Control and Numerics : Continuous versus discrete approaches

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INSTITUTE OF MATHEMATICS "SIMION STOILOW" OF THE ROMANIAN ACADEMY, Bucharest, March 2011

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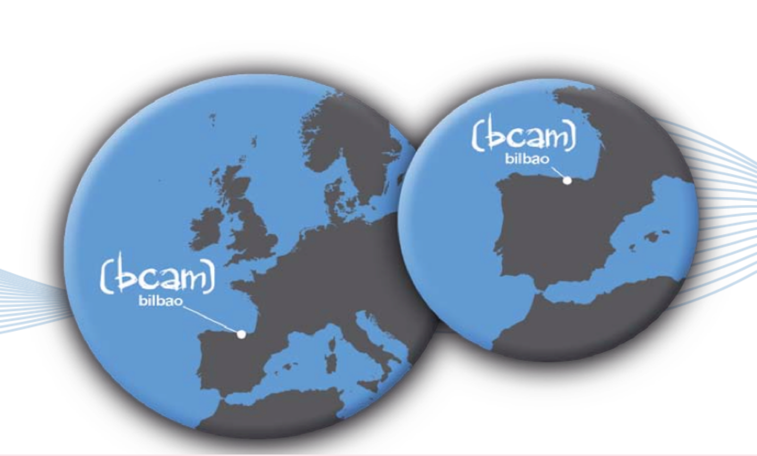
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GENERAL

Los rumanos, «muy parecidos» a los vascos

La comunidad extranjera más numerosa de Euskadi es también la más integrada socialmente

22.08.10 - 02:45 - ARTURO PUENTE | BILBAO.

El rumano no solo es el colectivo de extranjeros más numeroso en Euskadi -15.290 empadronados, según los últimos datos oficiales-, sino uno de los más integrados socialmente. Está presente en todos los municipios, ya sea en la construcción, en el servicio de las terrazas, en el cuidado de personas mayores y en las explotaciones agrarias de los caseríos. Forma una comunidad muy extensa -uno de cada diez inmigrantes afincados en el País Vasco es de ese origen-, pero quizá debido su rápida adaptación pasa más desapercibida que otras.

Fieles rumanos, en la celebración ortodoxa de la Ascensión en un templo de Derio. :: PEDRO URRESTI

Alexander Sandu, un rumano establecido en Bilbao desde hace años -«ni me acuerdo de cuántos»-, apunta algunas razones de su integración. «Somos gente muy parecida a los vascos: profundamente sociales, vivimos para la familia y los amigos, nos gusta charlar delante de una taza de café y disfrutar de la buena mesa», explica. También el idioma ayuda a esa rápida asimilación. «Nuestra lengua se parece bastante al castellano, así que nos hacemos rápido con el vocabulario y las expresiones», señala.

Motivation

Control problems for PDE are interesting for at least two reasons:

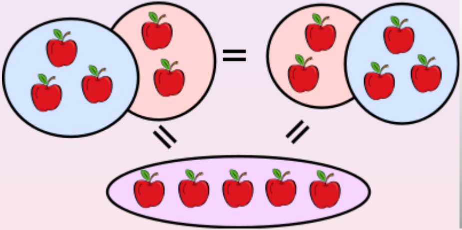
- They emerge in most real applications. PDE as the models of Continuum and Quantum Mechanics. Furthermore, in real world, there is always something to be optimized, controlled, optimally shaped, etc.
- Answering to these control problems often requires a deep understanding of the underlying dynamics and a better master of the standard PDE models.

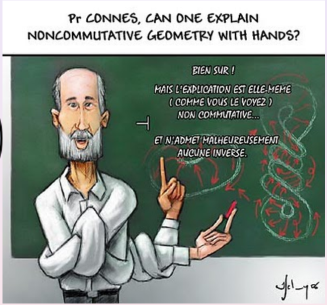
Surprisingly enough, this has led to an important ensemble of new tools and results and some fascinating problems are still widely open.
Furthermore, these kind of techniques are of application in some other fields, such as inverse problems theory and parameter identification issues.

These problems are also challenging and important from the viewpoint of numerical analysis and, often,

Classical intuition and/or “smooth calculus” fails....

Two ingredients: **Control** + **Numerics**
Do they commute?





Continuous versus discrete

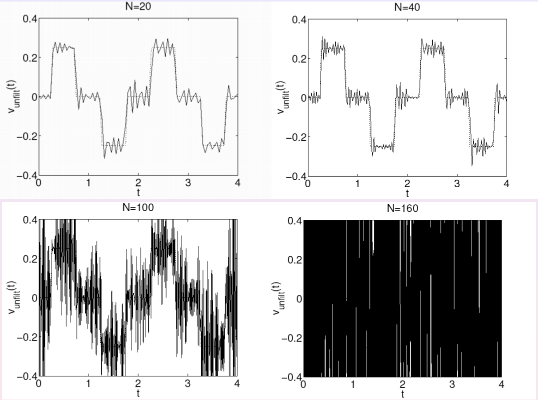
Two approaches:

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

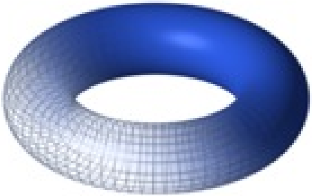
Do these processes lead to the same result?

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

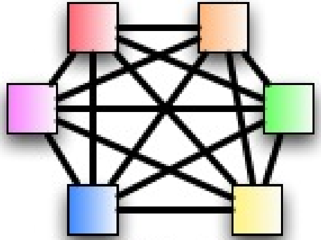
NO!!!!!!



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



A topological space:
the 2-Torus



A Graph:
the 6-clique

Important contributions by the romanian school:

- Sorin Micu, Fine estimates using moment problems and harmonic and complex analysis techniques
- Liviu Ignat, Bi-grid algorithms, harmonic analysis and dispersive estimates,...
- And many others: D., Cioranescu, M. Tucsnak, M. Negreanu, A. Marica, N. Cindea, C. Cazacu,...

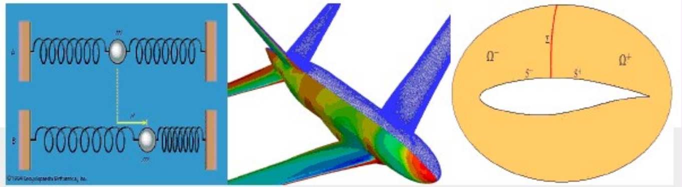
Connected also with the work by D. Tiba on optimal design and finite element approximations.

This is due to numerical spurious solutions.

Numerical analysis ensures that all solutions of the PDE can be approximated by the numerical ones but it does not guarantee that other virtual numerical realities emerge.

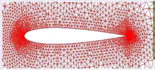
And in fact they often do and can generate damage.

These issues have been investigated systematically in the context of aeronautics in the search of optimal shapes.



Discrete: Discretization + gradient

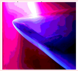
- Advantages: Discrete clouds of values. No shocks. Automatic differentiation, ...
- Drawbacks:
  - "Invisible" geometry.

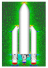


  - Scheme dependent.

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





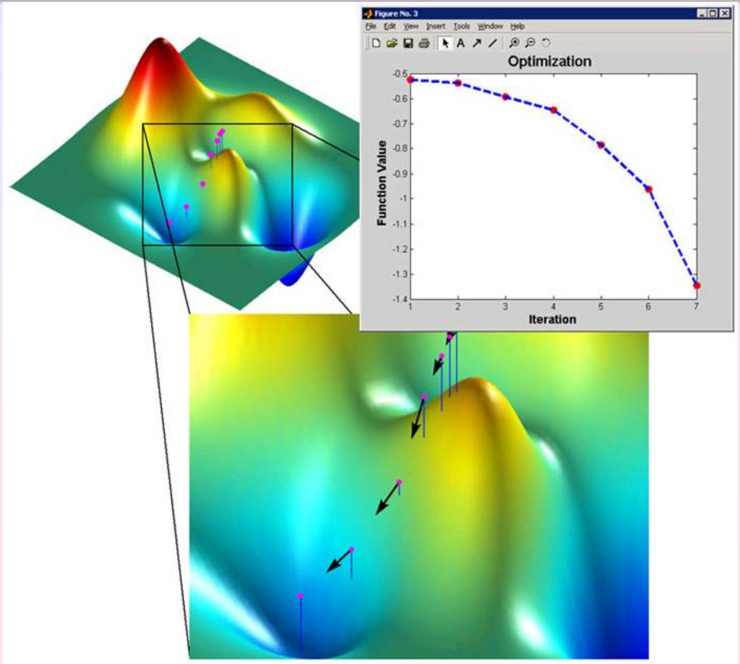

The idea: Alternating descent algorithms.

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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7

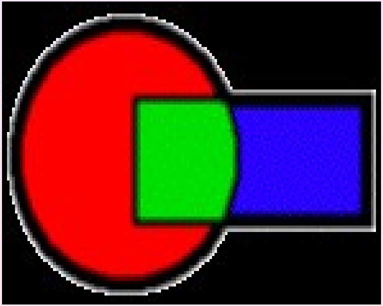
What if the u is vector valued ? $u = (x, y)$ and $J = J(x, y)$.
Alternating descent:

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

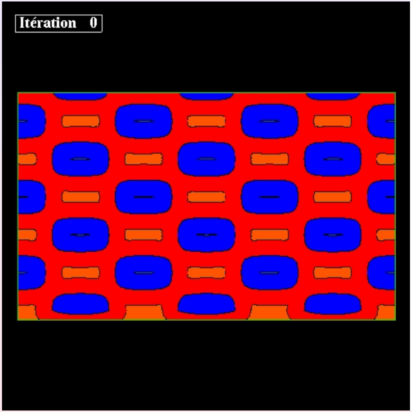
- **Motivation:**
  - x and y represent physical variables of different nature. Multiphysics problems.
  - Splitting the gradient into J_x and J_y may help on capturing the anisotropy of the graph.
  - Functionals J that are non-smooth with respect to some of the variables.
- **Question:** What's the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

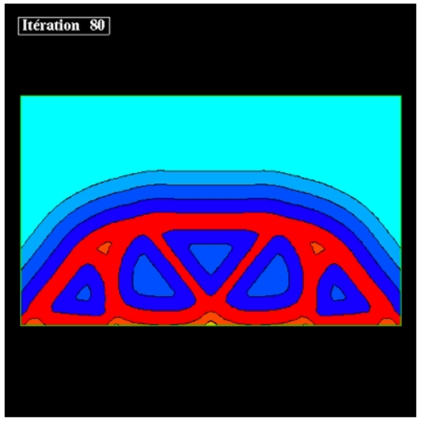
Inspired on domain decomposition techniques (Karl Hermann Amandus Schwarz (1843 – 1921)) and Marius Sophus Lie (1842 – 1899):

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



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

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

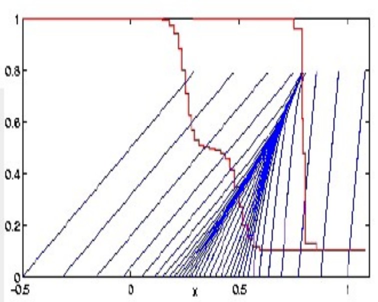
- There is a change of variable reducing the problem to the linear heat equation. This leads to explicit solutions.
- One can show explicitly the presence of shocks. G.B. Whitham, Linear and nonlinear waves, New York, Wiley-Interscience, 1974.

- Viscous version:

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

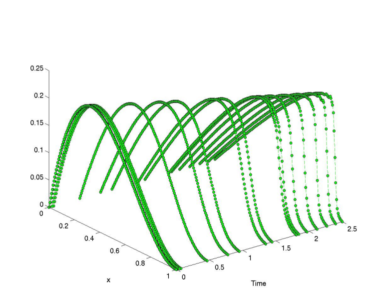
- Inviscid one:

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



Solutions may develop shocks or quasi-shock configurations.

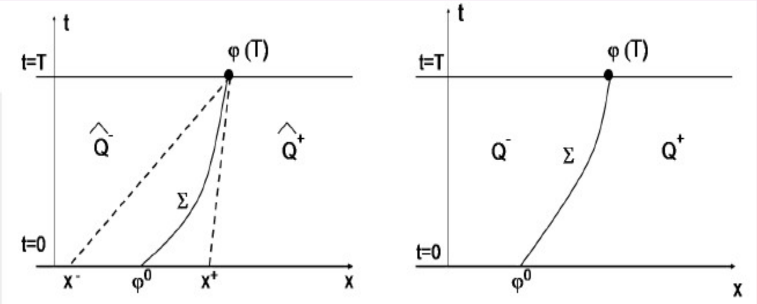
- For shock solutions, classical calculus fails: The derivative of a discontinuous function is a Dirac delta;
- For quasi-shock solutions the sensitivity (gradient) is so large that classical sensitivity calculus is meaningless.



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

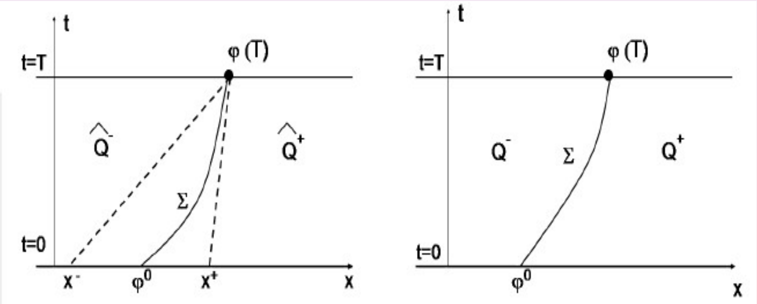
$$\varphi'(t)[u]_{\varphi(t)} = \left[u^2/2\right]_{\varphi(t)}$$

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:

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



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

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

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,...)

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.

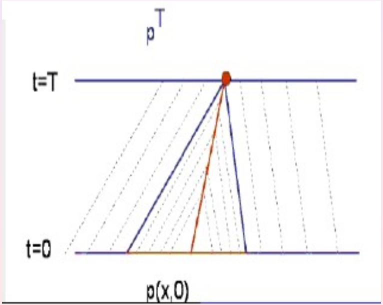
Gateaux derivative:

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

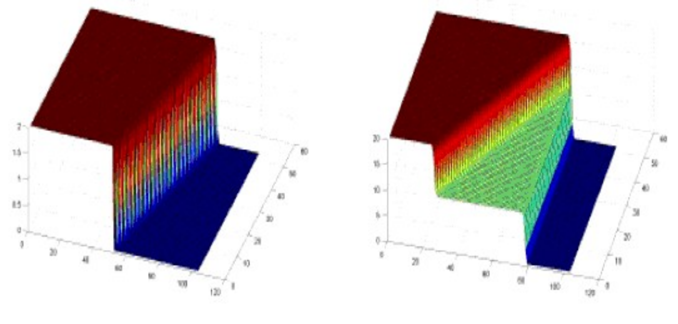
(p,q) = adjoint state

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

- 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

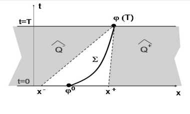
- Generalized tangent vectors $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ s. t.

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

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

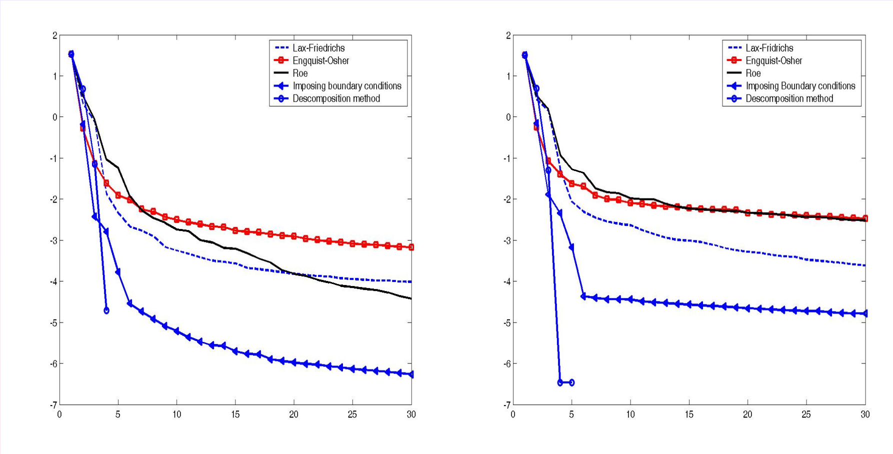
$$\delta J = -\left[\frac{(u(x,T)-u^d(x))^2}{2}\right]_{\varphi(T)} \frac{[u^0]_{\varphi^0}}{[u(\cdot,T)]_{\varphi(T)}}\delta\varphi^0.$$

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:

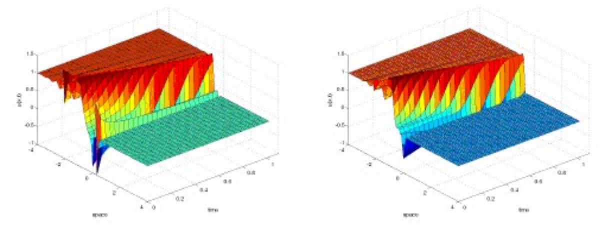
- Step 1: Use variations that only care about the shock location
- Step 2: Use variations that do not move the shock and only affect the shape away from it.



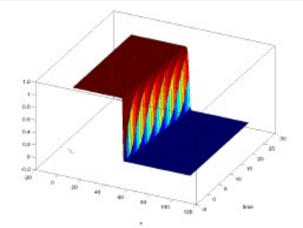
Splitting+Alternating wins!

Why?

Soare și umbră!

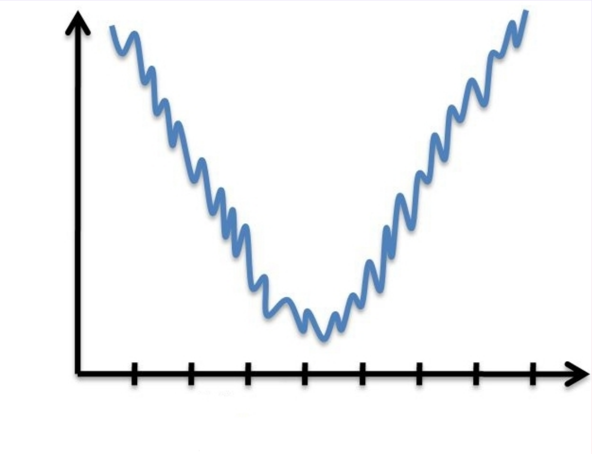


Results obtained applying Engquist-Osher's scheme and the one based on the complete adjoint system



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,...