

# Control and numerical simulation of conservation laws in large time horizons

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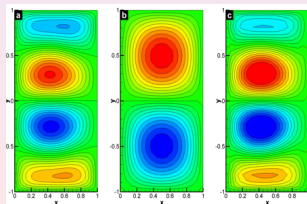
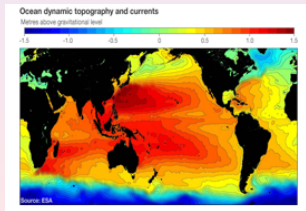
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# Climate modelling

- Climate modeling is a grand challenge computational problem, a research topic at the frontier of computational science.
- Simplified models for geophysical flows have been developed aim to: capture the important geophysical structures, while keeping the computational cost at a minimum.
- Although successful in numerical weather prediction, these models have a prohibitively high computational cost in climate modeling.



Xu Wang, [www.ima.umn.edu/wangzhu/](http://www.ima.umn.edu/wangzhu/)

## Thames barrier

- The Thames Barrier's purpose is to prevent London from being flooded by exceptionally high tides and storm surges.
- A storm surge generated by low pressure in the Atlantic Ocean, past the north of Scotland may then be driven into the shallow waters of the North Sea. The surge tide is funnelled down the North Sea which narrows towards the English Channel and the Thames Estuary. If the storm surge coincides with a spring tide, dangerously high water levels can occur in the Thames Estuary. This situation combined with downstream flows in the Thames provides the triggers for flood defence operations.



# Tsunamis

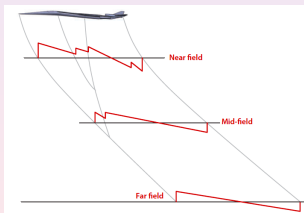
- Some isolated waves (solitons) are large and travel without loss of energy.
- This is the case of tsunamis and rogue waves.

Warning: Hence, there is no use trying sending a counterwave to stop a tsunami!



## Sonic boom

- Goal: the development of supersonic aircraft that are sufficiently quiet so that they can be allowed to fly supersonically over land.
- The pressure signature created by the aircraft must be such that, when it reaches the ground, (a) it can barely be perceived by the human ear, and (b) it results in disturbances to man-made structures that do not exceed the threshold of annoyance for a significant percentage of the population.



Juan J. Alonso and Michael R. Colonno, Multidisciplinary Optimization with Applications to Sonic-Boom Minimization, *Annu. Rev. Fluid Mech.* 2012, 44:505 – 26.

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# Geometric integration

## Numerical integration of the pendulum

## Joint work with L. Ignat &amp; A. Pozo

Consider the 1-D conservation law with or without viscosity:

$$u_t + [u^2]_x = \varepsilon u_{xx}, x \in \mathbb{R}, t > 0.$$

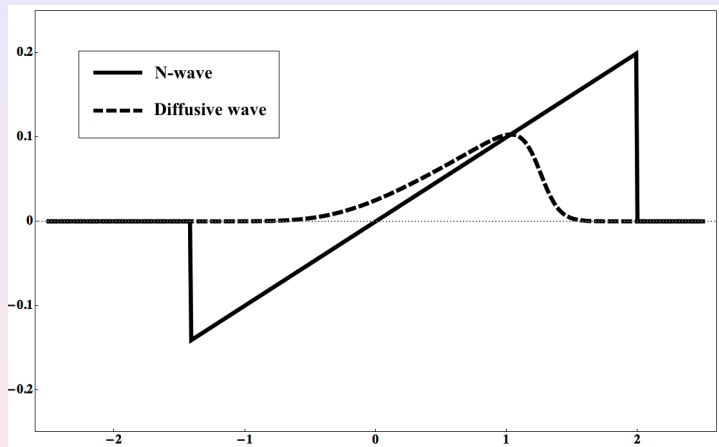
Then:

- If  $\varepsilon = 0$ ,  $u(\cdot, t) \sim N(\cdot, t)$  as  $t \rightarrow \infty$ ;
- If  $\varepsilon > 0$ ,  $u(\cdot, t) \sim u_M(\cdot, t)$  as  $t \rightarrow \infty$ ,

$u_M$  is the constant sign self-similar solution of the viscous Burgers equation (defined by the mass  $M$  of  $u_0$ ), while  $N$  is the so-called hyperbolic N-wave, defined as:

$$N(x, t) := \begin{cases} \frac{x}{t}, & \text{if } -2(pt)^{\frac{1}{2}} < x < (2qt)^{\frac{1}{2}} \\ 0 & \text{otherwise} \end{cases}$$

$$p := -2 \min_{y \in \mathbb{R}} \int_{-\infty}^y u^0(x) dx, \quad q := 2 \max_{y \in \mathbb{R}} \int_{-\infty}^y u^0(x) dx$$



## Conservative schemes

Let us consider now numerical approximation schemes

$$\begin{cases} u_j^{n+1} = u_n^j - \frac{\Delta t}{\Delta x} (g_{j+1/2}^n - g_{j-1/2}^n), & j \in \mathbf{Z}, n > 0. \\ u_j^0 = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u_0(x) dx, & j \in \mathbf{Z}, \end{cases}$$

The approximated solution  $u_\Delta$  is given by

$$u_\Delta(t, x) = u_j^n, \quad x_{j-1/2} < x < x_{j+1/2}, \quad t_n \leq t < t_{n+1},$$

where  $t_n = n\Delta t$  and  $x_{j+1/2} = (j + \frac{1}{2})\Delta x$ .

Is the large time dynamics of these discrete systems, a discrete version of the continuous one?

## 3-point conservative schemes

## 1 Lax-Friedrichs

$$g^{LF}(u, v) = \frac{u^2 + v^2}{4} - \frac{\Delta x}{\Delta t} \left( \frac{v - u}{2} \right),$$

## 2 Engquist-Osher

$$g^{EO}(u, v) = \frac{u(u + |u|)}{4} + \frac{v(v - |v|)}{4},$$

## 3 Godunov

$$g^G(u, v) = \begin{cases} \min_{w \in [u, v]} \frac{w^2}{2}, & \text{if } u \leq v, \\ \max_{w \in [v, u]} \frac{w^2}{2}, & \text{if } v \leq u. \end{cases}$$

## Numerical viscosity

We can rewrite three-point monotone schemes in the form

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{(u_{j+1}^n)^2 - (u_{j-1}^n)^2}{4\Delta x} = R(u_j^n, u_{j+1}^n) - R(u_{j-1}^n, u_j^n)$$

where the numerical viscosity  $R$  can be defined in a unique manner as

$$R(u, v) = \frac{Q(u, v)(v - u)}{2} = \frac{\lambda}{2} \left( \frac{u^2}{2} + \frac{v^2}{2} - 2g(u, v) \right).$$

For instance:

$$R^{LF}(u, v) = \frac{v - u}{2},$$

$$R^{EO}(u, v) = \frac{\lambda}{4} (v|v| - u|u|),$$

$$R^G(u, v) = \begin{cases} \frac{\lambda}{4} \text{sign}(|u| - |v|)(v^2 - u^2), & v \leq 0 \leq u, \\ \frac{\lambda}{4} (v|v| - u|u|), & \text{elsewhere.} \end{cases}$$

# Properties

These three schemes are well-known to satisfy the following properties:

- They converge to the entropy solution
- They are monotonic
- They preserve the total mass of solutions
- They are OSLC consistent:

$$\frac{u_{j-1}^n - u_{j+1}^n}{2\Delta x} \leq \frac{2}{n\Delta t}$$

- $L^1 \rightarrow L^\infty$  decay with a rate  $O(t^{-1/2})$
- Similarly they verify uniform  $BV_{\text{loc}}$  estimates

## Main result

## Theorem (Lax-Friedrichs scheme)

Consider  $u_0 \in L^1(\mathbf{R})$  and  $\Delta x$  and  $\Delta t$  such that  $\lambda \left| u^n \right|_{\infty, \Delta} \leq 1$ ,  $\lambda = \Delta t / \Delta x$ . Then, for any  $p \in [1, \infty)$ , the numerical solution  $u_\Delta$  given by the Lax-Friedrichs scheme satisfies

$$\lim_{t \rightarrow \infty} t^{\frac{1}{2}(1-\frac{1}{p})} \left| u_\Delta(t) - w(t) \right|_{L^p(\mathbf{R})} = 0,$$

where the profile  $w = w_{M_\Delta}$  is the unique solution of

$$\begin{cases} w_t + \left( \frac{w^2}{2} \right)_x = \frac{(\Delta x)^2}{2} w_{xx}, & x \in \mathbf{R}, t > 0, \\ w(0) = M_\Delta \delta_0, \end{cases}$$

with  $M_\Delta = \int_{\mathbf{R}} u_\Delta^0$ .



## Main result

## Theorem (Engquist-Osher and Godunov schemes)

Consider  $u_0 \in L^1(\mathbf{R})$  and  $\Delta x$  and  $\Delta t$  such that  $\lambda \left| u^n \right|_{\infty, \Delta} \leq 1$ ,  $\lambda = \Delta t / \Delta x$ . Then, for any  $p \in [1, \infty)$ , the numerical solutions  $u_\Delta$  given by Engquist-Osher and Godunov schemes satisfy the same asymptotic behavior but for the hyperbolic  $N$ -wave  $w = w_{p_\Delta, q_\Delta}$  unique solution of

$$\begin{cases} w_t + \left( \frac{w^2}{2} \right)_x = 0, & x \in \mathbf{R}, t > 0, \\ w(0) = M_\Delta \delta_0, & \lim_{t \rightarrow 0} \int_0^x w(t, z) dz = \begin{cases} 0, & x < 0, \\ -p_\Delta, & x = 0, \\ q_\Delta - p_\Delta, & x > 0, \end{cases} \end{cases}$$

with  $M_\Delta = \int_{\mathbf{R}} u_\Delta^0$  and  $p_\Delta = -\min_{x \in \mathbf{R}} \int_{-\infty}^x u_\Delta^0(z) dz$  and  $q_\Delta = \max_{x \in \mathbf{R}} \int_x^\infty u_\Delta^0(z) dz$ .

## Example

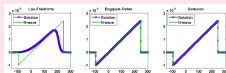
Let us consider the inviscid Burgers equation with initial data

$$u_0(x) = \begin{cases} -0.05, & x \in [-1, 0], \\ 0.15, & x \in [0, 2], \\ 0, & \text{elsewhere.} \end{cases}$$

The parameters that describe the asymptotic N-wave profile are:

$$M = 0.25, \quad p = 0.05 \quad \text{and} \quad q = 0.3.$$

We take  $\Delta x = 0.1$  as the mesh size for the interval  $[-350, 800]$  and  $\Delta t = 0.5$ . Solution to the Burgers equation at  $t = 10^5$ :





## Similarity variables

Let us consider the change of variables given by:

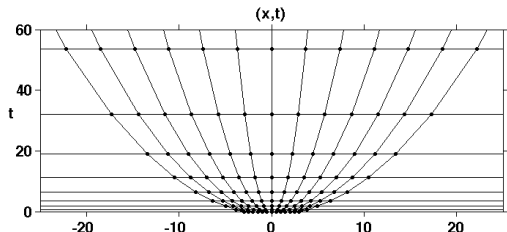
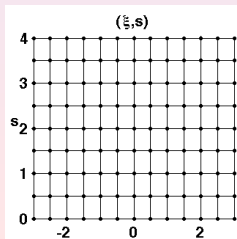
$$s = \ln(t + 1), \quad \xi = x/\sqrt{t + 1}, \quad w(\xi, s) = \sqrt{t + 1} u(x, t),$$

which turns the continuous Burgers equation into

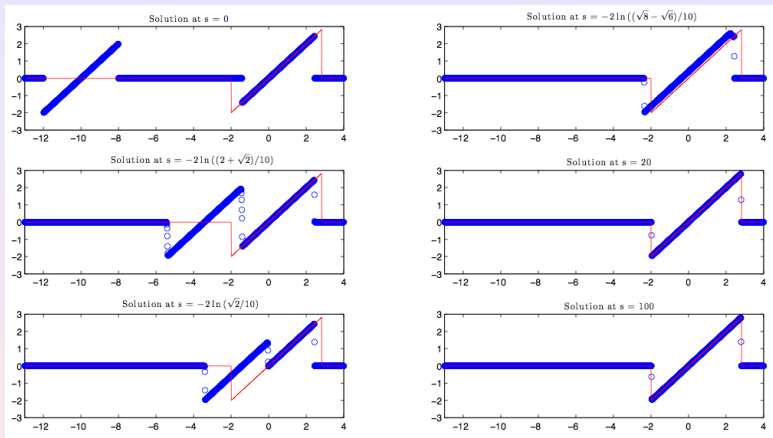
$$w_s + \left( \frac{1}{2} w^2 - \frac{1}{2} \xi w \right)_\xi = 0, \quad \xi \in \mathbf{R}, s > 0.$$

The asymptotic profile of the N-wave becomes a steady-state solution:

$$N_{p,q}(\xi) = \begin{cases} \xi, & -\sqrt{2p} < \xi < \sqrt{2q}, \\ 0, & \text{elsewhere,} \end{cases}$$



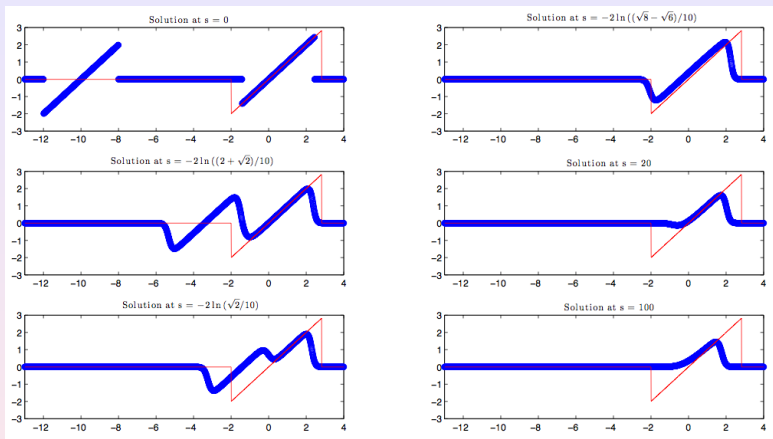
## Examples



Convergence of the numerical solution using Engquist-Osher scheme (circle dots) to the asymptotic N-wave (solid line). We take  $\Delta\xi = 0.01$  and  $\Delta s = 0.0005$ .

Snapshots at  $s = 0$ ,  $s = 2.15$ ,  $s = 3.91$ ,  $s = 6.55$ ,  $s = 20$  and  $s = 100$ .

## Examples



Numerical solution using the Lax-Friedrichs scheme (circle dots), taking  $\Delta\xi = 0.01$  and  $\Delta s = 0.0005$ . The N-wave (solid line) is not reached, as it converges to the diffusion wave.

Snapshots at  $s = 0$ ,  $s = 2.15$ ,  $s = 3.91$ ,  $s = 6.55$ ,  $s = 20$  and  $s = 100$ .

## Physical vs. Similarity variables

Comparison of numerical and exact solutions at  $t = 1000$ . We choose  $\Delta\xi$  such that the  $\left| \cdot \right|_{1,\Delta}$  error is similar. The time-steps are  $\Delta t = \Delta x/2$  and  $\Delta s = \Delta\xi/20$ , respectively, enough to satisfy the CFL condition.

For  $\Delta x = 0.1$ :

	Nodes	Time-steps	$\left  \cdot \right _{1,\Delta}$	$\left  \cdot \right _{2,\Delta}$	$\left  \cdot \right _{\infty,\Delta}$
Physical	1501	19987	0.0867	0.0482	0.0893
Similarity	215	4225	0.0897	0.0332	0.0367

For  $\Delta x = 0.01$ :

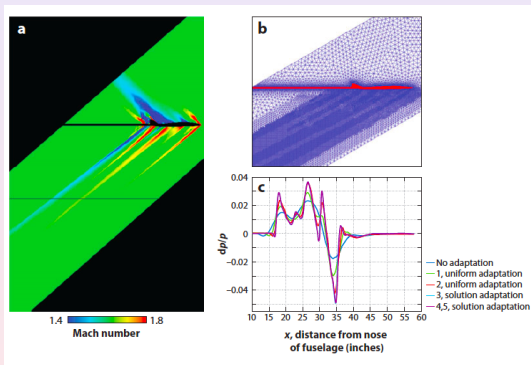
	Nodes	Time-steps	$\left  \cdot \right _{1,\Delta}$	$\left  \cdot \right _{2,\Delta}$	$\left  \cdot \right _{\infty,\Delta}$
Physical	15001	199867	0.0093	0.0118	0.0816
Similarity	2000	39459	0.0094	0.0106	0.0233

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The problem of inverse design, motivated by the problem of sonic-boom, and more precisely by the determination of the profile of the initial signature so to make sure it is acceptable when reaching earth, according to present regulations, can be formulated as an optimization or control problem in which the initial datum of the PDE under consideration.



Juan J. Alonso and Michael R. Colonno, Multidisciplinary Optimization with Applications to Sonic-Boom Minimization, *Annu. Rev. Fluid Mech.* (BCAM) 2012, 44:505 – 26.

Consider the minimization of the functional

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

associated to the solutions of the Burgers equation

$$\begin{cases} \partial_t u + \partial_x(u^2) - \varepsilon u_{xx} = 0 \\ u(x, 0) = u^0(x). \end{cases}$$

The minimization problem above can be proved to have a solution for a large class of targets and within reasonable classes of initial data.

What about its numerical computation?

## The discrete approach

The discrete version of the functional:

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

where  $u_\Delta = \{u_j^k\}$  solves a numerical discretization of the PDE based on some of the conservative schemes for conservation laws mentioned above.

In view of the very different asymptotic behavior of numerical solutions in large times, we also expect a different performance of the discrete optimization achieved.

In fact, we expect Engquist-Osher to perform well, but Lax-Friedrichs to have difficulties to recover the correct inverse design.



Is the iterative algorithm trapped in a local minimizer?

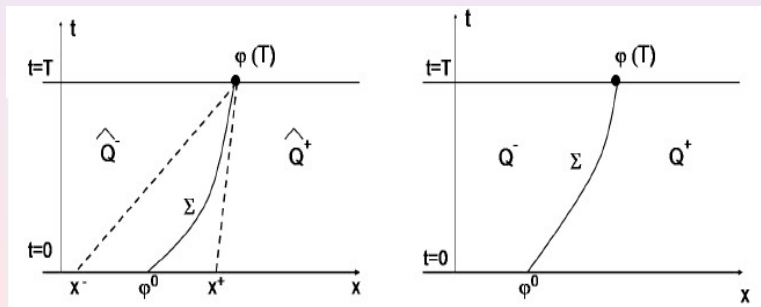
This is what the IPOPT software do (N. Allihverdi)

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

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





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

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

The difficulty may be overcome 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:

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

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

## Continuous versus discrete

Two approaches:

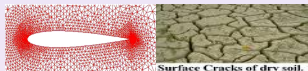
- **Continuous:** PDE + Optimal shape design  $\rightarrow$  implement that numerically.
- **Discrete:** Replace PDE and optimal design problem by discrete version  $\rightarrow$  Apply discrete tools

Do these processes lead to the same result?

$$\begin{aligned} &\text{OPTIMAL DESIGN} + \text{NUMERICS} \\ &= \\ &\text{NUMERICS} + \text{OPTIMAL DESIGN?} \end{aligned}$$

**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.



## 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 handled 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.

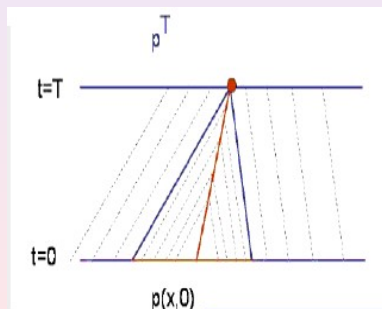
Gateaux derivative:

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

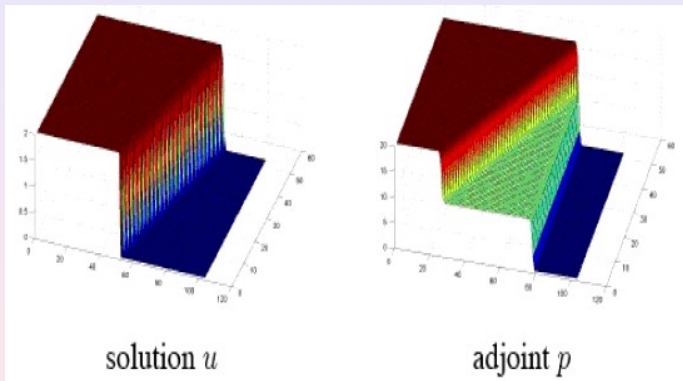
$(p, q) =$  adjoint state

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

- 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:





## The multi-dimensional case: Joint work with R. Lecarós

Consider the multi-dimensional scalar conservation, in the presence of one single shock curve:

$$\begin{aligned} \partial_t u + \operatorname{div}_x(f(u)) &= 0, & \text{in } Q_- \cup Q_+ \\ [u]n_\Sigma^t + [f(u)]n_\Sigma^x &= 0, & \text{on } \Sigma \\ u(x, 0) &= u^0(x), & x \in \mathbb{R}^2 \setminus \Sigma^0, \end{aligned}$$

The linearized system reads

$$\begin{aligned} \partial_t \delta u + \operatorname{div}_x(f'(u)\delta u) &= 0, & \text{in } Q_- \cup Q_+ \\ \operatorname{div}_\Sigma \left( \delta \varphi \left| n_\Sigma^x \right| \left( [f(u)]_{\Sigma^t}, [u]_{\Sigma^t} \right) \right) &= ([f'(u)\delta u]_{\Sigma^t}, [\delta u]_{\Sigma^t}) \cdot n_\Sigma, & \text{on } \Sigma \\ \delta u(x, 0) &= \delta u^0(x), & x \in \mathbb{R}^2 \setminus \Sigma^0 \\ \delta \varphi(x, 0) &= \delta \varphi^0(x), & x \in \Sigma^0 \end{aligned}$$

The Gateaux derivative of  $J$  can be written as follows

$$\delta J(u^0)[\delta u^0, \delta \varphi^0] = \int_{\mathbb{R}^2} p(x, 0) \delta u^0 dx - \int_{\Sigma^0} q(x, 0) [u]_{\Sigma^0} \delta \varphi^0 d\sigma,$$

where the adjoint state pair  $(p, q)$  satisfies the system

$$\begin{aligned} \partial_t p + f'(u) \cdot \nabla p &= 0, & \text{in } Q_- \cup Q_+ \\ [p]_{\Sigma^t} &= 0, & \text{on } \Sigma \\ q(x, t) &= p(x, t), & (x, t) \in \Sigma([f(u)]_{\Sigma^t}, [u]_{\Sigma^t}) \cdot \nabla_{\Sigma} q \\ &= 0, & \text{on } \Sigma \\ p(x, T) &= u(x, T) - u^d(x), & x \in \mathbb{R}^2 \setminus \Sigma^T \\ q(x, T) &= \frac{[(u(\cdot, T) - u^d)^2 / 2]_{\Sigma^T}}{[u]_{\Sigma^T}}, & x \in \Sigma^T. \end{aligned}$$

# Numerical experiment. Testing the alternating descent method.

The time is  $T = 0.2$ . The equation

$$u_t + \left(\frac{u^2}{2}\right)_x + \left(\frac{u^4}{4}\right)_y = 0 \quad (1)$$

$$u^0(x, y) = \begin{cases} 0.4 & x \leq 0.2 \wedge y \leq 0.4 \\ 0 & \text{other wise} \end{cases}$$

and  $u^d$  is the solution of (2) at time  $t = T$ , with initial datum  $u^*$ , given by

$$u^*(x, y) = \begin{cases} 0.7 & x \leq 0.8 \wedge y \leq 0.75 \\ 0 & \text{other wise} \end{cases}$$

# The discrete approach

Initial condition  $u^0$

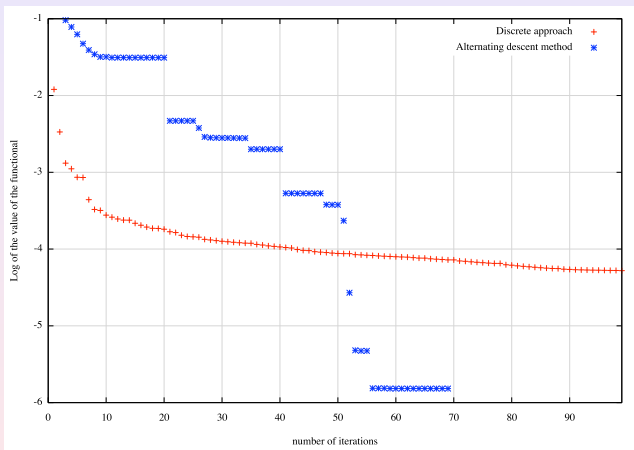
Solution at time  $T$ ,  $u^T$

# The alternating descent method in 2D

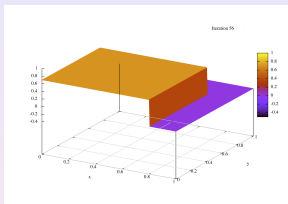
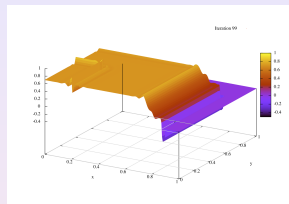
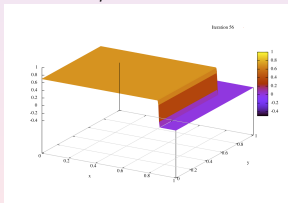
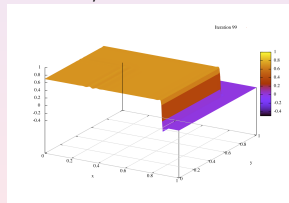
Initial condition  $u^0$

Solution at time  $T$ ,  $u^T$

# Comparison



## Comparison

ADM:  $u^0$ , iteration  $k = 43$ DM:  $u^0$ , iteration  $k = 99$ ADM:  $u^T$ , iteration  $k = 43$ DM:  $u^T$ , iteration  $k = 99$

## Numerical experiment. Testing the alternating descent method.

The time is  $T = 0.2$ . The equation

$$u_t + \left(\frac{u^2}{2}\right)_x + \left(\frac{u^4}{4}\right)_y = 0 \quad (2)$$

$$u^0(x, y) = \begin{cases} 0.4 & x \leq 0.3 \wedge y \leq 0.3 \\ 0 & \text{other wise} \end{cases}$$

and  $u^d$  is the solution of (2) at time  $t = T$ , with initial datum  $u^*$ , given by

$$u^*(x, y) = \begin{cases} 0.7 & x^2 + y^2 \leq (0.7)^2, x, y \geq 0 \\ 0.7 & x \leq 0.7, y \leq 0 \\ 0.7 & y \leq 0.7, x \leq 0 \\ 0 & \text{other wise} \end{cases}$$



# The discrete approach

Initial condition  $u^0$

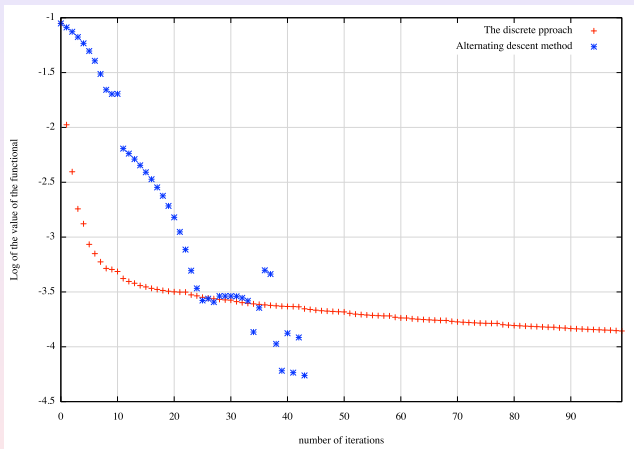
Solution at time  $T$ ,  $u^T$

# The alternating descent method in 2D

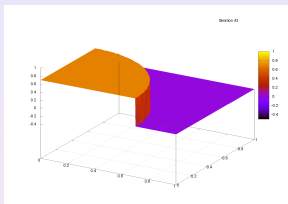
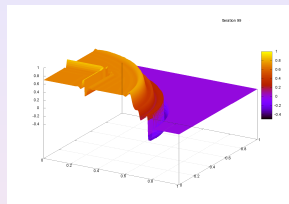
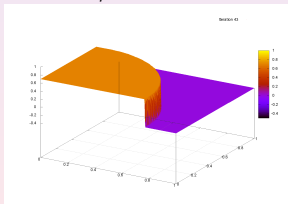
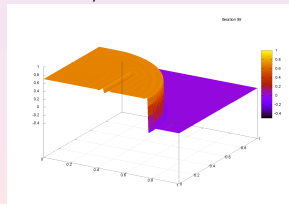
Initial condition  $u^0$

Solution at time  $T$ ,  $u^T$

## Comparison between the methods



## Comparison between the methods

ADM:  $u^0$ , iteration  $k = 43$ DM:  $u^0$ , iteration  $k = 99$ ADM:  $u^T$ , iteration  $k = 43$ DM:  $u^T$ , iteration  $k = 99$

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- 2 Long time numerical simulations
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- 5 Conclusions

Lots to be done on:

- Development of numerical algorithms preserving large time asymptotics for nonlinear PDEs (other works of our team on dispersive equations, dissipative wave equations,...)
- The analysis of how time-evolution controls are approximated by these numerical methods.
- Rigorous analysis of linearization around shocks, numerical approximation of the linearized system, etc.
- Use of geometric methods in combination with PDE ones to implement descent algorithms with moving shocks.
- Important applications.

All this needs to be made in a multidisciplinary environment so to assure impact on Engineering and Sciences

