x_1)$, shows that the characteristic lines emanating from $x_0$ and $x_1$ intersect in some time $t^*$ at some $x^*$. The solution will then be discontinuous at $(x^*,\, t^*)$ since the values $u_0(x_0)$ and $u_0(x_1)$ are incompatible.

The shock or discontinuity time $t^*$ can be computed by passing to the limit as $x_0 \to x_1$ in the identity

$$2u_0(x_0)t + x_0 = 2u_0(x_1)t + x_1.$$

This yields

$$t^* = \frac{x_1 - x_0}{2(u_0(x_0) - u_0(x_1))} = -\frac{x_0 - x_1}{2(u_0(x_0) - u_0(x_1))}. \tag{26}$$

As $x_0 \to x_1$ this gives

$$t^* = -\frac{1}{2u_0'(x_0)}. \tag{27}$$

The minimal shock time is then

$$t^* = \frac{1}{2\max_{x_0 \in \mathbb{R}} \Big( -u_0'(x_0) \Big)}. \tag{28}$$

## Vanishing viscosity

We analyze the behavior as $\nu \longrightarrow 0$ of the solutions of the viscous Burgers equation. As we shall see, they converge to the so called entropy solutions of the inviscid one.
As $\nu \longrightarrow 0^+$, the integrals in the Hopf-Cole representation of solutions concentrate at the points where $H$ achieves its minimum. The critical values of $H$ are characterized by:

$$H_y = -\frac{x-\xi}{2t} + u_0(\xi) = 0 \Leftrightarrow \xi = x - 2tu_0(\xi), \tag{29}$$

in which

$$H = -tu_0^2(\xi) + \int_{-\infty}^{\xi} u_0(\sigma)d\sigma. \tag{30}$$

The contribution of the integral [1]

$$\int_{\mathbb{R}} f(y) e^{-H/\nu} dy \tag{31}$$

around the minimum $y = \xi$ is

$$f(\xi) \sqrt{\frac{2\pi\nu}{H''(\xi)}} e^{-H(\xi)/\nu}. \tag{32}$$

In our case

$$H''(\xi) = \frac{1}{2t}. \tag{33}$$

We get

$$\int_{\mathbb{R}} (x-y) e^{-H/\nu} dy \sim (x-\xi) \sqrt{\frac{\pi\nu}{t}} e^{-[t u_0^2(\xi) + \int_{-\infty}^{\xi} u_0(\sigma) d\sigma]\nu}, \tag{34}$$

$$\int_{\mathbb{R}} e^{-H/\nu} dy \sim \sqrt{\frac{\pi\nu}{t}} e^{-[t u_0^2(\xi) + \int_{-\infty}^{\xi} u_0(\sigma) d\sigma]}. \tag{35}$$

[1] Carl M. Bender and Steven A. Orszag, Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory , Springer, 1999

Then

$$u_\nu(x,\ t) \sim \frac{(x-\xi)}{2t} \tag{36}$$

where $\xi$ is characterized by the equation

$$\xi = x - 2tu_0(\xi) \tag{37}$$

which is precisely the solution obtained by the method of characteristics:

$$u_\nu(x,\ t) \sim u_0(\xi) \tag{38}$$

This is valid when $H$ has only one minimum.
When $u_0$ is increasing and smooth there is only one solution and we recover the same solution as the one obtained by the method of characteristics.

When $H$ has several minima $\xi_1, \ldots, \xi_N$, each of them provides a contribution of the same form. But, in view of the exponential terms, only the absolute minimum of $H$ matters.
When there are two absolute minima $\xi_1$, $\xi_2$, the asymptotic form of $u_\nu$ would be:

$$u_\nu(x, t) \sim u_0(\xi_1) + u_0(\xi_2). \tag{39}$$

We now consider the Riemann problem

$$u_0(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0. \end{cases} \tag{40}$$

The system characterizing the minima can be written as

$$\begin{cases} \xi = x, & \text{si} \quad \xi < 0 \\ \xi + 2t = x, & \text{si} \quad \xi > 0. \end{cases} \tag{41}$$

When $x < 0$, this gives $\xi = x$ and then the limit is $u = u_0(\xi) = 0$. When $x > 2t$ we get $\xi = x - 2t$ and then the solution is $u \equiv 1$, which coincides with the result that the method of characteristic yields. By an approximation argument, in the intermediate zone we get $\xi = x/(1 + 2t)$ and

$$u(x, t) = \frac{x}{2t}. \tag{42}$$

The *rarefaction wave* $u = x/2t$ connects the value $u = 0$ to the left and $x = 1$ to the right.

This is the physical or *entropy* solution.

We now consider the Riemann problem

$$u_0(x) = \begin{cases} 1, & x < 0 \\ 0, & x > 0. \end{cases} \quad (43)$$

In this case we know there is a shock like solution.
The method of vanishing viscosity confirms this is the entropy or physical solution.
In this case, the function $H$ has two local minima, but when determining the global one we get either the value $u \equiv 0$ or $u \equiv 1$ depending on whether we are on the left or right of the shock.

## The Oleinick entropy condition

We claim that physical solutions of the Burgers equation satisfy

$$u_x \leq 1/2t. \tag{44}$$

Formally, if $u$ solves the Burgers equation $v = u_x$ satisfies

$$v_t + (2uv)_x = v_t + 2v^2 + 2uv_x = 0. \tag{45}$$

By the maximum principle we deduce that

$$v \leq w \tag{46}$$

where $w = w(t)$ is the solution of

$$w_t + 2w^2 = 0 \tag{47}$$

with initial datum $w(0) = \infty$: $w(t) = 1/2t$.
This formal argument can be fully justified for the physical solutions that are obtained as zero viscosity limits.

## Summary on entropy solutions of the Burgers equation

- Entropy solutions are the physical ones
- Entropy solutions are characterized by the zero viscosity limit.
- Entropy solutions are characterized also by the Oleinick inequality.
- Entropy solutions are unique (celebrated result by Kruzkov).

All this can be extended to multi-dimensional scalar conservation laws:

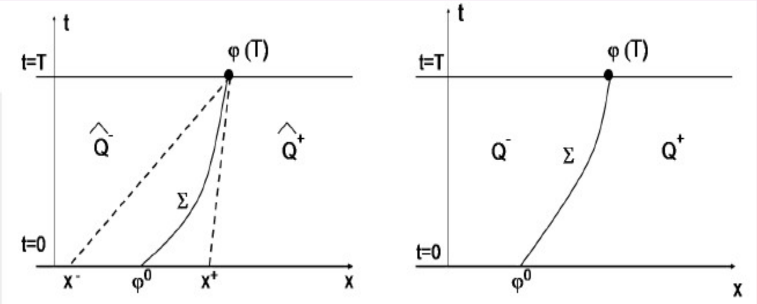
$$u_t + \mathrm{div}(\vec{f}(u)) = 0.$$

Note however that, in real applications, we often deal with systems, where theory if much more complex and only partially complete.

## Solution as a pair: flow+shock variables

Then the pair $(u, \varphi)$= (flow solution, shock location) 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 Rankine–Hugoniot equation

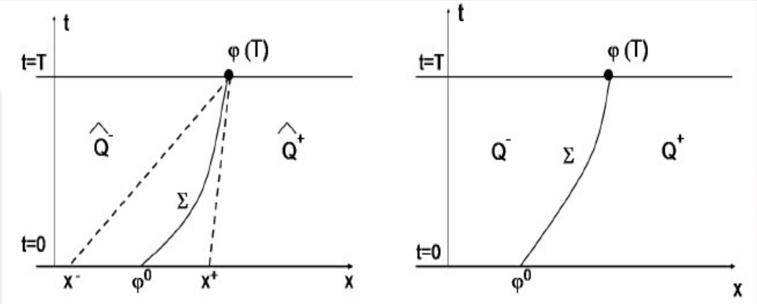
$$\varphi'(t)[u]_{\varphi(t)} = \left[u^2/2\right]_{\varphi(t)}$$

governs the behaviour of shock waves normal to the oncoming flow. It is named after physicists William John Macquorn Rankine (5 July 1820 – 24 December 1872) and Pierre Henri Hugoniot (1851 –1887).

Rankine, W. J. M. , On the thermodynamic theory of waves of finite longitudinal disturbances, Phil. Trans. Roy. Soc. London, 160, (1870).
Hugoniot, H., Propagation des Mouvements dans les Corps et spcialement dans les Gaz Parfaits, Journal de l'Ecole Polytechnique, 57, (1887); 58, (1889).

A new viewpoint: Solution = Solution + shock location. Then the pair $(u, \varphi)$ 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 linearized system

As we have seen, when applying descent algorithms, we have to compute the gradient of the functional $J$ to be minimized. This, in practice, requires computing the derivatives of the solutions of the underlying PDE with respect to the various design parameters. This ends up requiring the linearization of the nonlinear PDE's in the models under consideration.

When solutions are smooth and unique and depend stably on the various parameters entering in the system, linearization can be performed as in the context of ODE's:

$$x'(t) = f(x(t)); \; x(0) = x_0.$$

Let $x_\delta$ be the solution with initial datum $x_0 + \delta z_0$.

What is the derivative of $x_\delta$ with respect to $\delta$, that we denote by $z$?

The linearized state can be characterized as the unique solution of:

$$z'(t) = f'(x(t))z(t); \; z(0) = z_0.$$

The same analysis applies to the solutions of the viscous Burgers equation:

$$u_t - \nu u_{xx} + (u^2)_x = 0,\ x \in \mathbf{R},\ t > 0;\ u(x,0) = u_0(x),\ x \in \mathbf{R}.$$

If $u_\delta$ denotes the solution of the equation with initial datum $u_0(x) + \delta z_0(x)$ the linearized state $z$ derivative of $u_\delta$ with respect to $\delta$ is characterized as the solution of

$$z_t - \nu z_{xx} + (2uz)_x = 0,\ x \in \mathbf{R},\ t > 0;\ z(x,0) = z_0(x),\ x \in \mathbf{R}.$$

This linearization is fully justified in the $L^2(\mathbf{R})$-setting, in particular. More precisely, when $u_0$ and $z_0$ are in $L^2(\mathbf{R})$, both solution belong to $C([0,\infty); L^2(\mathbf{R})) \cap L^2(0,T; H^1(\mathbf{R}))$ and $z$ is the derivative of $u_\delta$ with respect to $\delta$ in that space.
As we shall see, this fails to be true in the inviscid case.

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,...)

In the inviscid case, the simple and "natural" rule

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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,...)

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.

## Continuous versus discrete

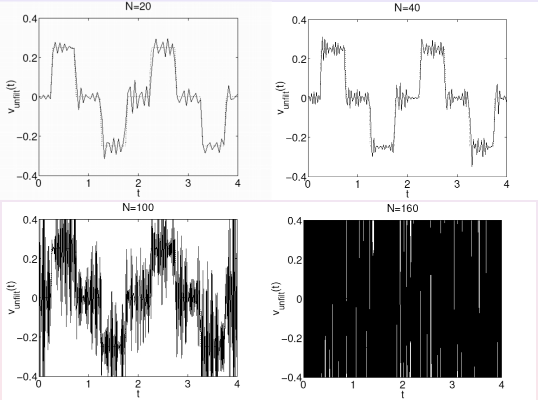
Two approaches:

- **Continuous:** PDE+ Optimal shape design $\longrightarrow$ implement that numerically.
- **Discrete:** Replace PDE and optimal design problem by discrete version $\longrightarrow$ Apply discrete tools

Do these processes lead to the same result?

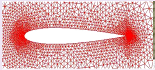
OPTIMAL DESIGN + NUMERICS
=
NUMERICS + OPTIMAL DESIGN?

NO!!!!!!



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.

# SHOCKS: A MUST

- Discrete approach: You do not see them
- Continuous approach: They make life difficult

# SHOCKS: A MUST

- Discrete approach: You do not see them
- Continuous approach: They make life difficult

## A new method

A new method: Splitting + alternating descent algorithm.

*C. Castro, F. Palacios, E. Z., M3AS, 2008.*

Ingredients:

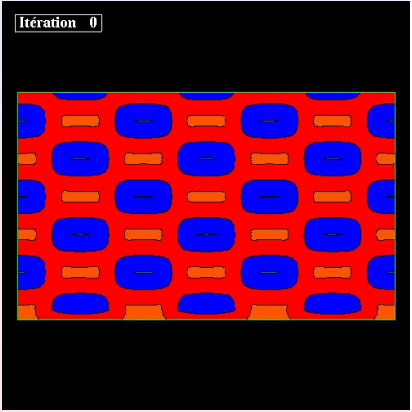
- The shock location is part of the state.

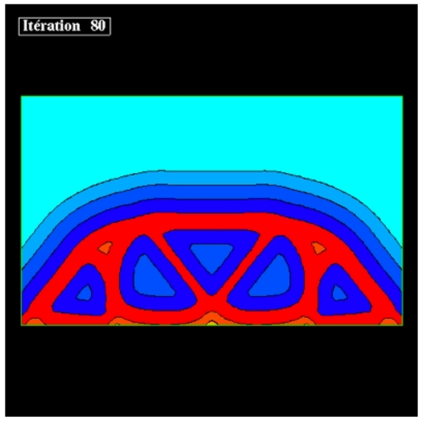
  State = Solution as a function + Geometric location of shocks.

- 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.

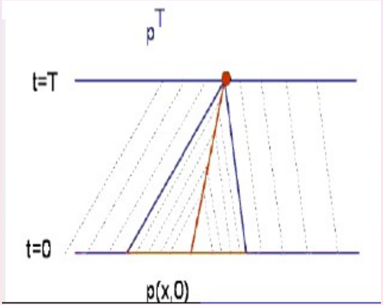
Gateaux derivative:

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

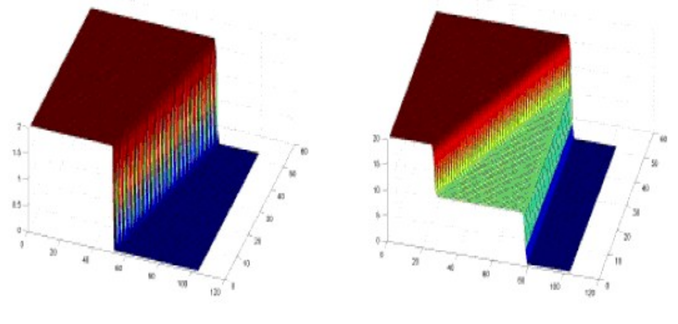
$(p,q)$ = adjoint state

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

- 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 adjoint system

Adjoint system = shorcut = all derivaties in one shot!

Consider the functional

$$J(\varepsilon) = \frac{1}{2} < Bu, u >, \quad B = \text{ symmetric}$$

$$u = u(\varepsilon) = \text{state}, \quad A(\varepsilon)u(\varepsilon) = b(\varepsilon).$$

Then,

$$\delta J(0) =< Bu, \delta u >, \quad A(0)\delta u = \delta b - \delta A(0)u(0).$$

$$A^*(0)p = Bu \quad (\text{adjoint system}),$$

and

$$< Bu, \delta u >=< A^*(0)p, \delta u >=< p, A(0)\delta u >=< p, \delta b - \delta A(0)u(0) > .$$

## 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, [2] Godunov's, Lax-Friedfrichs and Engquits-Osher schemes fulfil the OSLC condition.

[2] 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

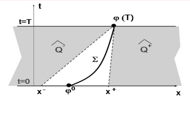
- Generalized tangent vectors $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ s. t.

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

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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## An open problem: Alternating descent / steepest descent.

- **Steepest descent:**

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

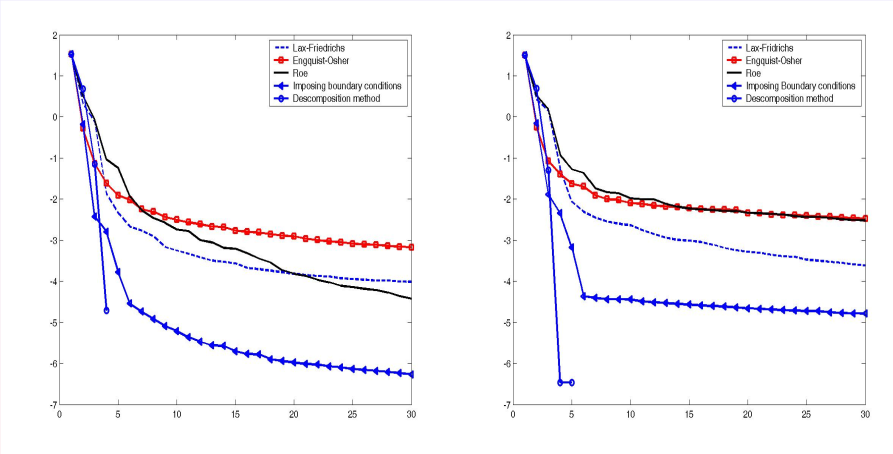
Discrete version of continuous gradient systems

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

- **Alternating descent:** $J = J(x, y)$

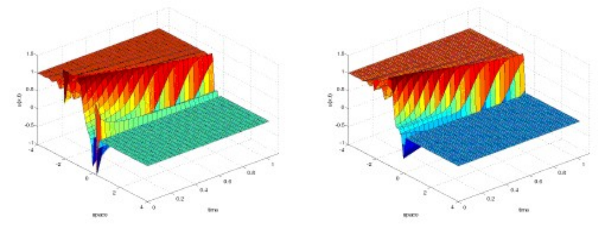
$$u_{k+1/2} = u_k - \rho J_x(u_k); \quad u_{k+1} = u_{k+1/2} - \rho J_y(u_k).$$

What's the continuous analog? Does it correspond to a class of dynamical systems for which the stability is understood?

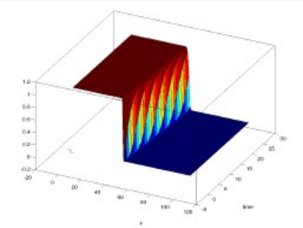



Splitting+Alternating wins!


Sol y sombra!

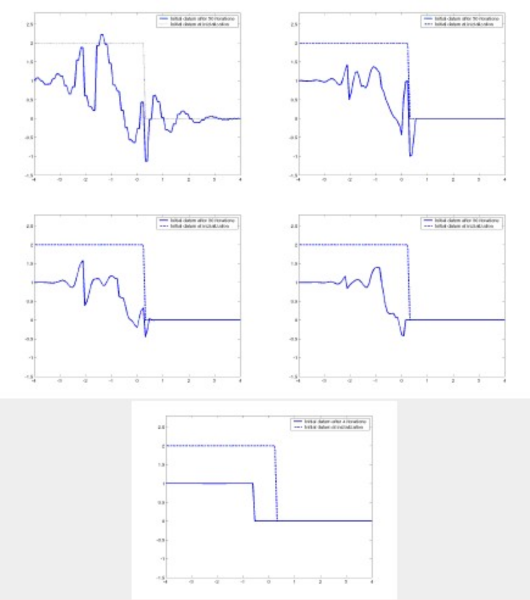


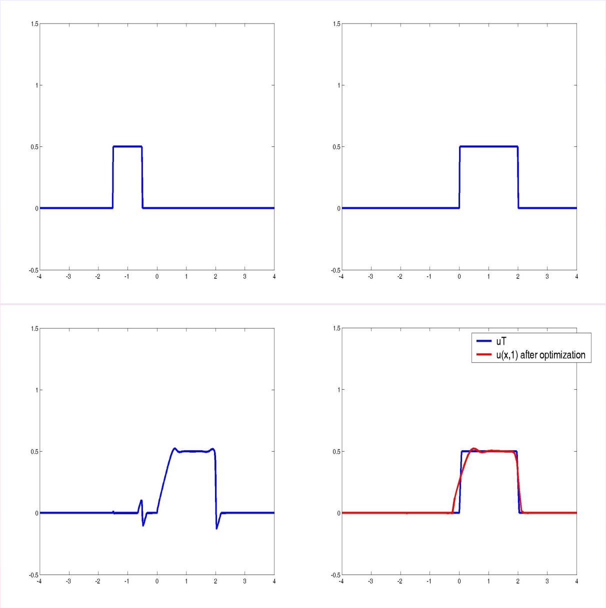
Results obtained applying Engquist-Osher's scheme and the one based on the complete adjoint system



Splitting+Alternating method.

# After 30 iterations:



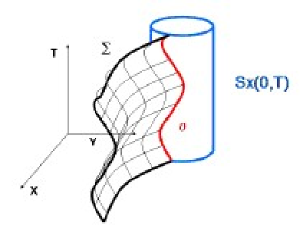

uT
u(x,1) after optimization

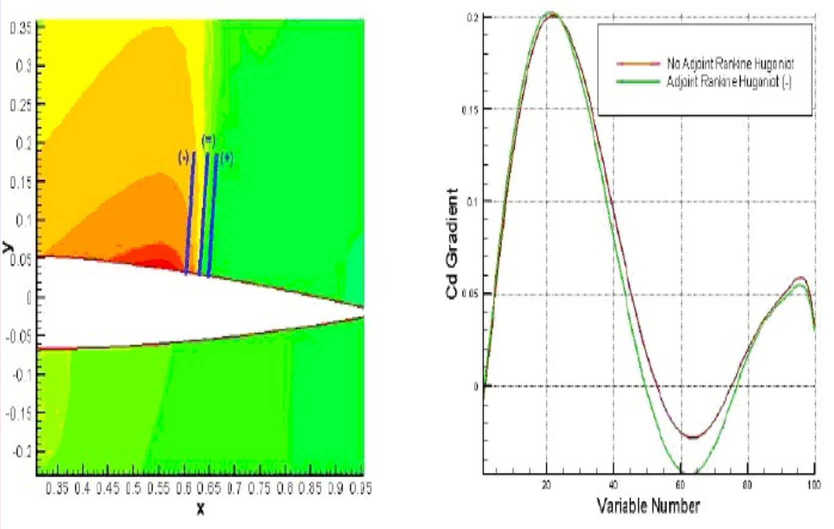
Splitting+alternating is more efficient:

- 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.

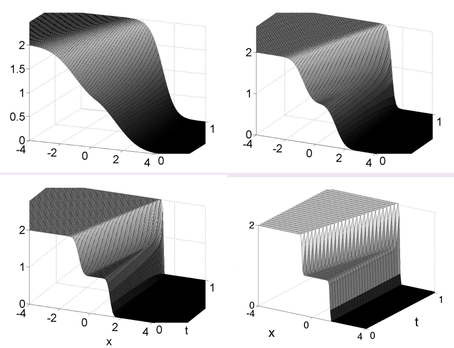
Numerical schemes for PDE + shock detection + shape, shock deformation + mesh adaptation,...






Influence of shock wave location (Drag Minimization).

# Viscous models




Adjoint solutions for different viscous values of the viscosity parameter: $\nu = 0.5$ (upper left), $\nu = 0.1$ (upper right) and $\nu = 0.01$ (lower left) and the exact adjoint solution (lower right).

## Related open problems.

Vanishing viscosity limit of the viscous adjoint system towards the unexpected inviscid one.

$$-\partial_t p - \nu p_{xx} - u\partial_x p = 0$$

$$\lim_{\nu \to 0} ????$$

$$\begin{cases} -\partial_t p - u\partial_x p = 0, \quad \text{in } Q^- \cup Q^+, \\ [p]_\Sigma = 0, \\ q(t) = p(\varphi(t), t), \text{ in } t \in (0, T) \\ q'(t) = 0, \text{ in } t \in (0, T) \end{cases}$$

Similar problems arise in other contexts.

- Zero dispersion limit? (J. Correia)
- For instance, the limit of

$$-\mathrm{div}(|\nabla u|^{p-2}\nabla u) = f$$

as $p \to \infty$ has been intensively investigated (J. M. Urbano,...)
Consider the linearized ajoint system

$$-\mathrm{div}(|\nabla u|^{p_2}\nabla p) = 1.$$

What's its limit?
Is it the adjoint of the linearized $\infty$-Laplacian?

## Flux identification.

$$\begin{cases} \partial_t u + \partial_x(f(u)) = 0, & \text{in } \mathbf{R} \times (0, T), \\ u(x,0) = u^0(x), & x \in \mathbf{R}. \end{cases}$$

This time the control is the nonlinearity $f$. It is actually an inverse problem.


- F. James and M. Sepúlveda, Convergence results for the flux identification in a scalar conservation law. *SIAM J. Control Optim.* **37**(3) (1999) 869-891.
- C. Castro and E. Zuazua, Flux identification for 1-d scalar conservation laws in the presence of shocks, preprint, 2009.

- 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.

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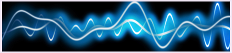

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