Control and numerical simulation of conservation laws in long time horizons

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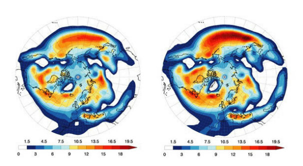
- (Hyperbolic) PDE
- Control
- Shocks
- Long time

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 with the 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.



P. L. Vidale, `http://www.met.reading.ac.uk/ vidale/`

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.

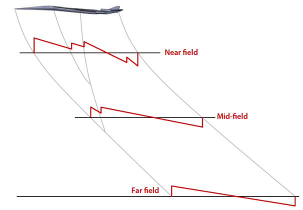
Tsunamis

- 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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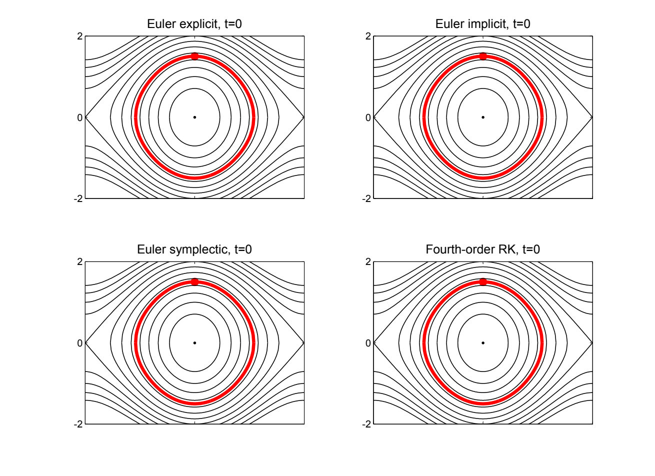
Geometric integration

Numerical integration of the pendulum



- Standard convergence of numerical schemes referes to convergence in finite time intervals $[0, T]$, $T < \infty$.
- standard convergence does not ensure a correct asymptotic behavior as $t \to \infty$ for the numerical solutions.
- Numerical schemes that do preserve the asymptotic behavior of the ODE solutions are said to be *simplectic* or *geometric*.

Joint work with L. Ignat & A. Pozo, Math of Computation, 2014

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

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

Then[2] :

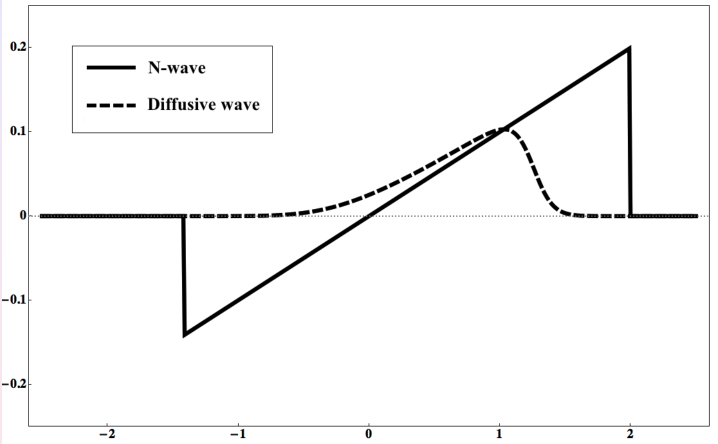
- If $\varepsilon = 0$, $u(\cdot, t) \sim N(\cdot, t)$ as $t \to \infty$;
- If $\varepsilon > 0$, $u(\cdot, t) \sim u_M(\cdot, t)$ as $t \to \infty$,

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:

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

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

[2] Y. J. Kim & A. E. Tzavaras, *Diffusive N-Waves and Metastability in the Burgers Equation*, SIAM J. Math. Anal. **33**(3) (2001), 607–633.


N-wave
Diffusive wave
0.2
0.1
0
−0.1
−0.2
−2
−1
0
1
2

Why in the inviscid case the asymptota is given by a N-wave?

Note that the equation can then be written as

$$u_t + 2uu_x = 0.$$

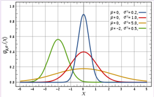
This is a transport equation, driven by the field $2u$. Thus, characteristics departing from points where $u < 0$ move towards the left while those in the region $u > 0$ to the right.

And why in the viscous case to a viscous wave?

This occurs already for the heat equation where the asymptotic behavior of solutions is given by the gaussian heat kernel [3]

$$u_t - u_{xx} = 0,$$

$$G(x,t) = (4\pi t)^{-1/2} exp(-|x|^2/4t).$$



Exercise: Prove that, if $f \in L^1(\mathbf{R}, 1+|x|)$ then

$$f(x) = \int f(x)dx\delta + [F]',$$

with $F \in L^1(\mathbf{R})$.

[3] J. Duoandikoetxea and E. Z.. Moments, masses de Dirac et décomposition de fonctions C. R. Acad. Sci. Paris. 315(6). 693-698. 1992.

There is no contradiction!!!

- Vanishing viscosity refers to the limit as $\varepsilon \to 0$ and t fixed;
- While the large time behavior refers to passing to the limit as $t \to \infty$ for ε fixed.

Both limit processes do not necessarily commute, $\varepsilon \to 0$ and $t \to \infty$, the same as they do not in the numerical approximation of ODEs, where the issue is rather $\Delta t \to 0$ versus $t \to \infty$.

Outline

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

$$v = v(x, t) = \int_{-\infty}^{x} u(s, t) ds \tag{1}$$

solves

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

Define then

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

that satisfies

$$w_t - w_{xx} + \frac{1}{\nu} | w_x |^2 = 0. \tag{3}$$

On the other hand,

$$z = w/\nu \tag{4}$$

satisfies

$$z_t - z_{xx} + \mid z_x \mid^2 = 0. \tag{5}$$

Introduce, at last,

$$\eta(x, t) = e^{-z} \tag{6}$$

that solves the heat equation

$$\eta_t - \eta_{xx} = 0. \tag{7}$$

Undoing the change of variables

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

Then

$$u(x, t) = -\nu \frac{\eta_x(x, \nu t)}{\eta(x, \nu t)}. \tag{8}$$

The solution η of this heat equation can be obtained by convolution with the heat kernel:

$$G(x,\ t) = (4\pi t)^{-1/2} \exp\left(- \mid x \mid^2 \Big/ 4t\right), \tag{9}$$

so that

$$\eta(x,\ t) = \Big[G(\cdot,\ t) * \eta_0(\cdot)\Big](x), \tag{10}$$

where η_0 is the initial datum of η.
On the other hand,

$$G_x(x,\ t) = -\frac{x}{4\sqrt{\pi}t^{3/2}} \exp\left(- \mid x \mid^2 \Big/ 4t\right). \tag{11}$$

In this way we get

$$u_\nu(x,\ t) = \frac{\int_{\mathbb{R}}(x-y)e^{-H(x,y,t)/\nu}dy}{2t\int_{\mathbb{R}}e^{-H(x,y,t)/\nu}dy} \tag{12}$$

where

$$H(x,\ y,\ t) = \frac{|\ x-y\ |^2}{4t} + \int_{-\infty}^{y} u_0(\sigma)d\sigma. \tag{13}$$

The contribution of the integral as $\nu \to 0^+$[4]

$$\int_{\mathbb{R}} f(y) e^{-H/\nu} dy \tag{14}$$

around the minimum $y = \xi$ is

$$f(\xi) \sqrt{\frac{2\pi\nu}{H''(\xi)}} e^{-H(\xi)/\nu}. \tag{15}$$

In our case

$$H''(\xi) = \frac{1}{2t}. \tag{16}$$

We get

$$\int_{\mathbb{R}} (x-y) e^{-H/\nu} dy \sim (x-\xi) \sqrt{\frac{\pi\nu}{t}} e^{-[tu_0^2(\xi) + \int_{-\infty}^{\xi} u_0(\sigma) d\sigma]\nu}, \tag{17}$$

$$\int_{\mathbb{R}} e^{-H/\nu} dy \sim \sqrt{\frac{\pi\nu}{t}} e^{-[tu_0^2(\xi) + \int_{-\infty}^{\xi} u_0(\sigma) d\sigma]}. \tag{18}$$

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

Then

$$u_\nu(x,\ t) \sim \frac{(x-\xi)}{2t} \tag{19}$$

where ξ is characterized by the equation

$$\xi = x - 2tu_0(\xi), \tag{20}$$

corresponding to the minima of H.
Thus

$$u_\nu(x,\ t) \sim u_0(\xi). \tag{21}$$

This is, precisely, the solution obtained by the method of characteristics:

$$u_\nu(x,\ t) \sim u_0(\xi). \tag{22}$$

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.

When there are two absolute minima ξ_1, ξ_2, the asymptotic form of u_ν would be:

$$u_\nu(x, t) \sim u_0(\xi_1) + u_0(\xi_2). \tag{23}$$

What does it mean?

We now consider the Riemann problem

$$u_0(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0. \end{cases} \tag{24}$$

We get:

- 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.
- In the intermediate zone we get $\xi = x/(1 + 2t)$ and

$$u(x,\ t) = \frac{x}{2t}. \tag{25}$$

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.

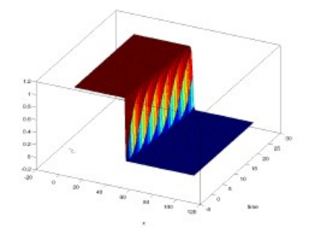
For the Riemann problem

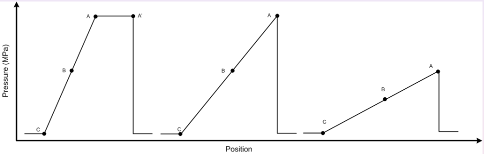
$$u_0(x) = \begin{cases} 1, & x < 0 \\ 0, & x > 0 \end{cases} \tag{26}$$

we get 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.





Shock versus rarefaction waves

The Oleinick entropy condition

Physical solutions of the Burgers equation satisfy

$$u_x \leq 1/2t. \tag{27}$$

Formally, $v = u_x$ satisfies

$$v_t + (2uv)_x = v_t + 2v^2 + 2uv_x = 0. \tag{28}$$

By the maximum principle we deduce that

$$v \leq w \tag{29}$$

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

$$w_t + 2w^2 = 0 \tag{30}$$

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.

Note that this is compatible with the structure of shock waves

Summary on entropy solutions of the Burgers equation

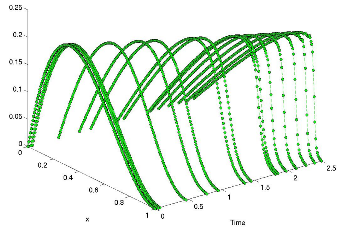
- Entropy solutions are the physical ones
- Entropy solutions are characterized by the zero viscosity limit.
- Entropy solutions are characterized also by the Oleinick inequality.
- Entropy solutions are unique (celebrated result by Kruzkov).

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.

As we have seen solutions may develop shocks or quasi-shock configurations.



References on the 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 differential 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).
- G.B. Whitham, Linear and nonlinear waves, New York, Wiley-Interscience, 1974.
- L. C. Evans, Partial Differential Equations, AMS, 1998.

Outline

Let us consider now numerical approximation schemes

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

The approximated solution u_Δ is given by

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

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

Is the large tine 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

$$g^{G}(u,v) = \begin{cases} \min\limits_{w\in[u,v]} \frac{w^2}{2}, & \text{if } u \le v, \\ \max\limits_{w\in[v,u]} \frac{w^2}{2}, & \text{if } v \le u. \end{cases}$$

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

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

For instance:

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

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

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

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:

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

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

Main result

Theorem (Lax-Friedrichs scheme)

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

$$\lim_{t\to\infty} t^{\frac{1}{2}(1-\frac{1}{p})} \Big| u_\Delta(t) - w(t) \Big|_{L^p(\mathbb{R})} = 0,$$

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 $M_\Delta = \int_{\mathbb{R}} u^0_\Delta$.

Main result

Theorem (Engquist-Osher and Godunov schemes)

Consider $u_0 \in L^1(\mathbf{R})$ and Δx and Δt such that $\lambda \Big| u^n \Big|_{\infty,\Delta} \leq 1$, $\lambda = \Delta t/\Delta x$. Then, for any $p \in [1,\infty)$, the numerical solutions u_Δ 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

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

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

Example

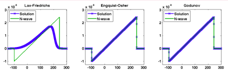
Let us consider the inviscid Burgers equation with initial data

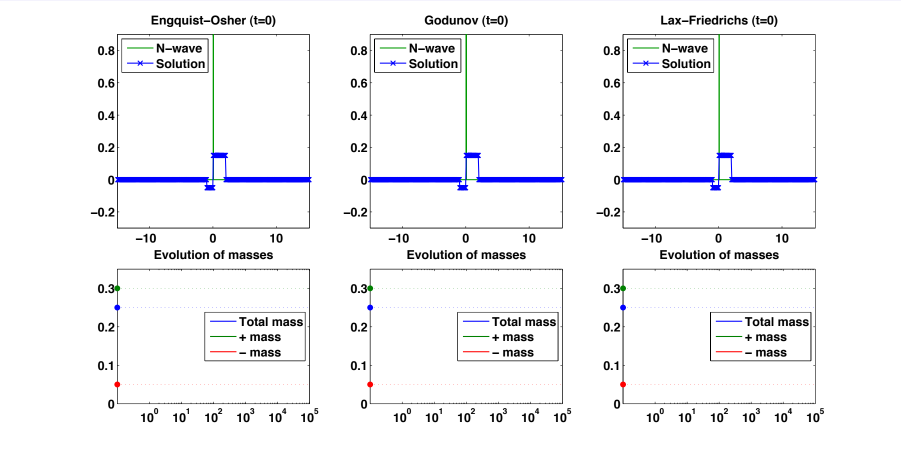
$$u_0(x) = \begin{cases} -0.05, & x \in [-1, 0], \\ 0.15, & x \in [0, 2], \\ 0, & \text{elsewhere.} \end{cases}$$

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 $t = 10^5$:




Engquist–Osher (t=0)
Godunov (t=0)
Lax–Friedrichs (t=0)
N–wave
Solution
Evolution of masses
Total mass
+ mass
– mass

Similarity variables

Let us consider the change of variables given by:

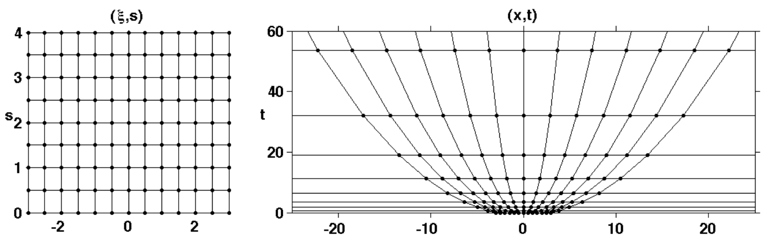
$$s = \ln(t+1), \qquad \xi = x/\sqrt{t+1}, \qquad w(\xi,s) = \sqrt{t+1}\; u(x,t),$$

which turns the continuous Burgers equation into

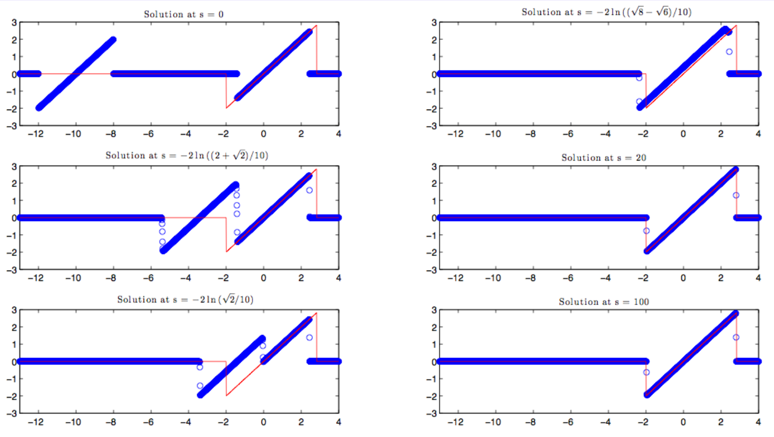
$$w_s + \left(\frac{1}{2}w^2 - \frac{1}{2}\xi w\right)_\xi = 0, \quad \xi \in \mathbf{R}, s > 0.$$

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

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



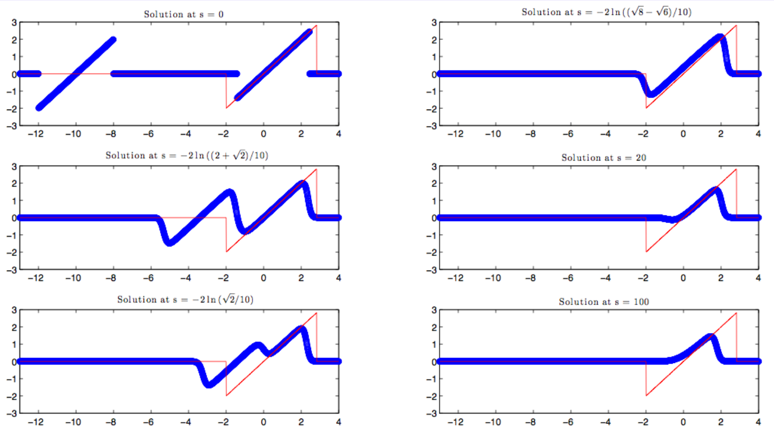
Examples



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 $s = 100$.

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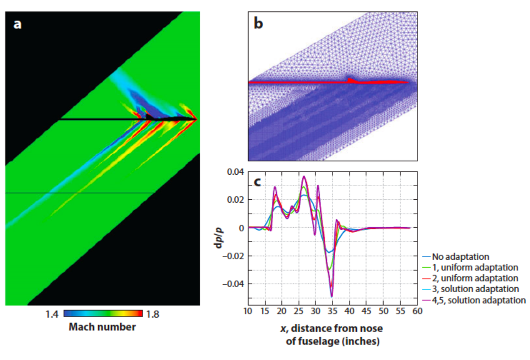
The problem of inverse design, motivated by the problem of sonic-boom, and more precisely by the determination of the profile of the initial signature so to make sure it is acceptable when reaching earth, according to present regulations, can be formulated as an optimization or control problem in which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

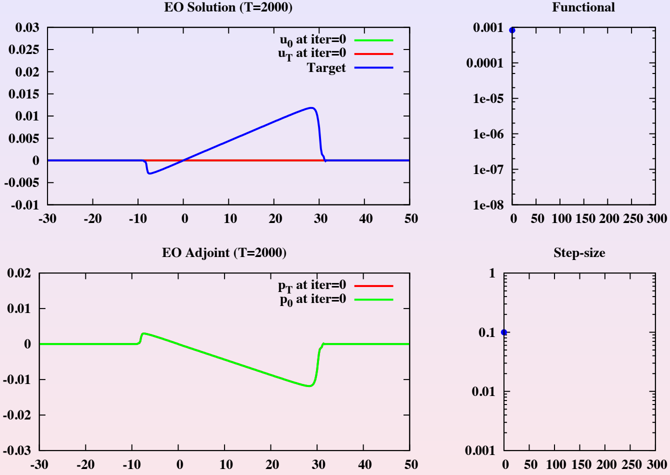
The discrete approach

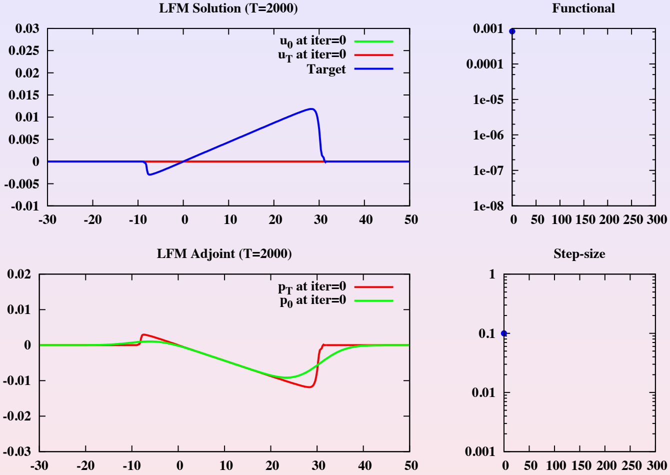
The discrete version of the functional:

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

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.

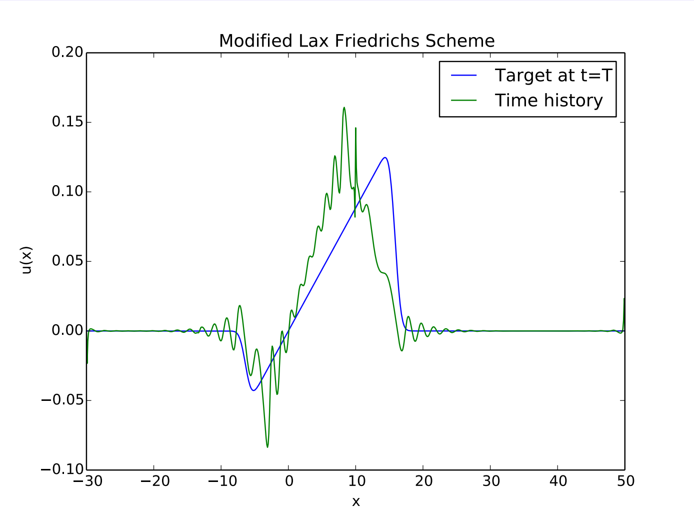
In view of the very different asymptotic behavior of numerical solutions in large times, we also expect a different performance of the discrete optimization achieved.
In fact, we expect Engquist-Osher to perform well, but Lax-Friedrisch to have difficulties to recover the correct inverse design.


EO Solution (T=2000)
u_0 at iter=0
u_T at iter=0
Target
0.03
0.025
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-30 -20 -10 0 10 20 30 40 50
Functional
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
0 50 100 150 200 250 300
EO Adjoint (T=2000)
p_T at iter=0
p_0 at iter=0
0.02
0.01
0
-0.01
-0.02
-0.03
-30 -20 -10 0 10 20 30 40 50
Step-size
1
0.1
0.01
0.001
0 50 100 150 200 250 300

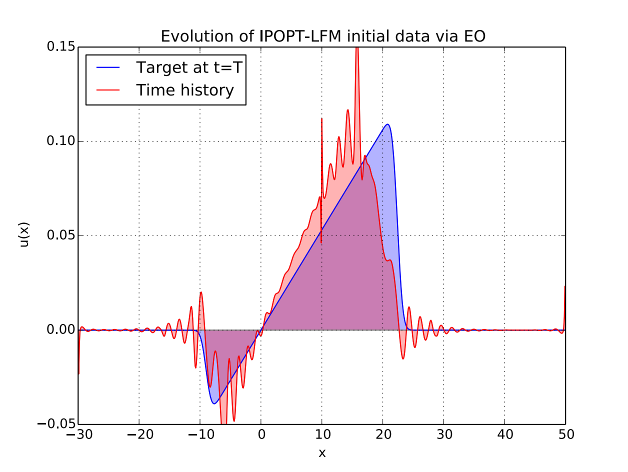


Is the iterative algorithm trapped in a local minimizer?

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



And this is the **bad** performance of the recovered initial profile when employing EO dynamics.



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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,...)
- Impact on inverse design.
- Important applications.

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

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