Conservation Laws, Hydrodynamic Limits and Numerical Schemes

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Contents

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  - Possible loss of regularity, weak solutions and entropy criterion
  - Basis for numerical simulations: Upwinding.
- Hydrodynamic Limits
  From statistical physics to fluid dynamics
- Numerical schemes

Motivation

Many problems in physics have the form

of **Conservation Laws** $\partial_t U + \nabla_x \cdot F(U) = 0$

where

- U can be a scalar or a vector, thus $F(U)$ a vector or a matrix,
- x can be one- or multi-dimensional

(Difficulties increases, for analysis and numerics, as the size of x and of U increases).

or **Balance Laws** $\partial_t U + \nabla_x \cdot F(U) = S(U)$.

Goal: To design a "good and efficient" numerical method

- mathematical and physical criterion
- non linearities
- conservation of equilibria ($\nabla_x \cdot F(U_{\mathrm{eq}}) = S(U_{\mathrm{eq}})$).

Example

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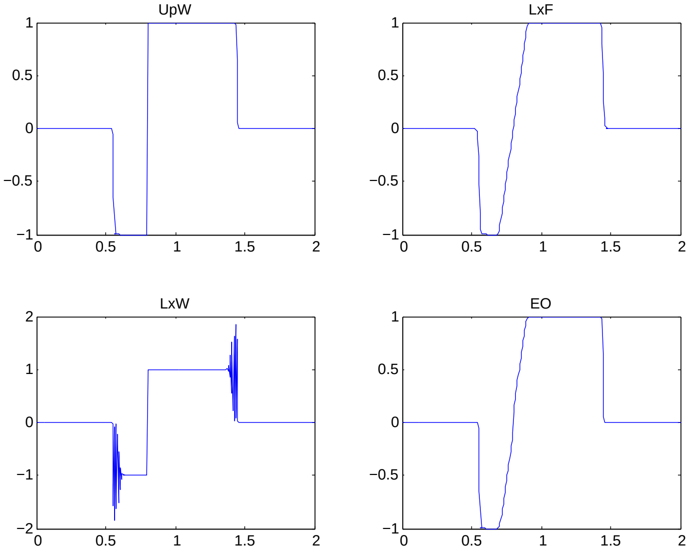


What does "conservation" mean?

Density of a passive tracer immersed in a fluid

- $\rho(t,x)$ = density of "particles":
  $\int_\Omega \rho(t,y)\,\mathrm{d}y$ = Mass contained in Ω at time t
- $u(t,x)$ = (God-given) velocity of the fluid
- **Mass balance**

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho(t,y)\,\mathrm{d}y = -\int_{\partial\Omega} \rho(t,y)u(t,y)\cdot\nu(y)\,\mathrm{d}\sigma(y).$$

- Integrating by parts yields the PDE $\partial_t\rho + \nabla_x\cdot(\rho u) = 0$.

Moto

To design numerical schemes by mimicking the physical derivation of the equation (Finite Volume Schemes)

The cornerstone is the notion of **flux**

- Given a physical quantity U, its evolution in a domain Ω is driven by gain/loss through the boundaries described by a **flux** Q so that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} U(t,y)\,\mathrm{d}y = -\int_{\partial\Omega} Q(t,y)\cdot\nu(y)\,\mathrm{d}\sigma(y).$$

- Then, **a physical law** prescribes how Q depends on U.
- Example: U =temperature, Fourier's law: $Q = -k\nabla_x U$.
  It leads to the **Heat Eq.** $\partial_t U = \nabla_x \cdot (k\nabla U)$. But this eq. does not belong to the framework of Hyperbolic problems...
  Main differences: **Infinite Speed of Propagation & Regularizing Effects**

See F. Boyer's lectures on FV methods for elliptic/parabolic eq.!

Examples

Transport eq.

$\partial_t \rho + \nabla_x \cdot (\rho u) = 0$

Kinetic eq. (Statistical physics)

Description in phase space $\partial_t f + \nabla_x \cdot (\xi f) = \text{Interaction terms}$, with $f(t, x, \xi)$ depending on space **and** velocity.

Non linear models: traffic flows

Lighthill-Whitham-Richards' model: ρ=density of vehicles, the velocity is $u(t, x) = V_0(1 - \rho)$ **depends on** ρ!

$$\partial_t \rho + \partial_x (V_0 \rho (1 - \rho)) = 0, \qquad \text{the flux is } V_0 \rho (1 - \rho)$$

Non linear models: Burgers eq.

A toy model for gas dynamics

$$\partial_t \rho + \partial_x (\rho^2/2) = 0$$

Examples Contn'd

Waves eq. (linear system)

$\partial_t u + c\partial_x v = 0, \qquad \partial_t v + c\partial_x u = 0$

- leads to $\partial^2_{tt} u - c^2 \partial^2_{xx} u = 0$.
- Set $W_\pm = u \pm v$, then $\partial_t W_\pm \pm c\partial_x W_\pm = 0$ that is a system of transport eq. (or a kinetic model with 2 velocities).

Euler system

$$\partial_t \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} + \partial_x \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (\rho u^2/2 + p)u \end{pmatrix} = 0$$

with $E = u^2/2 + e$, $p = p(\rho, e)$. (For instance $p = 2\rho e$.)

Moto

A numerical scheme for a complex system should first work on simple equations!

The **NON-CONSERVATIVE** transport equation

$$\partial_t \rho + u \partial_x \rho = 0$$

Define the Characteristics

Assume that $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is C^1 and satisfies $|u(t,x)| \leq C(1+|x|)$. Then we can apply the **Cauchy-Lipschitz theorem** and define the **Characteristic Curves**

$$\frac{\mathrm{d}}{\mathrm{d}s} X(s;t,x) = u(s, X(s;t,x)), \qquad X(t;t,x) = x.$$

$X(s;t,x)$ is the position occupied at time s by a particle which starts from position x at time t.

Go back to the PDE

- Chain Rule:
  $$\frac{\mathrm{d}}{\mathrm{d}s}\Big[\rho(s, X(s;t,x))\Big] = (\partial_t \rho + u \cdot \nabla_x \rho)(s, X(s;t,x)) = 0$$
- Integrate between $s = 0$ and $s = t$: $\rho(t,x) = \rho_{\mathrm{Init}}(X(0;t,x))$.

The **CONSERVATIVE** transport equation

$$\partial_t \rho + \partial_x(\rho u) = \partial_t \rho + u\partial_x \rho + \rho \partial_x u = 0$$

becomes $\dfrac{\mathrm{d}}{\mathrm{d}s}\Big[\rho(s, X(s;t,x))\Big] = -\rho\partial_x u(s, X(s;t,x))$.
Therefore $\rho(t,x) = \rho_{\mathrm{Init}}(X(0;t,x))\ J(0;t,x)$ with

$$J(s;t,x) = \exp\Big(- \int_s^t \partial_x u(\sigma, X(\sigma;t,x))\,\mathrm{d}\sigma \Big).$$

Interpretation: J is the jacobian of $y = X(s;t,x)$

$$\begin{cases} \partial_s\big(\partial_x X(s;t,x)\big) = (\partial_x u)(s, X(s;t,x))\ \partial_x X(s;t,x), \\ \partial_x X(t;t,x) = 1. \end{cases}$$

We deduce that

$$\partial_x X(s;t,x) = \exp\Big(+ \int_t^s \partial_x u(\sigma, X(\sigma;t,x)\,\mathrm{d}\sigma \Big) = J(s;t,x)$$

and $\mathrm{d}y = J(s;t,x)\,\mathrm{d}x$.

Fundamental observations

- Maximum principle: for the non-conservative case if $0 \leq \rho_{\mathrm{Init}}(x) \leq M$, then $0 \leq \rho(t,x) \leq M$; for the conservative case if $\rho_{\mathrm{Init}}(x) \geq 0$ then $\rho(t,x) \geq 0$.
- Mass conservation: for the conservative case
$$\int_{\mathbb{R}} \rho(t,x)\,\mathrm{d}x = \int_{\mathbb{R}} \rho_{\mathrm{Init}}(y)\,\mathrm{d}y.$$
- For $\rho_{\mathrm{Init}} \in C^1$, we get solutions in C^1 (no gain of regularity)
- The discussion extends to the multi-dimensional framework.
- The formulae generalize to data in $L^p(\mathbb{R})$, $1 \leq p \leq \infty$: it provides a (unique) solution in $C^0([0,T], L^p(\mathbb{R}))$ for $1 \leq p < \infty$, in $C^0([0,T], L^\infty(\mathbb{R}) - \mathrm{weak} - \star)$ for $p = \infty$.

Hints for proving uniqueness (Conservative case)

Weak solution

For any trial function $\phi \in C_c^1([0,\infty) \times \mathbb{R})$,

$$-\int_0^\infty \int_{\mathbb{R}} \rho(t,x)\big(\partial_t \phi(t,x) + u(t,x)\partial_x \phi(t,x)\big)\,\mathrm{d}x\,\mathrm{d}t - \int_{\mathbb{R}} \rho_{\mathrm{Init}}(x)\phi(0,x)\,\mathrm{d}x = 0.$$

Hölmgren's method

Let $\psi \in C_c^\infty((0,+\infty) \times \mathbb{R})$ with $\psi(t,\cdot) = 0$ for $t \geq T$. Solve $\partial_t \phi + u\partial_x \phi = \psi$ with final data $\phi\big|_{t=T} = 0$. Precisely, we have

$$\phi(t,x) = \int_T^t \psi(\sigma, X(\sigma;t,x))\,\mathrm{d}\sigma \in C_c^1([0,+\infty) \times \mathbb{R}).$$

thus, when $\rho_{\mathrm{Init}} = 0$, $\displaystyle\int_0^\infty \int_{\mathbb{R}} \rho(t,x)\psi(t,x)\,\mathrm{d}x\,\mathrm{d}t = 0.$

Fundamental example

Linear Transport with Constant Speed

Let $c \in \mathbb{R}$. Consider the PDE

$$\partial_t \rho + c \partial_x \rho = \partial_t \rho + \partial_x (c\rho) = 0.$$

Exact solution is known: $\rho(t, x) = \rho_{\text{Init}}(x - ct)$.

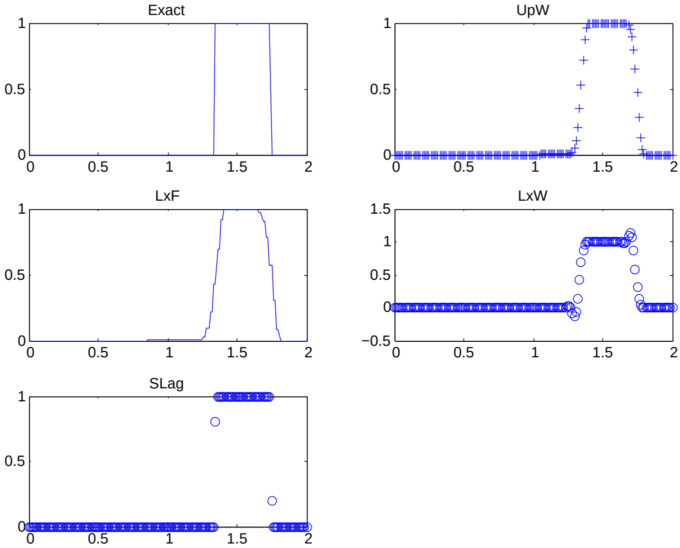
To be compared with the solution of the heat equation $\partial_t \rho = k \partial^2_{xx} \rho$ which is given by

$$\rho(t, x) = \frac{1}{\sqrt{4\pi t/k}} \int_{\mathbb{R}} e^{-k|x-y|^2/(4t)} \rho_{\text{Init}}(y) \, \mathrm{d}y.$$

(Infinite speed of propagation and regularization of the data.)

Exercise: Find the solution of $\partial_t \rho_\epsilon + \partial_x (c\rho_\epsilon) = \epsilon \partial^2_{xx} \rho_\epsilon$ and its limit as $\epsilon \to 0$.

Behavior of different schemes (initial data=step, speed>0)



Nonlinear problems

Linear transport: For C^k data, we get a C^k solution.

Let us try to reproduce the reasoning for a non linear problem:

$$\text{Burgers eq.} \quad \partial_t \rho + \partial_x \rho^2/2 = 0 = (\partial_t + \rho \partial_x)\rho.$$

We still get $\rho(t,x) = \rho_{\rm Init}(X(0;t,x))$. BUT now the characteristics depend on the solution itself

$$\frac{\mathrm{d}}{\mathrm{d}s} X(s;t,x) = \rho(s, X(s;t,x)), \qquad X(t;t,x) = x.$$

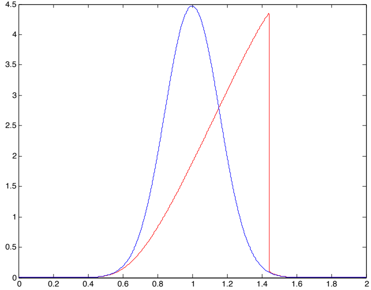
Singularities might appear in finite time

Let $v(t,x) = \partial_x \rho(t,x)$: $(\partial_t + \rho\partial_x)v = -v^2$. Along characteristics we recognize the **Ricatti eq.**

$$\frac{\mathrm{d}}{\mathrm{d}s}\big[v(s, X(s;t,x))\big] = -v^2(s, X(s;t,x))$$

We get $v(t,x) = \left(t + \dfrac{1}{\partial_x \rho_{\rm Init}(X(0;t,x))}\right)^{-1}$. Blow up when $\partial_x \rho_{\rm Init} \leq 0$.

Loss of regularity for nonlinear problems



- ρ remains bounded but $\partial_x \rho$ becomes singular
- Characteristics not well-defined: Cauchy-Lipschitz th. does not apply

Another way to think of the loss of regularity

- Sol constant along characteristics
- $\frac{\mathrm{d}}{\mathrm{d}t} X(t;0,x) = f'\big((\rho(t;X(t;0,x))\big) = f'\big(\rho_{\mathrm{Init}}(x)\big)$ hence $X(t;0,x) = x + tf'\big(\rho_{\mathrm{Init}}(x)\big) = \phi_t(x)$
- To find $\rho(t,x)$ by means of $\rho_{\mathrm{Init}}(x)$, one needs to invert $x \mapsto \phi_t(x)$. But $\phi_t'(x) = 1 + tf''\big(\rho_{\mathrm{Init}}(x)\big)\rho_{\mathrm{Init}}'(x)$ might change sign.

(We need) Weak solution for Scalar Conservation Laws

Definition

For any trial function $\phi \in C^1_c([0,\infty) \times \mathbb{R})$,

$$-\int_0^\infty \int_{\mathbb{R}} \big(\rho \partial_t \phi + f(\rho) \partial_x \phi\big)(t,x)\,\mathrm{d}x\,\mathrm{d}t - \int_{\mathbb{R}} \rho_{\mathrm{Init}}(x)\phi(0,x)\,\mathrm{d}x = 0.$$

Rankine-Hugoniot conditions

RH

Discontinuities satisfy $[\![f(\rho)]\!] = \dot{s}[\![\rho]\!]$.

Non uniqueness

Burgers eq. with $\rho_{\mathrm{Init}} = 0$: $\rho_1(t,x) = 0$ and
$\rho_2(t,x) = \mathbf{1}_{0<x<t/2} - \mathbf{1}_{-t/2<x<0}$ are both weak solutions!

How to select among weak sol.: entropy criterion

Observe that for **smooth** solutions of $\partial_t \rho + \partial_x f(\rho) = 0$, we have

$$\partial_t \eta(\rho) + \partial_x q(\rho) = 0, \qquad q'(z) = \eta'(z) f'(z).$$

But, discontinuous solutions DO NOT verify this relation. ▸ Det

Definition

A weak solution ρ is said to be entropic, if, *for any convex function* η, we have

$$-\int_0^\infty \int_{\mathbb{R}} \left(\eta(\rho)\partial_t \phi + q(\rho)\partial_x \phi\right)(t,x)\,\mathrm{d}x\,\mathrm{d}t - \int_{\mathbb{R}} \eta(\rho_{\mathrm{Init}})(x)\phi(0,x)\,\mathrm{d}x \leq 0$$

for any non negative trial function $\phi \geq 0$. ("$\partial_t \eta(\rho) + \partial_x q(\rho) \leq 0$")

Kruzkov's Theorem

The SCL admits a unique weak-entropic solution with $\rho \in C^0([0,T]; L^1_{\mathrm{loc}}(\mathbb{R}))$. ▸ ExBu

Admissible discontinuities

Go back to the Rankine-Hugoniot condition: $[\![q(u)]\!] \leq \dot{s}[\![\eta(u)]\!]$.
Use Kruzkhov's entropies

$$\eta_k(u) = |u-k|, \qquad q_k(u) = (f(u)-f(k))\mathrm{sgn}(u-k).$$

- with $k < \min(u_\ell, u_r)$, and $k > \max(u_\ell, u_r)$: back to RH.
- with $k = \theta u_\ell + (1-\theta)u_r$ it leads to

$$\mathrm{sgn}(u_r - u_\ell)\Big(\theta f(u_\ell) + (1-\theta)f(u_r) - f(\theta u_\ell + (1-\theta)u_r)\Big) \leq 0$$

Letting $\theta \to 0$, $\theta \to 1$, it yields the Lax criterion

$$f'(u_r) \leq \dot{s} \leq f'(u_\ell).$$

- In particular, when the flux f is **convex**, admissible discontinuities satisfy $u_r \leq u_\ell$. ▸ ExBu

Entropy and vanishing viscosity approach

- Owing to regularizing effects, one can prove the existence of solutions for the regularized problem

$$\partial_t \rho_\epsilon + \partial_x f(\rho_\epsilon) = \epsilon \partial^2_{xx} \rho_\epsilon$$

- Compare Euler and Navier-Stokes: ϵ plays the role of "viscosity". Besides, "good" numerical schemes induce such kind of regularization.

Program

- Solve the nonlinear parabolic eq. with $\epsilon > 0$
- Establish **uniform** estimates
- Deduce compactness properties
- Pass to the limit $\epsilon \to 0$
- Show uniqueness by using entropies

Entropy and vanishing viscosity approach

- Owing to regularizing effects, one can prove the existence of solutions for the regularized problem

$$\partial_t \rho_\epsilon + \partial_x f(\rho_\epsilon) = \epsilon \partial^2_{xx} \rho_\epsilon$$

- Entropy estimates

$$\begin{aligned}\partial_t \eta(\rho_\epsilon) + \partial_x q(\rho_\epsilon) &= \epsilon \eta'(\rho_\epsilon) \partial^2_{xx} \rho_\epsilon \\ &= \epsilon \partial_x \big(\eta'(\rho_\epsilon) \partial_x \rho_\epsilon \big) - \epsilon \eta''(\rho_\epsilon) |\partial_x \rho_\epsilon|^2\end{aligned}$$

  leads to

$$\frac{\mathrm{d}}{\mathrm{d}t} \int \eta(\rho_\epsilon)\,\mathrm{d}x + \epsilon \int \eta''(\rho_\epsilon) |\partial_x \rho_\epsilon|^2\,\mathrm{d}x = 0.$$

- In particular, with $\eta(\rho) = \rho^2/2$, we deduce that

  ρ_ϵ is bounded in $L^\infty(0, T; L^2(\mathbb{R}))$,

  $\sqrt{\epsilon}\partial_x \rho_\epsilon$ is bounded in $L^2((0, T \times \mathbb{R})$.

Entropy and vanishing viscosity approach, Contn'd

- We know that

$$\rho_\epsilon \text{ is bounded in } L^\infty(0,T;L^2(\mathbb{R}))$$

$$\sqrt{\epsilon}\partial_x \rho_\epsilon \text{ is bounded in } L^2((0,T)\times\mathbb{R})$$

- Similarly we can obtain L^∞ estimates (use for instance $\eta(\rho) = \left[\rho - \|\rho_{\text{Init}}\|_\infty\right]_-^2$)
- Therefore

$$\partial_t \rho_\epsilon + \partial_x f(\rho_\epsilon) = \sqrt{\epsilon}\partial_x\left(\sqrt{\epsilon}\partial_x \rho_\epsilon\right) \xrightarrow[\epsilon\to 0]{} 0$$

and, on the same token,

$$\partial_t \eta(\rho_\epsilon) + \partial_x q(\rho_\epsilon) = \underbrace{\sqrt{\epsilon}\partial_x\left(\sqrt{\epsilon}\eta'(\rho_\epsilon)\partial_x\rho_\epsilon\right)}_{\xrightarrow[\epsilon\to 0]{} 0} \underbrace{-\epsilon\eta''(\rho_\epsilon)|\partial_x\rho_\epsilon|^2}_{\leq 0}$$

Numerical schemes for transport equations

Let $c \in \mathbb{R}$ be a fixed constant. The solution of the PDE $\partial_t u + c\partial_x u = 0$ is explicitely known by means of the initial data

$$u(t,x) = u_{\mathrm{Init}}(x - ct).$$

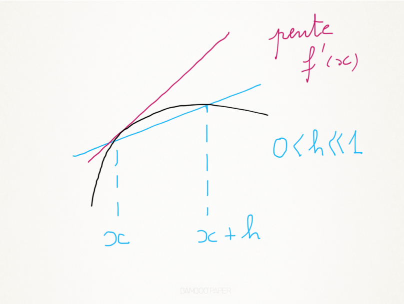
What do "natural" schemes on this simple equation ?
We know u_j^n=approximation of the solution at time $n\Delta t$ and on the grid points

$$x_0 = 0 < x_1 = \Delta x < \ldots x_j = j\Delta x < x_{j+1} = (j{+}1)\Delta x < \ldots < x_N = L$$

(note that $N = L/\Delta x$). We want to update with

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = ???$$

To approximate the derivative



$$\frac{f(x+h)-f(x)}{h} \xrightarrow[h\to 0]{} f'(x), \qquad \frac{f(x)-f(x-h)}{h} \xrightarrow[h\to 0]{} f'(x),$$

$$\frac{f(x+h)-f(x-h)}{2h} \xrightarrow[h\to 0]{} f'(x).$$

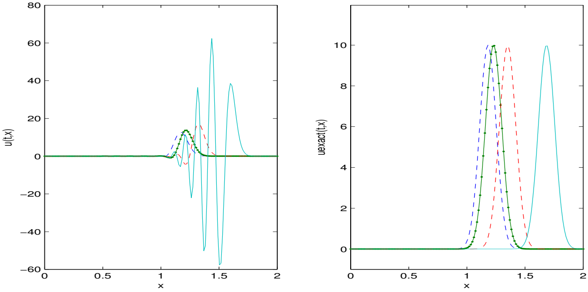
To approximate the derivative

$$\left|\frac{f(x+h)-f(x)}{h} - f'(x)\right| \leq C\ h,$$

$$\left|\frac{f(x)-f(x-h)}{h} - f'(x)\right| \leq C\ h,$$

look less appealing than $\left|\dfrac{f(x+h)-f(x-h)}{2h} - f'(x)\right| \leq C\ h^2$

But..



UpWinding

The centered scheme

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

goes wrong. Upwinding:

$$\frac{u_j^{n+1}-u_j^n}{\Delta t} = -c\begin{cases} \dfrac{u_{j+1}^n - u_j^n}{\Delta x} & \text{if } c<0, \\ \dfrac{u_j^n - u_{j-1}^n}{\Delta x} & \text{if } c>0 \end{cases}$$

does the job! ▸ UPW

Stability: CFL condition

If $\frac{|c|\Delta t}{\Delta x} \leq 1$, then u_j^{n+1} appears as a convex combination of $u_{j-1}^n, u_j^n, u_{j+1}^n$. In particular, L^∞ estimates are preserved.

Code for transport eq.: Init.

```
c=1.37; %Speed
lg=2; %Size domain
cfl=0.9; %CFL nb: try with ¿1
J=150;% nb of cells
x=linspace(0,lg,J)'; % Grid
dx=x(2)-x(1); %Space step
dt=dx*cfl/c;% Time step
a=c*dt/dx; %Speed coef
Tfin=.5 % Final time
t=0;
eps=0.01;
u0=zeros(J,1);
u0((x>lg/2-lg/10)&(x<lg/2+lg/10))=1.;%Disc. data
u0=(1/sqrt(eps))*exp(-(x-lg/2).*(x-lg/2)/eps);% Cont. data
```

Code for transport eq.: Useful Matrices

```
e=ones(J,1);
ACent=spdiags([-e,0*e,e],-1:1,J,J);
APlus=spdiags([-e,e,0*e],-1:1,J,J);
AMinus=spdiags([0*e,-e,e],-1:1,J,J);
APlus(1,J)=-1;
AMinus(J,1)=1;
ACent(1,J)=1;ACent(J,1)=1;
matlap=spdiags([e,-2*e,e],-1:1,J,J);
matlap(1,J)=1;
matlap(J,1)=1;
```

Code for transport eq.: Time loop

```
while (k=1:Ntfin)
UpW=UpW-c*dt/dx*APlus*UpW; % Upwind
LxF=LxF-c*dt/dx/2*ACent*LxF + matlap*LxF/2; %Lax-Friedrihs
LxW=LxW-c*dt/dx/2*ACent*LxW
+(c*dt/dx)^2/2*matlap*LxW;%Lax-Wendroff
uexact=(1/sqrt(eps))*exp(-(x-c*k*dt-lg/2).*(x-c*k*dt-lg/2)/eps);
%Sol exacte
end
```

Finite Volume Schemes for Conservation Laws

How can we extend the notion of UpWinding for nonlinear problems

$$\partial_t U + \partial_x F(U) = 0 \ ?$$

Integrate over cells $(t^n, t^{n+1}) \times (x_{j-1/2}, x_{j+1/2})$:

$$\int_{x_{j-1/2}}^{x_{j+1/2}} U(t^{n+1}, y)\,\mathrm{d}y - \int_{x_{j-1/2}}^{x_{j+1/2}} U(t^n, y)\,\mathrm{d}y + \int_{t^n}^{t^{n+1}} \left\{ F(U(s, x_{j+1/2})) - F(U(s, x_{j-1/2})) \right\} \mathrm{d}s = 0.$$

The numerical unknown U_j^n is intended to approximate the mean value $\dfrac{1}{\Delta x}\displaystyle\int_{x_{j-1/2}}^{x_{j+1/2}} U(t^n, y)\,\mathrm{d}y$. We mimic the balance formula:

$$\frac{\Delta x}{\Delta t}(U_j^{n+1} - U_j^n) + F_{j+1/2}^n - F_{j-1/2}^n = 0$$

and we seek a relevant definition for the numerical flux $F_{j+1/2}^n$.

Example: the Rujsanow scheme

Let us consider a mere SCL $\partial_t \rho + \partial_x f(\rho) = 0$. Set $a = \max |f'(\rho)|$ and rewrite

$$\partial_t \rho + \partial_x \underbrace{\left(\frac{f(\rho) + a\rho}{2}\right)}_{\text{Velocity } f'(\rho)+a>0} + \partial_x \underbrace{\left(\frac{f(\rho) - a\rho}{2}\right)}_{\text{Velocity } f'(\rho)-a<0} = 0.$$

It leads to

$$\frac{\rho_j^{n+1} - \rho_n^j}{\Delta t} = -\frac{1}{2\Delta x}\Big(f(\rho_j^n) + a\rho_j^n - f(\rho_{j-1}^n) - a\rho_{j-1}^n$$
$$+ f(\rho_{j+1}^n) - a\rho_{j+1}^n - f(\rho_j^n) + a\rho_j^n\Big)$$
$$= \underbrace{-\frac{1}{2\Delta x}\left(f(\rho_{j+1}^n) - f(\rho_{j-1}^n)\right)}_{\text{Centered Approx.}} + \underbrace{\frac{a}{\Delta x}\left(\rho_{j+1}^n - 2\rho_j^n - +\rho_{j-1}^n\right)}_{\text{Diffusion}}.$$

It correponds to the discretization of the **modified equation**

$$\partial_t \rho + \partial_x f(\rho) = \epsilon \partial_{xx}^2 \rho, \qquad \epsilon = a\Delta x.$$

Example: the Rujsanow scheme, Cont'd

The Rusjanow scheme can be rewritten in terms of numerical fluxes

$$\frac{\Delta x}{\Delta t}(\rho_j^{n+1} - \rho_n^j) + F_{j+1/2}^n - F_{j-1/2}^n = 0, \qquad F_{j+1/2}^n = \mathbb{F}(\rho_{j+1}^n, \rho_j^n),$$

with $\mathbb{F}(\rho_{j+1}^n, \rho_j^n) = \dfrac{1}{2}(f(\rho_{j+1}^n) - a\rho_{j+1}^n + f(\rho_j^n) + a\rho_j^n).$

Properties and extensions

- The flux is consistent $\mathbb{F}(\rho, \rho) = f(\rho)$.
- L^∞ stability under CFL condition $\frac{a\Delta t}{\Delta x} < 1$.
- The method can be designed by reasoning locally.
- The method adapts to system using for a the spectral radius of the jacobian matrix $\nabla_U F(U)$.

Elements for the numerical analysis of scheme for SCL

PDE: $\partial_t \rho + \partial_x f(\rho) = 0$

Scheme: $\dfrac{h}{\Delta t}(\rho_j^{n+1} - \rho_j^n) + F_{j+1/2}^n - F_{j-1/2}^n = 0$, $F_{j+1/2}^n = \mathbb{F}(\rho_{j+1}^n, \rho_j^n)$.

Flux-Consistency $\mathbb{F}(\rho, \rho) = f(\rho)$.

Lax-Wendroff Theorem

Let $\Delta t/h$ be constant and let ρ^h be the piecewise constant function associated to the discretization and the scheme. Suppose that ρ^h is uniformly bounded in L^∞ and that it converges in L^1_{loc} and a.e. to ρ as h goes to 0. Then ρ is a weak solution of the PDE.

Note that this statement does not ensure the uniform bound nor the convergence of (a subsequence of) the approximation, and it says nothing about the entropy criterion!

Elements for the numerical analysis of scheme for SCL, II

Assume we can rewrite the scheme in the Incremental Form

$$\rho_j^{n+1} = \rho_j^n - C_{j-1/2}^n(\rho_j^n - \rho_{j-1}^n) + D_{j+1/2}^n(\rho_{j+1}^n - \rho_j^n)$$

Harten-Le Roux Lemma

Assume $C_{j-1/2}^n \geq 0$, $D_{j+1/2}^n \geq 0$ with $C_{j-1/2}^n + D_{j+1/2}^n \leq 1$. Then the scheme is L^∞-stable.
(With furthermore $C_{j+1/2}^n + D_{j+1/2}^n \leq 1$, the scheme is TVD).

Cond 1=UpWinding, cond. 2=CFL.
A convex combination appears in

$$\rho_j^{n+1} = (1 - C_{j-1/2}^n - D_{j+1/2}^n)\rho_j^n + C_{j-1/2}^n\rho_{j-1}^n + D_{j+1/2}^n\rho_{j+1}^n.$$

Kinetic equations: collisional models

Conservation laws="macroscopic" version of a more detailed physics

N particles $\underbrace{\longrightarrow}_{N\to\infty}$ Statistical physics $\underbrace{\longrightarrow}_{\text{mean free path } \to 0}$ Hydrodynamic

General form: $$\underbrace{\partial_t f + \xi \partial_x f}_{\text{Transport}} = \frac{1}{\tau} \underbrace{Q(f)}_{\text{Collision}}$$

where Q is intended to describe "interaction between particles" and τ is a relaxation time.

Q has a specific structure

- Q usually acts only on ξ: integral or differential operator
- Q preserves the maximum principle ($f \geq 0$).
  For example : $Q(f) = Q^+(f) - \nu(f)\ f$
  and think of an iterative process with the Duhamel formula:
  $\partial_t f_{n+1} + \xi \cdot \nabla_x f_{n+1} + \nu(f_n) f_{n+1} = Q^+(f_n)$.

Kinetic equations: collisional models

General form

$$\partial_t f + \xi \partial_x f = \frac{1}{\tau} Q(f)$$

where Q is intended to describe "interaction between particles"

and Q has some fundamental properties, crucial both on a physical and a mathematical viewpoints

- Conservation: There exists functions $m(\xi)$ such that $\int m(\xi) Q(f)\, \mathrm{d}\xi = 0$
- Equilibrium: $Q(f) = 0$ iff f has a specific dependence wrt ξ: $f = M(\xi)$.
- Dissipation: There exists some function Ψ such that $\int \Psi(f) Q(f)\, \mathrm{d}\xi \leq 0$

Example: Boltzmann eq. describes binary collision dynamics, with mass, momentum, energy conservation.

Example: the BGK operator

$Q(f) = M_{n,u,\theta} - f$ with $M_{n,u,\theta}(\xi) = \frac{n}{(2\pi\theta)^{N/2}} \exp\Big(-\frac{|\xi-u|^2}{2\theta}\Big)$.

where

$$\int \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} f \,\mathrm{d}\xi = \begin{pmatrix} n \\ nu \\ nu^2 + Nn\theta \end{pmatrix} = \int \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} M_{n,u,\theta}(\xi)\,\mathrm{d}\xi$$

Properties

- Conservation of mass, momentum, energy: $\displaystyle\int (1,\xi,\xi^2) Q(f)\,\mathrm{d}\xi = 0$,
- Equilibrium: $Q(f) = 0$ iff $f(\xi) = M_{n,u,\theta}(\xi)$,
- Entropy dissipation $\displaystyle\int Q(f)\ln(f)\,\mathrm{d}\xi \leq 0$.

From BGK to Euler

Go back to BGK: $\partial_t f + \xi \cdot \nabla_x f = \frac{1}{\tau}\big(M_{n,u,\theta} - f\big)$

- Due to conservation we have

$$\partial_t \int \begin{pmatrix} 1 \\ \xi \\ \xi^2/2 \end{pmatrix} f \, \mathrm{d}\xi + \nabla_x \int \xi \begin{pmatrix} 1 \\ \xi \\ \xi^2/2 \end{pmatrix} f \, \mathrm{d}\xi = 0$$

It recasts as

$$\partial_t \begin{pmatrix} n \\ nu \\ (nu^2 + Nn\theta)/2 \end{pmatrix} + \nabla_x \begin{pmatrix} nu \\ \mathbb{P} \\ Q \end{pmatrix} = 0$$

but $\mathbb{P}$ and Q, **moments of** f cannot be expressed by means on n, u, θ: the system is not closed.

From BGK to Euler, II

Go back to BGK: $\partial_t f + \xi \cdot \nabla_x f = \frac{1}{\tau}\big(M_{n,u,\theta} - f\big)$

- Due to conservation we have

$$\partial_t \int \begin{pmatrix} 1 \\ \xi \\ \xi^2/2 \end{pmatrix} f \,\mathrm{d}\xi + \nabla_x \int \xi \begin{pmatrix} 1 \\ \xi \\ \xi^2/2 \end{pmatrix} f \,\mathrm{d}\xi = 0$$

- Due to equilibrium and dissipation we expect as $\tau \to 0$ that $f \simeq M_{n,u,\theta}$
- Then, replace f by $M_{n,u,\theta}$ in the conservation eq. and we get...

$$\begin{aligned}
&\partial_t n + \mathrm{div}_x(nu) = 0,\\
&\partial_t(nu) + \mathrm{Div}_x(nu \otimes u + n\theta\mathbb{I}) = 0,\\
&\partial_t\Big(\frac{nu^2}{2} + N\frac{n\theta}{2}\Big) + \mathrm{div}_x\Big(\big(\frac{nu^2}{2} + N\frac{n\theta}{2} + n\theta\big)u\Big) = 0.
\end{aligned}$$

the Euler system for (n, u, θ) with pressure law $p = n\theta$.

From BGK to Euler, III

The kinetic framework also provides an entropy for the Euler system. We have

$$\partial_t \int f \ln(f)\,\mathrm{d}\xi + \nabla_x \int \xi f \ln(f)\,\mathrm{d}\xi \leq 0.$$

Set $\eta(U) = \displaystyle\int M_{\rho,u,\theta}(\xi) \ln(M_{\rho,u,\theta}(\xi))\,\mathrm{d}\xi$, with $U = (\rho, \rho u, \rho u^2/2 + N\rho\theta/2)$.

Proposition

$U \mapsto \eta(U)$ is convex. The associated entropy flux reads $\displaystyle\int \xi M_{\rho,u,\theta}(\xi) \ln(M_{\rho,u,\theta}(\xi))\,\mathrm{d}\xi = u\eta(U)$.

A BGK-like toy model [Perthame-Tadmor '91]

Let $a : \mathbb{R} \to \mathbb{R}$ ("velocity function") and consider

$$\partial_t f + a(\xi)\partial_x f = \frac{1}{\epsilon}(M[\rho_f] - f), \qquad \rho_f(t,x) = \int_{\mathbb{R}} f(t,x,\xi)\,\mathrm{d}\xi,$$

Here, the "Maxwellian" is

$$M[\rho](\xi) = \mathbf{1}_{0\le\xi\le\rho} - \mathbf{1}_{\rho\le\xi\le 0}$$

Mass conservation ($\rho_+ = \max(0,\rho) \ge 0$, $\rho_- = \min(0,\rho) \le 0$)

$$\int_{\mathbb{R}} (M[\rho_f]-f)\,\mathrm{d}\xi = \int_0^{[\rho_f]_+} \mathrm{d}\xi - \int_{[\rho_f]_-}^0 \mathrm{d}\xi - \rho_f = [\rho_f]_+ + [\rho_f]_- - \rho_f = 0.$$

leads to the local conservation law

$$\partial_t \int_{\mathbb{R}} f\,\mathrm{d}\xi + \partial_x \int_{\mathbb{R}} a(\xi) f\,\mathrm{d}\xi = 0$$

Entropy dissipation

Lemma ▸ Bk4

Assume $-1 \leq f(\xi) \leq 1$ and $\operatorname{sgn}(\xi) f(\xi) \geq 0$. Let H be a non decreasing funtion. Then $\displaystyle\int (M[\rho_f] - f) H \,\mathrm{d}\xi \leq 0$.

$$
\begin{aligned}
I &= \int (M[\rho_f] - f)(H(\xi) - H(\rho_f))\,\mathrm{d}\xi \\
&= \int_0^{[\rho_f]_+} \underbrace{(1-f)}_{\geq 0}\underbrace{(H(\xi) - H(\rho_f))}_{\leq 0}\,\mathrm{d}\xi + \int_{[\rho_f]_+}^{\infty} \underbrace{(-f)}_{\leq 0}\underbrace{(H(\xi) - H(\rho_f))}_{\geq 0}\,\mathrm{d}\xi \\
&+ \int_{[\rho_f]_-}^{0} \underbrace{(-1-f)}_{\leq 0}\underbrace{(H(\xi) - H(\rho_f))}_{\geq 0}\,\mathrm{d}\xi + \int_{-\infty}^{[\rho_f]_-} \underbrace{(-f)}_{\geq 0}\underbrace{(H(\xi) - H(\rho_f))}_{\leq 0}\,\mathrm{d}\xi.
\end{aligned}
$$

Consequence

For η convex, we have $\displaystyle\partial_t \int \eta'(\xi) f \,\mathrm{d}\xi + \partial_x \int a(\xi)\eta'(\xi) f \,\mathrm{d}\xi \leq 0$.

Can we guess the limit $\epsilon \to 0$? (Yes, we can!)

Let $A'(\rho) = a(\rho)$, $A(0) = 0$, so that $\int_{\mathbb{R}} a(\xi) M[\rho]\, \mathrm{d}\xi = A(\rho)$

Write $f = M[\rho_f] - \epsilon(\partial_t f + a(\xi)\partial_x f)$ so that

$$\partial_t \rho + \partial_x \int_{\mathbb{R}} a(\xi) M[\rho]\, \mathrm{d}\xi - \epsilon \partial_x \left(\int_{\mathbb{R}} a(\xi) \big(\partial_t f + a(\xi)\partial_x f\big)\, \mathrm{d}\xi \right) = 0$$

$$= \partial_t \rho + \partial_x A(\rho) - \epsilon \left(\partial^2_{tx} \int_{\mathbb{R}} a(\xi)\ f\, \mathrm{d}\xi + \partial^2_{xx} \int_{\mathbb{R}} a(\xi)^2\ f\, \mathrm{d}\xi \right) = 0.$$

Then, we suspect that $f \simeq M[\rho]$ with ρ solution of the scalar conservation law

$$\partial_t \rho + \partial_x A(\rho) = 0.$$

Note: We have used, when $\phi(0) = 0$,

$$\int_{\mathbb{R}} \phi'(\xi) M[\rho](\xi)\, \mathrm{d}\xi = \int_0^{\rho_+} \phi'(\xi)\, \mathrm{d}\xi - \int_{\rho_-}^{0} \phi'(\xi)\, \mathrm{d}\xi = \phi(\rho_+) + \phi(\rho_-) = \phi(\rho).$$

Step 1. Existence of solutions and a priori estimates

Initial data

Let $f_0 : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ verify $-1 \leq f_0 \leq 1$, $\mathrm{sgn}(\xi) f_0(x,\xi) \geq 0$ and

$$\int_{\mathbb{R}} \int_{\mathbb{R}} f_0(x,\xi)\, \mathrm{d}\xi\, \mathrm{d}x < \infty, \quad f_0(x,\xi) = 0 \text{ for } |\xi| \geq V.$$

Duhamel formula

$$\frac{\mathrm{d}}{\mathrm{d}s} \left[e^{s/\epsilon}\, f(t+s, x+sa(\xi), \xi) \right] = \frac{1}{\epsilon}\, e^{s/\epsilon}\, M[\rho_f](t+s, x+sa(\xi), \xi).$$

Iterative scheme

- $f^{(0)} = 0$,
- $f^{(n)}$ being given, set $\rho^{(n)}(t,x) = \int_{\mathbb{R}} f^{(n)}(t,x,\xi)\, \mathrm{d}\xi$ and

$$\begin{aligned} f^{(n+1)}(t,x,\xi) &= e^{-t/\epsilon} f_0(x - ta(\xi), \xi) \\ &\quad + \frac{1}{\epsilon} \int_0^t e^{-(t-s)/\epsilon}\, M[\rho^{(n)}](s, x-(t-s)a(\xi), \xi)\, \mathrm{d}s \end{aligned}$$

Convergence of the scheme

- $0 \leq \mathrm{sgn}(\xi) f^{(n)}(t, x, \xi) \leq 1$
- $\mathrm{supp}\big(f^{(n)}(t, x, \cdot)\big) \subset [-V_0, V_0]$ implies $M[\rho^{(n)}] = 0$ on $\complement[-V_0, V_0]$. Thus $\mathrm{supp}\big(f^{(n+1)}(t, x, \cdot)\big) \subset [-V_0, V_0]$.
- $\displaystyle\int |M[\rho_{f_1}] - M_{[\rho_{f_2}]}| \,\mathrm{d}\xi \leq \int |f_1 - f_2| \,\mathrm{d}\xi.$
- For a certain norm on $L^\infty(0, \infty; L^1(\mathbb{R} \times \mathbb{R}))$, we can find $0 < \eta < 1$ such that $\| f^{(n+1)} - f^{(n)} \| \leq \eta \| f^{(n)} - f^{(n-1)} \|$.
- Conclusion: existence-uniqueness for the nonlinear BGK model.

Step 2. Dissipation Properties

With the entropy dissipation ▸ ED, rewrite the collision term:

- Set $m_\epsilon(t,x,\xi) = \dfrac{1}{\epsilon}\displaystyle\int_{-\infty}^{\xi} \big(M[\rho_\epsilon] - f_\epsilon\big)(t,x,w)\,\mathrm{d}w$
- m_ϵ is a sequence of non negative measures on $(0,T)\times\mathbb{R}\times\mathbb{R}$.

  since for $h \geq 0$, with $H(\xi) = \displaystyle\int_{-\infty}^{\xi} h(z)\,\mathrm{d}z$

$$\int_{\mathbb{R}} m_\epsilon h\,\mathrm{d}\xi = -\int_{\mathbb{R}} \partial_\xi m_\epsilon\; H\,\mathrm{d}\xi \geq 0.$$

- The sequence $\big(m_\epsilon\big)_{\epsilon>0}$ is bounded in $\mathcal{M}^1((0,T)\times\mathbb{R}\times\mathbb{R})$.

  ▸ Cal

A few mathematical tools, Average lemma

A specific tool of kinetic theory

- Goal: Having information on f and $\xi \cdot \nabla_x f$, can we improve the regularity (compactness) of $\rho_\psi(x) = \int \psi(\xi)\, f(x,\xi)\,\mathrm{d}\xi$?
- Basic claim: *If both f and $\xi \cdot \nabla_x f$ belong to $L^2(\mathbb{R}^N \times \mathbb{R}^N)$, then ρ_ψ lies in $H^{1/2}(\mathbb{R}^N)$.*

Sketch of proof ALL2

- Fourier transform wrt to space
- Split into $|\xi \cdot k| \geq \delta|k|$ (Good) $|\xi \cdot k| \leq \delta|k|$ (Bad but with a small contribution)
- Optimize wrt δ: $|\widehat{\rho_\psi}(k)| \leq \dfrac{\left[F(k)G(k)\right]^{1/2}}{|k|^{1/2}}$ with $F, G \in L^2(\mathbb{R}^N)$.

Improvements and variants

- Replacing $\xi \cdot \nabla_x$ by $\partial_t + a(\xi) \cdot \nabla_x$ is not a big deal...
- Crucial: "having enough velocity" that is for any k$\in \mathbb{S}^{N-1}$, $\left|\left\{\xi \in B(0,R),\ \xi \cdot k = 0\right\}\right| = 0$
- Dealing with L^p spaces (ok at least for $p > 1$)
- Dealing with derivatives in the rhs

Theorem [Bouchut, Perthame-Souganidis].

Let f_n and g_n satisfy

$$(\partial_t + \xi \cdot \nabla_x) f_n = \sum_{j=1}^{N} \partial_{x_j} \partial_\xi^\alpha g_n^{(j)}$$

for some $\alpha \in \mathbb{N}^N$. Let Q be a open set in $\mathbb{R} \times \mathbb{R}^N$. We suppose that $\left(f_n\right)_{n\in\mathbb{N}}$ is bounded in $L^p(Q \times \mathbb{R}^N)$ for some $p > 1$ and the $\left(g_n^{(j)}\right)_{n\in\mathbb{N}}$'s are relatively compact in $L^p(Q \times \mathbb{R}^N)$. Then, for any $\phi \in C_c^\infty(\mathbb{R}^N)$, the sequence defined by $\rho_n(t,x) = \int_{\mathbb{R}^N} f_n \phi \,\mathrm{d}\xi$ is relatively compact in $L^p(Q)$.

Step 3. Compactness

We have

$$\partial_t f_\epsilon + a(\xi)\partial_x f_\epsilon = \partial_\xi m_\epsilon$$

with

- f_ϵ bounded in L^∞,
- m_ϵ bounded in $\mathcal{M}^1((0,T)\times\mathbb{R}\times\mathbb{R})$.
- Suppose $a(\xi) = A'(\xi) \neq 0$ for a. e. ξ.

Average lemma applies and ρ_ϵ converges strongly in $L^p((0,T)\times\mathbb{R})$, $1 \le p < \infty$. ALC

Suppose further $f_{\mathrm{Init},\epsilon}(x,\xi) \rightharpoonup M[\rho_{\mathrm{Init}}](x,\xi)$ (preparation of data): it guarantees

$$\lim_{h\to 0} \frac{1}{h}\int_0^h \int |\rho(t,x)-\rho_0(x)|\,\mathrm{d}x\,\mathrm{d}t = 0.$$

Step 4. Conclusion

Conservation law

We have $\partial_t \rho + \partial_x A(\rho) = 0$... but this is not enough

Entropies

$$\int_0^t \int_{\mathbb{R}} \left(\eta(\rho)\partial_t \psi + q(\rho)\partial_x \psi\right) \, \mathrm{d}x \, \mathrm{d}t \geq 0$$

for any positive $\psi \in C_c^\infty((0,\infty) \times \mathbb{R} \times \mathbb{R})$ and any pair entropy/entropy flux (η, q), with η convex and $\eta' A' = q'$. Indeed

$$\partial_t \eta(\rho_\epsilon) + \partial_x q(\rho_\epsilon) = \underbrace{-\int_{\mathbb{R}} \eta''(v) \, m_\epsilon \, \mathrm{d}v}_{\text{which is } \leq 0} + \underbrace{\text{remainder}}_{\text{which is small}}$$

Kinetic scheme for SCL

Let us start with a Time splitting

- Step 1: solve the linear transport equation

$$\partial_t f + a(\xi)\partial_x f = 0.$$

UpWind does the job ($a_\pm = \frac{a\pm|a|}{2}$).

$$\frac{\Delta x}{\Delta t}(f_j^{n+1/2}(\xi) - f_j^n(\xi)) \\ = -\{[a(\xi)]_+(f_j^n(\xi) - f_{j-1}^n(\xi)) + [a(\xi)]_-(f_{j+1}^n(\xi) - f_j^n(\xi))\}.$$

- Step 2: solve the stiff ODE

$$\partial_t f = \frac{1}{\tau}(M[\rho_f] - f).$$

BUT ρ_f does not change during this step ($\int Q(f)\,\mathrm{d}\xi = 0$): $\rho^{n+1} = \rho^{n+1/2} = \displaystyle\int f^{n+1/2}\,\mathrm{d}\xi$. We integrate by hand:

$$f_j^{n+1} = e^{-\Delta t/\tau} f_j^{n+1/2} + (1 - e^{-\Delta t/\tau})M_j^{n+1/2}.$$

Kinetic scheme for SCL

Now let $\tau \to 0$

- Step 2 degenerates to $f_j^{n+1} = M_j^{n+1/2}$ (projection to the equilibrium).
- Integrate Step 1 to obtain a scheme for the macroscopic quantity ρ

$$
\begin{aligned}
\rho_j^{n+1} = \int f_j^{n+1}\,\mathrm{d}\xi &= \int f^{n+1/2}\,\mathrm{d}\xi \\
&= \rho_j^n - \frac{\Delta t}{\Delta x}(F_{j+1/2}^n - F_{j-1/2}^n),
\end{aligned}
$$

with the numerical flux

$$
\begin{aligned}
F_{j+1/2}^n &= \int a_+(\xi) M[\rho_j^n]\,\mathrm{d}\xi + \int a_-(\xi) M[\rho_{j+1}^n]\,\mathrm{d}\xi \\
&= \mathbb{F}(\rho_{j+1}^n, \rho_j^n) = A_p(\rho_{j+1}^n) + A_m(\rho_j^n), \quad A_{p,m}(\rho) = \int_0^\rho a_{+,-}(z)\,\mathrm{d}z.
\end{aligned}
$$

Properties of the kinetic scheme

- We recover the Enquist-Osher scheme,
- Consistency of the flux $F^n_{j+1/2} = \mathbb{F}(\rho^n_{j+1}, \rho^n_j)$ with
  $$\mathbb{F}(\rho,\rho) = \int (a_+(z) + a_-(z))M[\rho](z)\,\mathrm{d}z = A(\rho)$$
- Incremental form:
  $$\rho^{n+1}_j = \rho^n_j + \frac{\Delta t}{\Delta x} D^n_{j+1/2}(\rho^n_{j+1} - \rho^n_j) - \frac{\Delta t}{\Delta x} C^n_{j-1/2}(\rho^n_j - \rho^n_{j-1})$$
  with

$$D^n_{j+1/2} = -\frac{\Delta t}{\Delta x}\frac{A_m(\rho^n_{j+1}) - A_m(\rho^n_j)}{\rho^n_{j+1} - \rho^n_j}, \qquad C^n_{j-1/2} = \frac{\Delta t}{\Delta x}\frac{A_p(\rho^n_j) - A_p(\rho^n_{j-1})}{\rho^n_j - \rho^n_{j-1}}$$

≥ 0 since $A'_m = a_- \leq 0$, $A'_p = a_+ \geq 0$. Stability is guaranteed under CFL condition: $|\frac{A_{m,p}(\rho+h) - A_{m,p}(\rho)}{h}| \geq |a_{-,+}(\rho)|$, thus $1 - C^n_{j-1/2} - D^n_{j+1/2} \geq 0$ when $\Delta t \max|a(\rho)| \leq \Delta x$

Entropy dissipation

Let η convex. By the dissipation lemma
$\displaystyle\int \eta'(\xi)(f_j^{n+1} - M[\rho_j^{n+1}])\,\mathrm{d}\xi \geq 0$, or $\eta(\rho_j^{n+1}) \leq \displaystyle\int \eta'(\xi) f_j^{n+1}\,\mathrm{d}\xi$.
But

$$\eta'(\xi)f_j^{n+1}(\xi) \leq \eta'(\xi)\Big(M[\rho_j^n](\xi)\Big(1 - \frac{\Delta t}{\Delta x}|a(\xi)|\Big) \\ + \frac{\Delta t}{\Delta x} a_+(\xi) M[\rho_{j-1}^n](\xi) + \frac{\Delta t}{\Delta x}(-a_-(\xi)) M[\rho_{j+1}^n](\xi)\Big).$$

Sum over j and ξ:

$$\sum_j \int \eta'(\xi) f_j^{n+1}(\xi)\,\mathrm{d}\xi \leq \sum_j \int \eta'(\xi) M[\rho_j^n](\xi)\,\mathrm{d}\xi = \sum_j \eta(\rho_j^n)$$

We conclude that $\displaystyle\sum_j \eta(\rho_j^{n+1}) \leq \sum_j \eta(\rho_j^n)$. ExBu

Kinetic scheme for the Euler system

Let us start with a Time splitting

- Step 1: solve the linear transport equation

$$\partial_t f + \xi \partial_x f = 0.$$

UpWind does the job ($\xi_\pm = \frac{\xi \pm |\xi|}{2}$).

$$\frac{\Delta x}{\Delta t}(f_j^{n+1/2}(\xi) - f_j^n(\xi)) \\ = -\{\xi_+(f_j^n(\xi) - f_{j-1}^n(\xi)) + \xi_-(f_{j+1}^n(\xi) - f_j^n(\xi))\}.$$

- Step 2: solve the stiff ODE

$$\partial_t f = \frac{1}{\tau}(M[\rho, u, \theta] - f).$$

BUT ρ, u, θ do not change during this step ($\int Q(f)\,\mathrm{d}\xi = 0$):
$(\rho, u, \theta)^{n+1} = (\rho, u, \theta)^{n+1/2} = \displaystyle\int (1, v, |\xi - u|^2/N) f^{n+1/2}\,\mathrm{d}\xi.$
We integrate by hand:

$$f_j^{n+1} = e^{-\Delta t/\tau} f_j^{n+1/2} + (1 - e^{-\Delta t/\tau}) M_j^{n+1/2}.$$

Kinetic scheme for the Euler system

Now let $\tau \to 0$

- Step 2 degenerates to $f_j^{n+1} = M_j^{n+1/2}$ (projection to the equilibrium).
- Integrate Step 1 to obtain a scheme for the macroscopic quantities $\rho, \rho u, \rho E = \rho u^2/2 + N\theta/2$

$$\begin{pmatrix} \rho_j^{n+1} \\ (\rho u)_j^{n+1} \\ (2\rho E)_j^{n+1} \end{pmatrix} = \int \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} f_j^{n+1} \, \mathrm{d}\xi = \int \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} f^{n+1/2} \, \mathrm{d}\xi$$

$$= \begin{pmatrix} \rho_j^{n} \\ (\rho u)_j^{n} \\ (2\rho E)_j^{n} \end{pmatrix} - \frac{\Delta t}{\Delta x}(F_{j+1/2}^n - F_{j-1/2}^n),$$

with the numerical fluxes

$$F_{j+1/2}^n = \int \xi_+ \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} M[\rho_j^n, u_j^n, \theta_j^n] \, \mathrm{d}\xi + \int \xi_- \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} M[\rho_{j+1}^n, u_{j+1}^n, \theta_{j+1}^n] \, \mathrm{d}\xi.$$

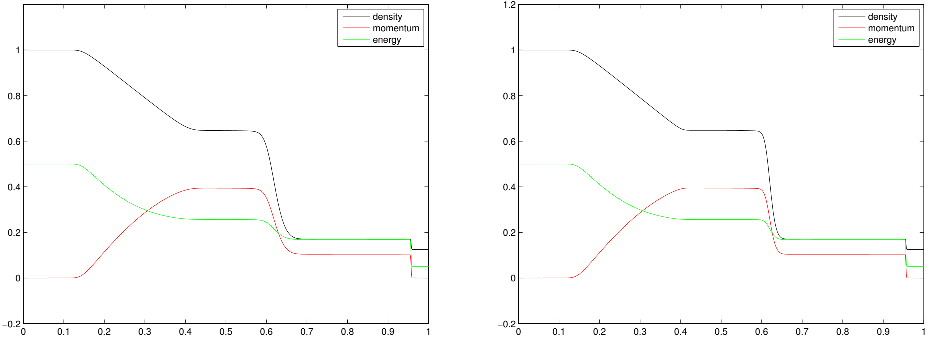
Properties of the scheme

- Work with generalized equilibrium having compact support, adapted to the characteristic speeds of the system $u-\sqrt{3\theta}, u, u+\sqrt{3\theta}$: replace the Maxwellian $M[\rho,u,\theta]$ by Kaniel's function

$$\mathscr{M}[\rho,u,\theta](\xi) = \frac{\rho}{2\sqrt{\theta}}\mathbf{1}_{|\xi-u|\leq\sqrt{3\theta}}$$

- Under CFL condition: $\max(|u_j^n| + \sqrt{3\theta_j^n}) \leq \Delta x/\Delta t$, then ρ^{n+1} and θ^{n+1} remain ≥ 0. Pos
- Possible extension to more complex pressure law.
- Pullin, Desphpande, Perthame...

Simulation of the Euler system (Rusjanow vs Kinetic)



Remarks on Isentropic Euler equations

Pressure law: $p = p(\rho)$. Example $p(\rho) = \kappa\rho^\gamma$, $\kappa > 0$, $\gamma > 1$ (but for "real" applications the formula can be much more complicated, with possible loss of convexity).

$$\begin{aligned} &\partial_t \rho + \partial_x(\rho u) = 0, \\ &\partial_t(\rho u) + \partial_x(\rho u^2 + p(\rho)) = 0 \end{aligned}$$

In non conservative form, with $U = (\rho, \rho u = J)$

$$\partial_t U + A(U)\partial_x U = 0, \qquad A(U) = \begin{pmatrix} 0 & 1 \\ -J^2/\rho^2 + p'(\rho) & 2J/\rho \end{pmatrix}$$

Eigenvalues $u \pm c(\rho)$, with $c(\rho) = \sqrt{p'(\rho)}$, the sound speed.

Entropy

Let $\Phi''(\rho) = \dfrac{p'(\rho)}{\rho}$ and set $\eta(U) = \dfrac{J^2}{2\rho} + \Phi(\rho)$. Then, $U \mapsto \eta(U)$ is convex and we have, for smooth solutions,

$\partial_t \eta(U) + \partial_x q(U) = 0$, with $q(U) = J(\dfrac{J^2}{2\rho^2} + \Phi(\rho))$

Kinetic schemes for the isentropic Euler system

Kaniel's function

Use $\mathscr{M}[\rho, u](\xi) = \dfrac{\rho}{2c(\rho)} \mathbf{1}_{|\xi - u| \leq c(\rho)}$. Idea based on the finite speed of propagation of the system.

Entropy and Gibbs principle

Minimize a functional $H(f) = \int \left(\frac{\xi^2}{2} f + \Psi(f) \right) \mathrm{d}\xi$, under moments constraints $\int (1, \xi) f \, \mathrm{d}\xi = (\rho, J)$. Denote $M[\rho, J]$ the minimizor. The construction is such that $\eta(\rho, J) = H(M[\rho, J])$. We get

$$M[\rho, J] = a \Big[\rho^{\gamma - 1} - b |\xi - J/\rho|^2 \Big]_+^{(3-\gamma)/2(\gamma-1)}$$

See Bouchut, Berthelin-Bouchut, Perthame

Comments on the isentropic case

- By construction the scheme $\#2$ is entropy decaying.
- But the CFL is slightly more constrained than with method $\#1$.
- There is no clear formula for general (non homogeneous) pressure laws
- Computation of the numerical fluxes involves the evaluation of integrals that could be numerically costly (except for $\gamma = 2$)... (to be compared with the resolution of Riemann problems)
- Kinetic schemes usually performs well in vacuum regions
- A new version of (stable and entropy-decaying) kinetic scheme on staggered grids: Berthelin-G.-Minjeaud.

A kinetic scheme on staggered grids for barotropic gas dynamics

$$\begin{cases} \partial_t \phi + \partial_x(\phi V) = 0, \\ \partial_t(\phi V) + \partial_x(\phi V^2 + \pi(\phi)) = 0. \end{cases}$$

The pressure $\phi \mapsto \pi(\phi)$ is strictly increasing and strictly convex;
the sound speed $\phi \mapsto c(\phi) = \sqrt{\pi'(\phi)}$ is strictly increasing.
[Not true for "real" gases like the Bizarrium.]
The system is hyperbolic, the characteristic speeds are $V \pm c(\phi)$.

Kinetic scheme

Define a "generalized Maxwellian" $M = (M_0, M_1)(\phi, V)$ with

$$\int M \,\mathrm{d}\xi = \begin{pmatrix} \phi \\ \phi V \end{pmatrix} = U, \quad \int \xi M \,\mathrm{d}\xi = \begin{pmatrix} \phi V \\ \phi V^2 + \pi(\phi) \end{pmatrix} = F(U).$$

Set $F^{\pm}(U) = \int_{\xi \gtrless 0} \xi M(\phi, V)(\xi) \,\mathrm{d}\xi.$

Consistency : $F(U) = F^+(U) + F^-(U)$.

Construction of the kinetic scheme

Principle : Fluxes are constructed from **moments of** M & **Upwinding**

Maxwellian

$$M_0(\phi, V)(\xi) = \frac{\phi}{2c(\phi)} \mathbf{1}_{|\xi - V| \leq c(\rho)},$$
$$M_1(\phi, V)(\xi) = V M_0(\phi, V)(\xi) + \tilde{M}(\phi, V)(\xi)$$

with $\tilde{M}(\phi, V)(\xi) = \xi L(\phi, V) \mathbf{1}_{|\xi| \leq |V| + c(\phi)}$.

Staggered grids: Mass flux

Density known at $x_{j+1/2}$, velocity at the interface x_j.
Upwinding is natural

$$\frac{h_{j+1/2}}{\Delta t}(\phi^{k+1}_{j+1/2} - \phi^k_{j+1/2}) + \mathscr{F}^k_{j+1} - \mathscr{F}^k_j = 0,$$
$$\mathscr{F}^k_j = \int_{\xi>0} \xi M_0(\phi_{j-1/2}, V^k_j)\,\mathrm{d}\xi + \int_{\xi<0} \xi M_0(\phi_{j+1/2}, V^k_j)\,\mathrm{d}\xi$$

Staggered grids: Momentum

- Set $\phi_j^k = \dfrac{h_{j+1/2}\phi_{j+1/2}^k + h_{j-1/2}\phi_{j-1/2}^k}{2h_j} = \dfrac{1}{h_j}\displaystyle\int \phi_h^k(y)\,\mathrm{d}y$.
- FV scheme
  $$\frac{h_j}{\Delta t}(\phi_j^{k+1}V_j^{k+1} - \phi_j^k V_j^{k+1}) + \tilde{\mathscr{F}}_{j+1/2}^k - \tilde{\mathscr{F}}_{j+1/2}^k = 0.$$
- **Pressure flux**: Since
  $$\int_{\xi>0} \xi \tilde{M}(\rho, V)\,\mathrm{d}\xi + \int_{\xi<0} \xi \tilde{M}(\rho', V')\,\mathrm{d}\xi = \frac{1}{2}(p(\rho) + p(\rho'))$$
  the pressure gradient is **centered** $p(\phi_{j+1/2}^k) - p(\phi_{j-1/2}^k)$.
- **Convection flux**: $\phi V \times V$ =Mass flux $\times$ V involves $\displaystyle\int_{\xi\gtrless 0} \xi M_0(\phi, V)(\xi) \times V\,\mathrm{d}\xi$. Idea: Upwind of V and average on $x_{j+1/2}$ of the mass fluxes known at x_j, x_{j+1}:
  $$V_j \frac{\mathscr{F}^+(\phi_{j-1/2}, V_j) + \mathscr{F}^+(\phi_{j+1/2}, V_{j+1/2})}{2} + V_{j+1}\frac{\mathscr{F}^-(\phi_{j+1/2}, V_j) + \mathscr{F}^-(\phi_{j+3/2}, V_{j+1})}{2}$$

Numerical Analysis

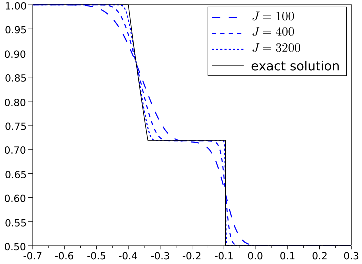
Under suitable CFL condition:

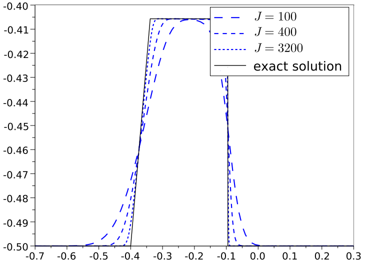
- Positivity of the density is preserved $\rho^k_{j+1/2} \geq 0$,
- The physical entropy is decaying: with $p(\rho) = \rho\Phi'(\rho) - \Phi(\rho)$,

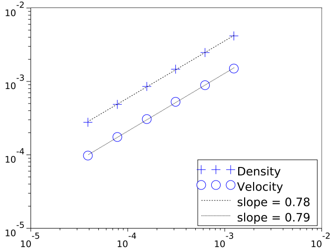
$$h_j \sum_j \phi_j^{k+1} |V_j^{k+1}|^2 + h_{j+1/2} \sum_j \Phi(\phi^{k+1}_{j+1/2}) \leq h_j \sum_j \phi_j^k |V_j^k|^2 + h_{j+1/2} \sum_j \Phi(\phi^k_{j+1/2}).$$

  It holds for general (convex) pressure laws.
  Proof: mixing of Bouchut's and Herbin-Latché techniques.
  Unusual: "work with 2 eq. rather than a system".
- Performs well in vacuum regions.

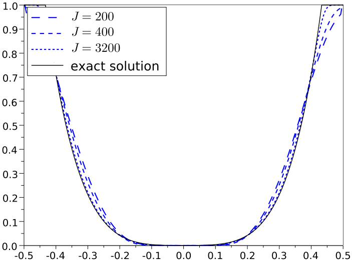
Numerical results (Density, Velocity, L^1-Error)

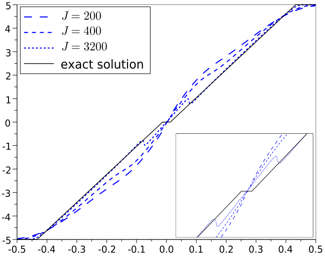


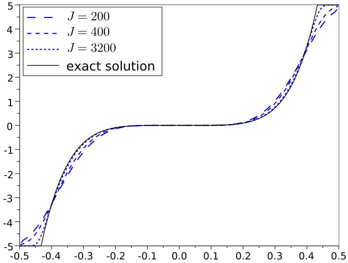




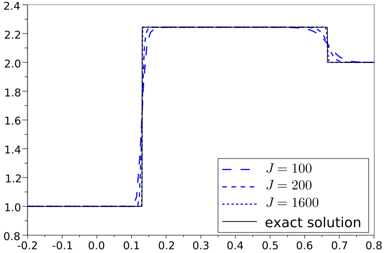
A simulation with vacuum (Density, Velocity, Momentum)

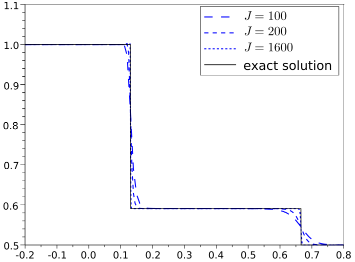


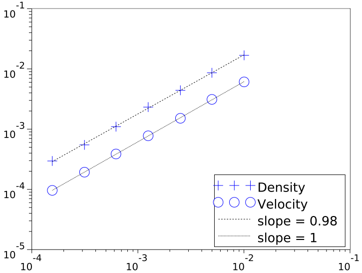




Simulation of a Van der Waals gas $k\left(\frac{\rho}{\rho^*-\rho}\right)^\gamma$







Rankine-Hugoniot condition ▸ WS

Let ρ be a weak solution of $\partial_t \rho + \partial_x f(\rho) = 0$.
Assume that ρ is C^1 in Ω^- and Ω^+, with a discontinuity curve $\Gamma = \{(x,t) = (s(t),t),\ t \geq 0\}$.

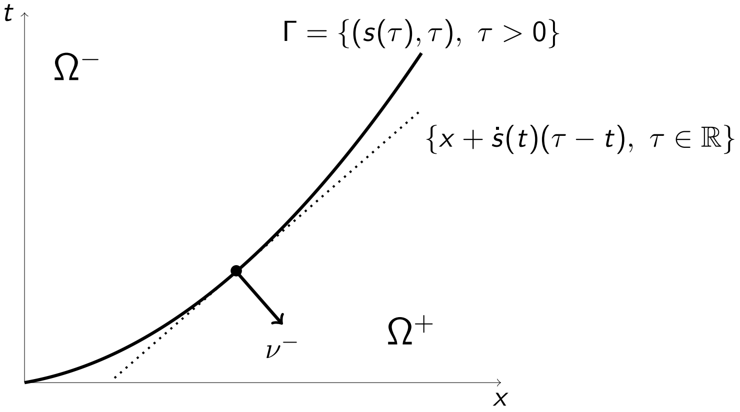


Figure: Courbe de discontinuité et relations de Rankine-Hugoniot

Rankine-Hugoniot condition ▸ WS

Let ρ be a weak solution of $\partial_t \rho + \partial_x f(\rho) = 0$.
Assume that ρ is C^1 in Ω^- and Ω^+, with a discontinuity curve $\Gamma = \{(x,t) = (s(t),t),\ t \geq 0\}$.

$$
\begin{aligned}
-\iint (\rho \partial_t \phi + f(\rho)\partial_x \phi)\,\mathrm{d}x\,\mathrm{d}t = 0 &= -\iint_{\Omega^-} \ldots \mathrm{d}x\,\mathrm{d}t - \iint_{\Omega^+} \ldots \mathrm{d}x\,\mathrm{d}t \\
= \iint_{\Omega^-} \big(\partial_t \rho + \partial_x f(\rho)\big)\phi\,\mathrm{d}x\,\mathrm{d}t &+ \iint_{\Omega^+} \big(\partial_t \rho + \partial_x f(\rho)\big)\phi\,\mathrm{d}x\,\mathrm{d}t \\
-\int_{\Gamma^-} (\rho \nu_t^- + f(\rho)\nu_x^-)\phi\,\mathrm{d}\gamma &- \int_{\Gamma^-} (\rho \nu_t^+ + f(\rho)\nu_x^+)\phi\,\mathrm{d}\gamma \\
= 0 + \int_{\Gamma} \big[(\rho^+ - \rho^-)\nu_t^- &+ (f(\rho^+) - f(\rho^-)\nu_x^-\big]\phi\,\mathrm{d}\gamma
\end{aligned}
$$

since $\nu^- = \begin{pmatrix} \nu_x^- \\ \nu_t^- \end{pmatrix} = -\nu^+ = \dfrac{1}{\sqrt{1 + |s'(t)|^2}} \begin{pmatrix} 1 \\ -s'(t) \end{pmatrix}$.

We arrive at $[\![\rho]\!]\dot{s} = [\![f(\rho)]\!]$

Discontinuous solutions and entropies ▸ Kr

For discontinuous solutions, we make the following quantity appear (by reproducing the computations that lead to RH relations)

$$
\begin{aligned}
&[\![\eta(\rho)]\!]\dot{s} - [\![q(\rho)]\!] = (\eta(\rho_r) - \eta(\rho_\ell))\dot{s} - (q(\rho_r) - q(\rho_\ell)) \\
&= \int_{\rho_\ell}^{\rho_r} \eta'(z)\dot{s}\,\mathrm{d}z - \int_{\rho_\ell}^{\rho_r} q'(z)\,\mathrm{d}z \\
&= \int_{\rho_\ell}^{\rho_r} \eta'(z)\dot{s}\,\mathrm{d}z - \int_{\rho_\ell}^{\rho_r} \eta' f'(z)\,\mathrm{d}z \qquad \text{(then integrate by parts)} \\
&= -\int_{\rho_\ell}^{\rho_r} \eta''(z)\Big(\frac{f(\rho_r) - f(\rho_\ell)}{\rho_r - \rho_\ell}(z - \rho_\ell) - \big(f(z) - f(\rho_\ell)\big)\Big)\,\mathrm{d}z \\
&= -\int_{\rho_\ell}^{\rho_r} \eta''(z)(z - \rho_\ell)\,\left(\frac{f(\rho_r) - f(\rho_\ell)}{\rho_r - \rho_\ell} - \frac{f(z) - f(\rho_\ell)}{z - \rho_\ell}\right)\mathrm{d}z.
\end{aligned}
$$

Since η is convex, $z \mapsto \eta''(z)(z - \rho_\ell)$ has a constant sign on the interval I defined by ρ_r and ρ_ℓ. Assuming that f is convex or concave on I, the integrand has a constant sign and $[\![\eta(\rho)]\!]\dot{s} - [\![q(\rho)]\!]$ vanishes iff $f(z) - f(\rho_\ell) = \dfrac{f(\rho_r) - f(\rho_\ell)}{\rho_r - \rho_\ell}(z - \rho_\ell)$ on I. It would mean that f is an affine function on I, a case that we exclude by assumption

(the flux is assumed "genuinely non linear").

Estimate of m_ϵ

▸ Bk4

Bear in mind that f_ϵ, $M[\rho_\epsilon]$, and thus m_ϵ have their support wrt the variable ξ in $[-V, V]$. Then, with $h_V(\xi) = h(\xi)\mathbf{1}_{|\xi|\leq V}$, $H_V(\xi) = \int_{-\infty}^{\xi} h_V(z)\,\mathrm{d}z$, we have

$$
\begin{aligned}
0 \leq \iiint m_\epsilon h(\xi)\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}t = \iiint m_\epsilon h_V(\xi)\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}t \\
&= -\iiint \frac{1}{\epsilon}\left(M[\rho_\epsilon] - f_\epsilon\right)\, H_V(\xi)\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}t \\
&= -\iiint (\partial_t + a(\xi)\partial_x) f_\epsilon\; H_V(\xi)\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}t \\
&\leq -\iint f_\epsilon H_V\,\mathrm{d}\xi\,\mathrm{d}x\Big|_{t=0}^{t=T} \\
&\leq 2V\,\|h_V\|_{L^\infty}\|f_\epsilon\|_{L^\infty(0,T;L^1)} \\
&\leq 4V\,\|h\|_{L^\infty}\|f_{\mathrm{Init}}\|_{L^1}.
\end{aligned}
$$

Stability analysis

$$f_j^{n+1/2}(\xi) = \left(1 - \frac{\Delta t}{\Delta x}|\xi|\right)\mathscr{M}_j^n(\xi) + \frac{\Delta t}{\Delta x}\xi_+ \mathscr{M}_{j-1}^n(\xi) + \frac{\Delta t}{\Delta x}(-\xi_-)\mathscr{M}_{j+1}^n(\xi)$$

vanishes for $|\xi| \geq \max(|u_j^n + \sqrt{3\theta_j^n})$ (support property of the equilibrium $\mathscr{M}$).

By CFL, this is a convex combination of ≥ 0 quantities:

$f_j^{n+1/2}(\xi) \geq 0$ and $\rho_j^{n+1} = \int f_j^{n+1/2}(\xi)\,\mathrm{d}\xi \geq 0$.

Similarly, we have

$$\begin{aligned} 2(\rho E)_j^{n+1} &= \int \xi^2 f_j^{n+1/2}(\xi)\,\mathrm{d}\xi \\ &= \int \left(|\xi - u_j^{n+1}|^2 - |u_j^{n+1}| + 2u_j^{n+1}\xi\right) f_j^{n+1/2}(\xi)\,\mathrm{d}\xi \\ &\geq 0 - |u_j^{n+1}|^2\rho_j^{n+1} + 2u_j^{n+1}\rho_j^{n+1}u_j^{n+1} = \rho_j^{n+1}|u_j^{n+1}|^2 \end{aligned}$$

Since $2E_j^{n+1} = |u_j^{n+1}|^2 + 3\theta_j^{n+1}$ we deduce that $\theta_j^{n+1} \geq 0$. ▸ PptE

Average Lemma: L^2 statement ▸ Bk5

- Fourier Transform wrt x.
- $\widehat{\rho}(k) = \int \widehat{f}(k,\xi)\psi(\xi)\,\mathrm{d}\xi = \int_{|\xi\cdot k|/\leq\delta|k|} \dots \mathrm{d}\xi + \int_{|\xi\cdot k|/>\delta|k|} \dots \mathrm{d}\xi.$
- $I1 \leq \sqrt{\int |\widehat{f}(k,\xi)|^2\,\mathrm{d}\xi}\sqrt{\int_{|\xi\cdot k|\leq\delta|k|} |\psi|^2\,\mathrm{d}\xi} \leq F(k)\sqrt{\delta}.$
- $I2 \leq \sqrt{\int |k\cdot\xi|^2|\widehat{f}(k,\xi)|^2\,\mathrm{d}\xi}\sqrt{\int_{|\xi\cdot k|>\delta|k|} \frac{|\psi(\xi)|^2}{|k\cdot\xi|^2}\,\mathrm{d}\xi} \leq \frac{G(k)}{\delta|k|^2}.$
- $I2$ (large $k\cdot\xi$'s)=Good, $I1$ (small $k\cdot\xi$'s)=Bad but Small
- Optimize wrt δ, use F, G bounded in L^2...
- We need "enough velocities":

$$\mathrm{meas}\big(\{\xi\in\mathbb{R}^N,\ |\xi|\leq R,\ |\xi\cdot k|\leq\epsilon\}\big) \leq C_R\epsilon^\gamma$$

Gain of compactness ▸ Comp

Set $\Delta_{t,x,\xi}\Phi_\epsilon = m_\epsilon = \nabla_{t,x,\xi} \cdot (\nabla_{t,x,\xi}\Phi_\epsilon)$.
Remind that $W^{1,p} \subset_{\mathrm{comp}} C^0$, hence $\mathscr{M}^1 = (C^0)' \subset_{\mathrm{comp}} W^{-1,p'}$, for $p > N$, $1 \le p' < N/(N-1)$.
Thus Φ_ϵ is compact in $W^{1,p'}_{\mathrm{loc}}$, with, here, $N = 3$, and $\nabla\Phi_\epsilon$ is compact in $L^{p'}_{\mathrm{loc}}$, $1 \le p' < 3/2$.

The assumption on the velocity becomes

$$\mathrm{meas}\big(\{\xi \in \mathbb{R}^N,\ |\xi| \le R,\ |\alpha + a(\xi)\cdot k| \le \epsilon\}\big) \le C_R\epsilon^\delta$$

Here $N = 1$ and we can get rid of k:

$$\mathrm{meas}\big(\{\xi \in \mathbb{R},\ |\xi| \le R,\ |\alpha + a(\xi)| \le \epsilon\}\big) \le C_R\epsilon^\delta$$

It is satisfied when $a'(\xi) = A''(\xi) \neq 0$ for a. e. ξ
(Genuinely Nonlinear problem)

Upwind scheme for the transport equation ▸ BkU

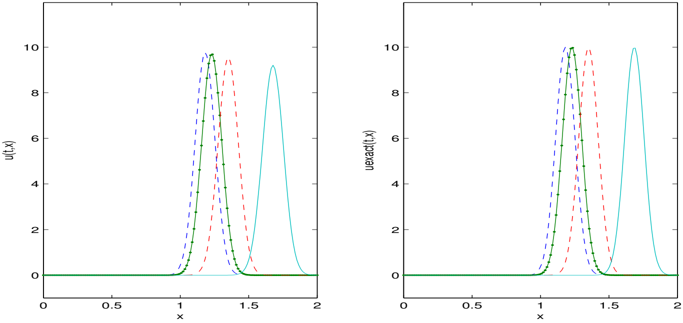


Figure: Upwind Scheme vs. Exact solution