Flow control in the presence of shocks

Enrique Zuazua

Ikerbasque & Basque Center for Applied Mathematics (BCAM)
Bilbao, Basque Country, Spain
zuazua@bcamath.org
http://www.bcamath.org/zuazua/

ADVANCED METHODS AND PERSPECTIVES IN NONLINEAR OPTIMIZATION AND CONTROL, Toulouse, February 2010

Outline

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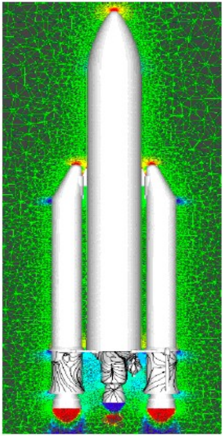
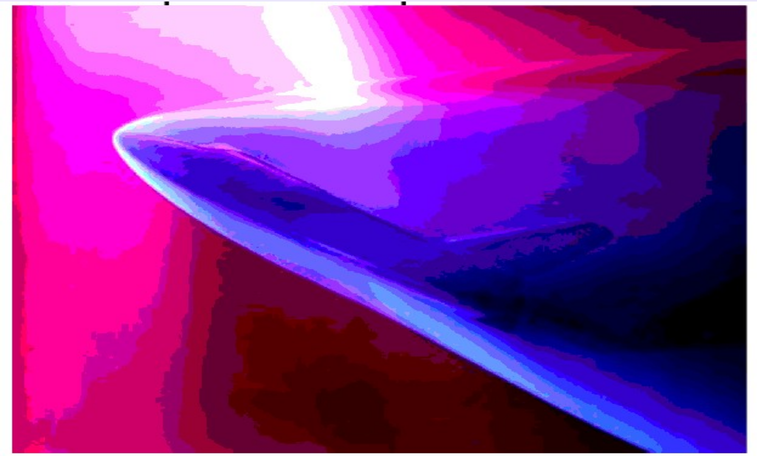
Meta or hypermotivation





More realistic/mathematical motivation

- Solve control, optimization, and/or optimal design problems involving solutions of Partial Differential Equations (as the main models of Continuum Mechanics) when solutions involve singularities.
- Classical intuition and/or "smooth calculus" fails....

Continuous versus discrete

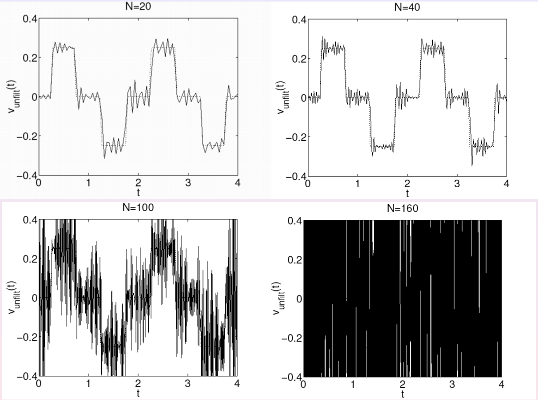
Two approaches:

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

Do these processes lead to the same result?

$$\text{OPTIMAL DESIGN} + \text{NUMERICS}$$
$$=$$
$$\text{NUMERICS} + \text{OPTIMAL DESIGN?}$$

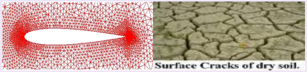
NO!!!!!!



E. Z., SIAM Review, 47 (2) (2005), 197-243.

Discrete: Discretization + gradient

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



    - Scheme dependent.

Continuous: Continuous gradient + discretization.

- Advantages: "Simpler" formal computations. Solver independent. Shock detection.
- Drawbacks:
    - Yields approximate gradients.
    - Subtle if shocks.
    - Hard to justify analytically. The one million dollar problem! http://www.claymath.org/millennium/Navier-Stokes_Equatio

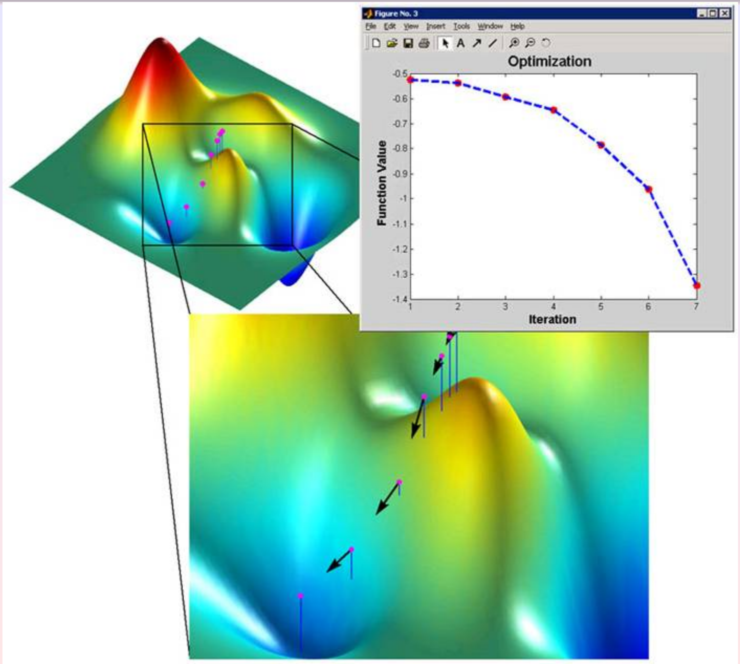
The idea: Alternating descent algorithms.

Steepest descent:

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

Discrete version of continuous gradient systems

$$u'(\tau) = -\nabla J(u(\tau)).$$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Optimization
Function Value
Iteration
-0.5
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-1
-1.1
-1.2
-1.3
-1.4
1
2
3
4
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6
7

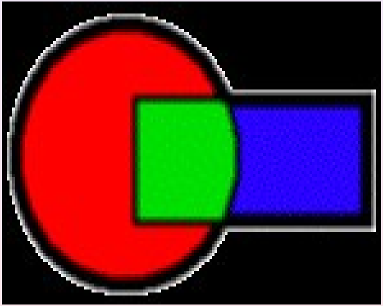
What if the u is vector valued ? $u = (x, y)$ and $J = J(x, y)$.
Alternating descent:

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

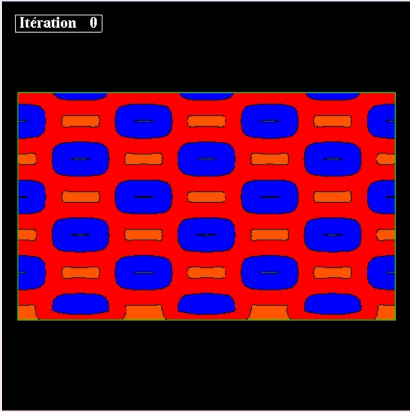
- **Motivation:**
  - x and y represent physical variables of different nature. Multiphysics problems.
  - Splitting the gradient into J_x and J_y may help on capturing the anisotropy of the graph.
  - Functionals J that are non-smooth with respect to some of the variables.
- **Question:** What's the continuous analog? Does it correspond to a class of dynamical systems for which the stability is understood?

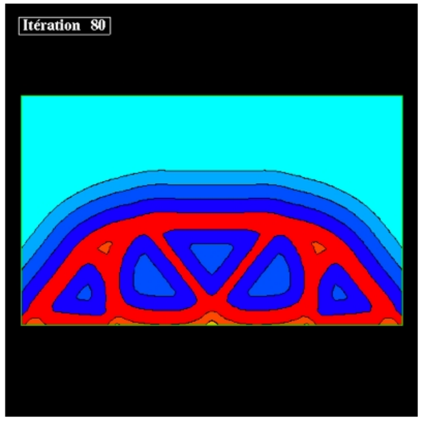
Inspired on domain decomposition techniques (Karl Hermann Amandus Schwarz (1843 – 1921)) and Marius Sophus Lie (1842 – 1899):

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



These kind of algorithms are used (without may be stating them that way) in various contexts. For instance in optimal design in elasticity where shape and topological derivatives are combined:





G. Allaire's web page, Ecole Polytechnique.

- In this case there is one single physics but two control or design parameters: external shape and inner topology.
- In some cases the possible presence of two distinguished physics and/or control parameters is not completely obvious. Part of the game is to identify the appropriate x and y !

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, 2 – 12 (1940).
- E. Hopf, The partial dfferential equation $u_t + uu_x = u_{xx}$, Comm. Pure Appl. Math. 3, 201 –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

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

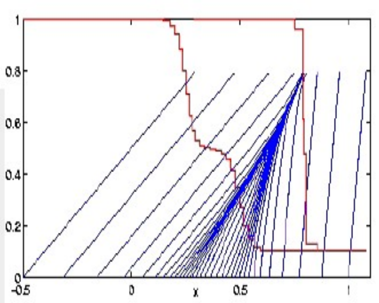
- There is a change of variable reducing the problem to the linear heat equation. This leads to explicit solutions.
- One can show explicitly the presence of shocks.
  G.B. Whitham, Linear and nonlinear waves, New York, Wiley-Interscience, 1974.

- Viscous version:

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

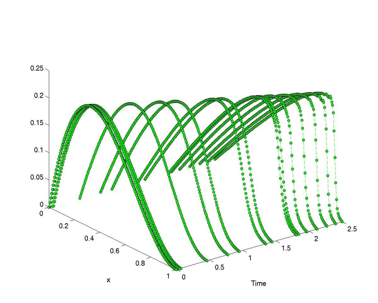
- Inviscid one:

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



Solutions may develop shocks or quasi-shock configurations.

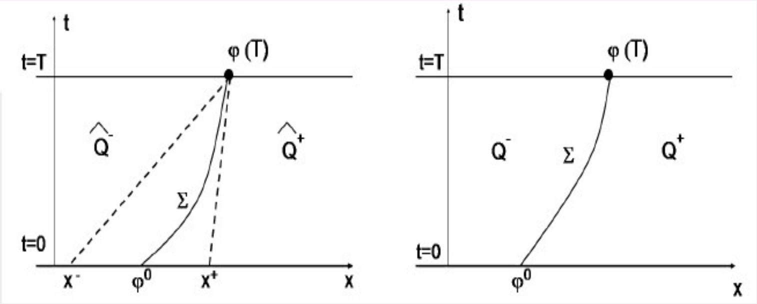
- For shock solutions, classical calculus fails: The derivative of a discontinuous function is a Dirac delta;
- For quasi-shock solutions the sensitivity (gradient) is so large that classical sensitivity calculus is meaningless.



Solution as a pair: flow+shock variables

Then the pair (u, φ)= (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

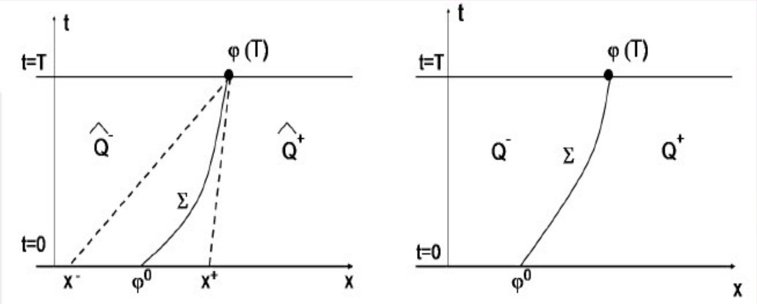
$$\varphi'(t)[u]_{\varphi(t)} = \left[u^2/2\right]_{\varphi(t)}$$

governs the behaviour of shock waves normal to the oncoming flow.

- 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, φ) solves:

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



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

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

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,...)

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.

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,....

An example: Inverse design of initial data

Consider

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

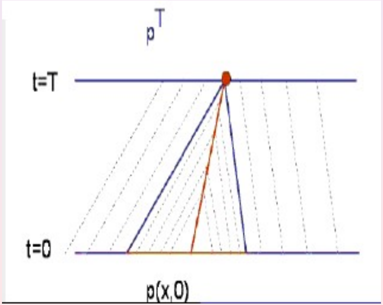
u^d = step function.
Gateaux derivative:

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

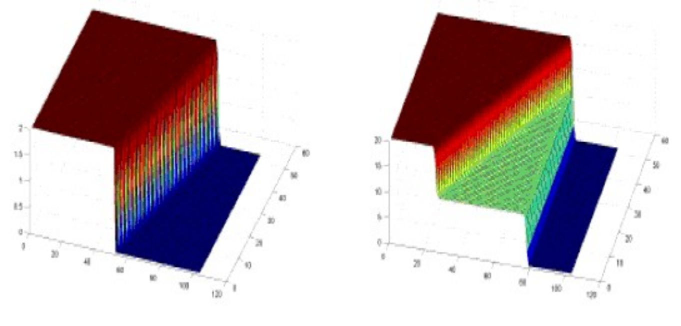
(p, q) = adjoint state

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

- 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 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

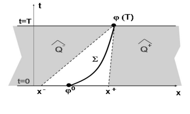
- Generalized tangent vectors $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ s. t.

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

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

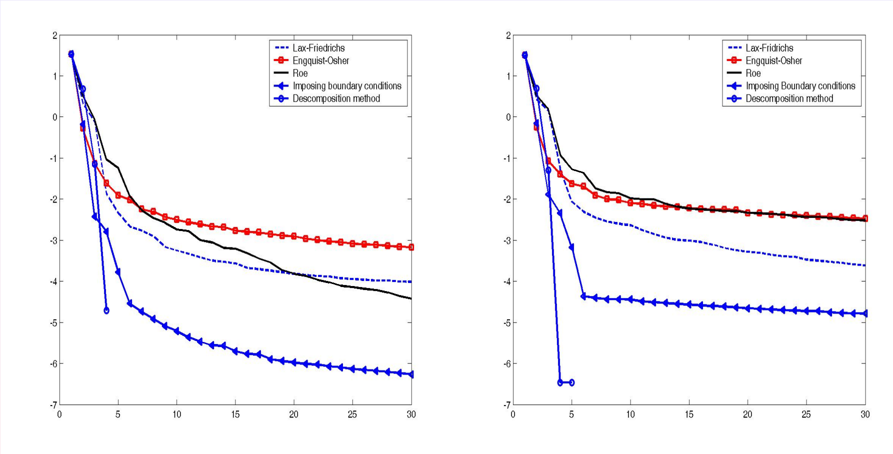
$$\delta J = -\left[\frac{(u(x,T) - u^d(x))^2}{2}\right]_{\varphi(T)} \frac{[u^0]_{\varphi^0}}{[u(\cdot, T)]_{\varphi(T)}} \delta\varphi^0.$$

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:

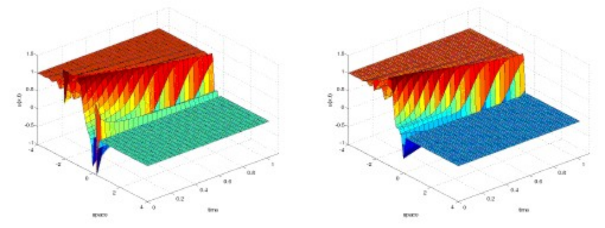
- Step 1: Use variations that only care about the shock location
- Step 2: Use variations that do not move the shock and only affect the shape away from it.



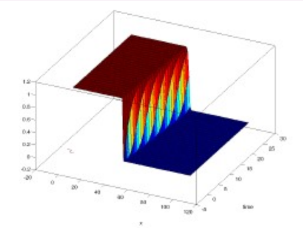
Splitting+Alternating wins!

Why?

Sol y sombra!

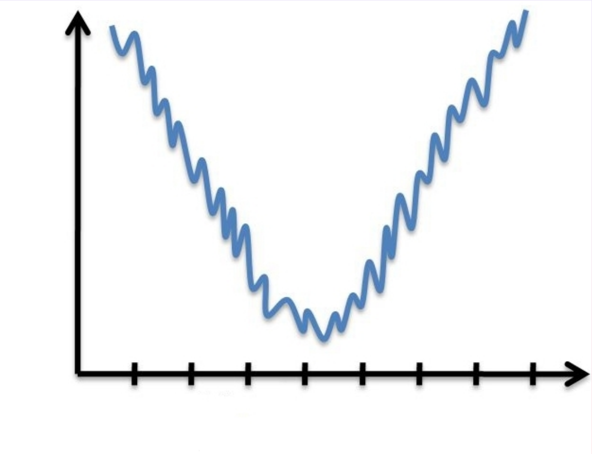


Results obtained applying Engquist-Osher's scheme and the one based on the complete adjoint system



Splitting+Alternating method.

- Numerical schemes replace shocks by oscillations.
- The oscillations of the numerical solution introduce oscillations on the approximation of the functional J:

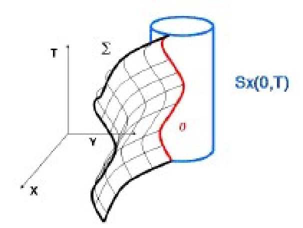


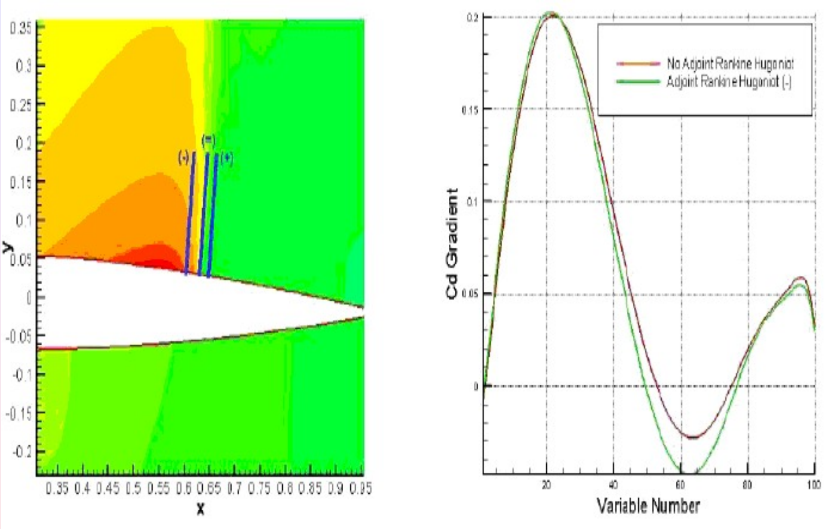
Splitting+alternating is more efficient:

- 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.

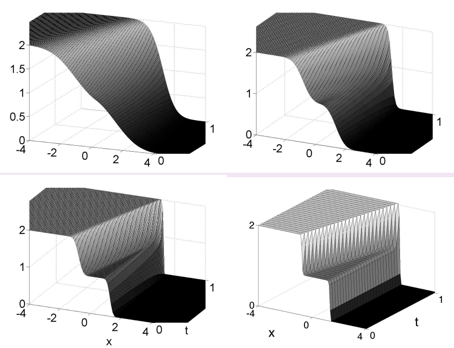
Numerical schemes for PDE + shock detection + shape, shock deformation + mesh adaptation,... Works by F. Lauzet (INRIA).





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).

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.

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