Kinetic Approximations

Philippe Helluy

University of Strasbourg, IRMA CNRS, Inria Tonus

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Plan

Convection-Diffusion Equation

Diffusion Equation

Consider the diffusion (or heat) equation

$$w_t - \mu w_{xx} = 0,$$

where:

- the unknown $w(x,t)$ is a function of $x \in \mathbb{R}$ and time t,
- $w_t = \frac{\partial w}{\partial t}$, $w_x = \frac{\partial w}{\partial x}$,

with an initial condition

$$w(x,0) = w_0(x).$$

The parameter μ is the diffusion coefficient.

Fourier Transform

The Fourier Transform on $\mathbb{R}$ is defined by ($i^2 = -1$)

$$\hat{w}(\xi) = \int_{x=-\infty}^{x=+\infty} w(x)\exp(-ix\xi)dx.$$

Convolution is defined by

$$(f * g)(x) = \int_{x=-\infty}^{x=+\infty} f(x-y)g(y)dy.$$

Some properties:

- $w(x) = \frac{1}{2\pi}\int_{\xi=-\infty}^{\xi=+\infty} \hat{w}(\xi)\exp(+ix\xi)d\xi$ (Inverse Fourier Transform)
- $\int |w|^2 = \int |\hat{w}|^2$ (Parseval's equality, the Fourier Transform is an isometry of $L^2(\mathbb{R})$)
- $(f * g)\hat{} = \hat{f}\hat{g}$ (transform of the convolution into a product)

Exact Solution

Fourier Transform in x ($\partial_x \to i\xi$)

$$\hat{w}_t = -\mu\xi^2 \hat{w}$$

so

$$\hat{w}(\xi, t) = \exp(-\mu\xi^2 t)\hat{w}_0.$$

Remarks:

- Energy decreases if $\mu > 0$ (increases otherwise)
- Convolution in x

$$w = E(\cdot, t) * w_0, \text{ with } E(x, t) = \frac{1}{2\sqrt{\pi\mu t}} \exp(\frac{-x^2}{4\mu t}).$$

- Smoothing effect when $\mu > 0$.

Issue if $\mu < 0$. Suppose that the spectrum of w_0 (the support of $\hat{w}_0$) is bounded, included in the interval $[-\phi, \phi]$, then

$$\|w(\cdot, t)\|_{L^2} \leq \exp(|\mu| \phi^2 t) \|w(\cdot, 0)\|_{L^2},$$

but this estimate cannot be improved: the solution 'explodes' in time.

Convection Equation

Convection (or transport) equation with velocity c

$$w_t + cw_x = 0, \quad w(\cdot, 0) = w_0(\cdot).$$

Fourier Transform

$$\hat{w}_t = -ic\xi\hat{w}.$$

We find

$$\hat{w}(\xi, t) = \exp(-ic\xi t)\hat{w}(\xi, 0).$$

Hence (Fourier shift)

$$w(x, t) = w_0(x - ct).$$

Convection-Diffusion

For the convection-diffusion equation

$$w_t + cw_x - \mu w_{xx} = 0, \quad w(x,0) = w_0(x),$$

where μ is the viscosity coefficient, we find

$$w = E(\cdot,t) * w_0, \text{ with } E(x,t) = \frac{1}{2\sqrt{\pi\mu t}}\exp(\frac{-(x-ct)^2}{4\mu t}).$$

Stability

From the previous formula, we can deduce:

- Maximum principle: if $0 \leq w_0 \leq M$ then $0 \leq w(\cdot, t) \leq M$, $t > 0$.
- Decay of energy $\mathcal{E}(t) = \int_x w(x,t)^2 dx$: $\mathcal{E}(t) \leq \mathcal{E}(0)$, $t > 0$.

Upwind scheme

We consider the transport equation

$$w_t + cw_x = 0, \quad x \in \mathbb{R}, \quad t \geq 0,$$

with initial condition $w(x, 0) = w_0(x)$ and $c > 0$.
Time step τ, space step h. Discretization at points $x_i = ih$, $t_n = n\tau$, $w_i^n \simeq w(x_i, t_n)$. Upwind scheme, $w_i^0 = w(x_i, 0)$ and

$$\frac{w_i^{n+1} - w_i^n}{\tau} + c\frac{w_i^n - w_{i-1}^n}{h} = 0.$$

Very natural: information comes from the left.

Maximum principle

We introduce the CFL number $\beta = c\tau/h$. Then:

$$w_i^{n+1} = (1-\beta)w_i^n + \beta w_{i-1}^n.$$

Under the condition $\beta \leq 1$ we have the discrete maximum principle. If for all i, $0 \leq w_i^0 \leq M$ then for all i and $n > 0$, $0 \leq w_i^n \leq M$.

Equivalent Equation

We can construct a continuous version of the previous scheme. We seek a function $\tilde{w}(x, t)$ (which we still denote w) that solves the difference equation

$$\frac{w(x, t+\tau) - w(x, t)}{\tau} + c\frac{w(x, t) - w(x-h, t)}{h} = 0.$$

This solution coincides with the discrete solution at the points $(x, t) = (x_i, t_n)$. What does w satisfy formally when h and τ tend to 0 with $c\tau/h = \beta$ fixed?

Energy stability

Shift operator (notation: $I^2 = -1$)

$$(\mathcal{D}_h w)(x) = w(x-h), \quad (\mathcal{D}_h w)^\wedge(\xi) = \exp(-Ih\xi)\hat{w}(\xi).$$

The finite difference equation becomes, with $c\tau/h = \beta$,

$$\hat{w}(\xi, t+\tau) = A(\xi, h)\hat{w}(\xi, t),$$

with $A(\xi, h) = (1 - \beta + \beta e^{-Ih\xi})$, the amplification coefficient. The scheme is stable in L^2 iff A is in the unit disk for all frequencies ξ. We retrieve the condition

$$\beta \leq 1.$$

Using Fourier

Shift operator (notation: $I^2 = -1$)

$$(\mathcal{D}_h w)(x) = w(x-h), \quad (\mathcal{D}_h w)^\wedge(\xi) = \exp(-Ih\xi)\hat{w}(\xi).$$

The difference equation becomes, with $c\tau/h = \beta$,

$$\hat{w}(\xi, t+\tau) = A(\xi,\tau)\hat{w}(\xi,t),$$

with $A(\xi, h) = (1-\beta+\beta e^{-Ih\xi})$. So we have

$$\frac{\hat{w}(\xi,t+\tau)-\hat{w}(\xi,t-\tau)}{2\tau} + \frac{1}{2\tau}\left(\frac{1}{A(\xi,-\tau)} - A(\xi,\tau)\right)\hat{w}(\xi,\tau) = 0.$$

With a Taylor expansion at $\tau = 0$ and inverse Fourier transform, we find

$$w_t + cw_x - \frac{c}{2}(1-\beta)hw_{xx} = 0 + O(h^2).$$

The upwind scheme introduces a numerical viscosity $\mu = \frac{c}{2}(1-\beta)h$. The consistency is therefore of order 1. We recover the CFL stability condition.

Remark on the equivalent equation

The equivalent equation often provides information on the CFL stability, but not always [5]. Example: heat equation

$$w_t - w_{xx} = 0,$$

discretized by the classical explicit scheme

$$\frac{u(x,t+\tau) - u(x,\tau)}{\tau} + \frac{-u(x-h,\tau) + 2u(x,\tau) - u(x+h,\tau)}{h^2} = 0.$$

The equivalent equation is

$$u_t - u_{xx} - \frac{1}{12}(1-6\beta)h^2 u_{xxxx} = O(h^4),$$

which is stable under the condition $\beta > 1/6$ while the scheme is stable if $\beta < 1/2$!

Hyperbolic Systems

Conservation Laws

First-order conservation laws system (CLS). Notation convention: vectors and matrices with capital letters, scalars with lowercase letters.

$$W_t + \sum_{i=1}^{d} \partial_i Q^i(W) = 0,$$

- Unknown vector: $W(X,t) \in \mathbb{R}^m$, $X = (x^1, \ldots, x^d) \in \mathbb{R}^d$ space variable, $t \geq 0$, time variable;
- $\partial_i = \frac{\partial}{\partial x^i}$. If $d = 1$ we note $w = W$, $x^1 = x$, $Q^1(W) = q(w)$ and $\partial_1 Q^1(W) = q(w)_x$.
- $Q^i(W)$: flux in the direction i. If $Q^i(W, \nabla_X W)$: second-order system...

For a spatial vector $N \in \mathbb{R}^d$ we can also define the flux in the direction N by

$$Q(W,N) = \sum_{i=1}^{d} Q^i(W) \cdot N_i(W) = Q(W) \cdot N(W).$$

Conservation ?

Integrate the CLS over a space domain Ω and note the "mass" contained in this domain at time t

$$M(t) = \int_{X\in\Omega} W(X,t).$$

The Stokes formula leads to

$$\frac{d}{dt}M(t) = \int_{X\in\partial\Omega} Q(W(X,t),N(X)),$$

where $N(X)$ is the outward normal vector to Ω at point X on the boundary $\partial\Omega$.
In other words, the variation of the mass in the domain over time is given by the integral of the flux on the boundary.

Hyperbolicity

The CLS is hyperbolic if for all directions N and all vector W the Jacobian matrix of the flux

$$A(W, N) = D_W Q(W, N)$$

is diagonalizable with real eigenvalues. We note $\lambda_i(W, N)$ the eigenvalues (often arranged in ascending order) and $R_i(W)$ the corresponding eigenvectors.
Note that in the scalar case $m = 1$ the system is necessarily hyperbolic.

Hyperbolicity?

Consider the linear CLS $W = (a, b)^\intercal$

$$\partial_t \begin{pmatrix} a \\ b \end{pmatrix} + \partial_x \left(\begin{pmatrix} 0 & \epsilon \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right) = 0, \quad \epsilon = \pm 1.$$

In Fourier space

$$IM(\xi,\tau) \begin{pmatrix} \hat{a}(\xi,\tau) \\ \hat{b}(\xi,\tau) \end{pmatrix} = 0, \quad M(\xi,\tau) = \begin{pmatrix} \tau & \epsilon\xi \\ \xi & \tau \end{pmatrix}.$$

There are non-trivial solutions if and only if $\det M(\xi,\tau) = 0$ which gives

$$\tau^2 - \epsilon\xi^2 = 0.$$

If $\epsilon = 1$, this resembles the equation of a hyperbola and the system is said to be hyperbolic. If $\epsilon = -1$, the system is said to be elliptic.

Examples: transport, Burgers

Consider $d = 1$, $m = 1$, and $q(w) = cw$. This gives the 1D transport equation

$$w_t + cw_x = 0.$$

The eigenvalue $\lambda_1 = c$.
The Burgers equation is obtained by choosing $q(w) = w^2/2$. This yields

$$w_t + \left(\frac{w^2}{2}\right)_x = 0.$$

For smooth solutions, the Burgers equation can also be written

$$w_t + ww_x = 0.$$

Here,

$$\lambda_1(w) = w.$$

In the Burgers equation, the wave speed is also the unknown conservative quantity w.

Example: Traffic Flow

Vehicle density on a highway lane $w(x,t) \geq 0$. Vehicle speed $v = v(w)$. Conservation law of vehicles

$$w_t + (v(w)w)_x = 0.$$

The flux is therefore

$$q(w) = wv(w).$$

Vehicle driver behavior law. For a maximum density $w = w_{max}$, the speed $v(w_{max}) = 0$. For a very fluid traffic, drivers travel at the maximum allowed speed $v(0) = v_{max}$. Therefore, we can take

$$v(w) = (1 - \frac{w}{w_{max}})v_{max}.$$

Here the wave speed is therefore

$$\lambda(w) = q'(w) = (1 - \frac{2w}{w_{max}})v_{max} \in [-v_{max}, v_{max}].$$

Other Examples

- Saint-Venant Model (or shallow water): $m = 2$, $d = 1$, water height $h(x,t)$, mean horizontal velocity $u(x,t)$, gravity $g = 9.81\text{m/s}^2$.

$$W = \begin{pmatrix} h \\ hu \end{pmatrix}, \quad Q^1(W) = \begin{pmatrix} hu \\ hu^2 + gh^2/2 \end{pmatrix},$$

$$\partial_t W + \partial_x Q^1(W) = 0.$$

- Compressible Gas;
- Maxwell's Equations;
- Multiphase Fluid;
- MHD Equations;
- *etc.*

Method of Characteristics

Consider a scalar 1D conservation law ($m = 1$, $d = 1$)

$$w_t + q(w)_x = 0.$$

Characteristic curve: parameterized curve $t \mapsto (x(t), t)$ in the (x, t) plane along which w is constant

$$\frac{d}{dt} w(x(t), t) = 0.$$

We find that $x'(t) = q'(w(x(t), t) = q'(w(x(0), 0)$ is constant. The characteristics are therefore straight lines. This allows to compute the solutions (strong solutions).

Critical Time

- Transport: if $q(w) = cw$ then $x(t) = ct + x_0$. Therefore $w(x,t) = w(x(0),0) = w(x - ct, 0)$.
- Burgers: if $q(w) = w^2/2$ then $x(t) = w(x_0, 0)t + x_0$. If the initial condition is decreasing and q convex, one can see that the characteristics intersect while transporting different values of w. The strong solution ceases to exist after a certain time that can be calculated as:

$$t = \frac{-1}{\inf_x q'(w_0(x))}.$$

The concept of a strong solution is not sufficient. It will be necessary to generalize.

Hyperbolicity and Transport

Hyperbolicity is a necessary condition for stability. Example: a one-dimensional ($d = 1$) linear CLS with constant coefficients:

$$W_t + Q(W)_x = 0, \quad Q(W) = AW.$$

If A is diagonalizable with real eigenvalues

$$\text{diag}(\lambda_1, \ldots, \lambda_m) = \Lambda = R^{-1}AR,$$

where the columns of R are the eigenvectors R_i. Positing $W = PY$, we have

$$Y_t + \Lambda Y_x = 0$$

and each component Y^i of Y is a solution to a transport equation with velocity λ_i. The eigenvalues can be interpreted as wave speeds.

Hyperbolicity and Stability

If an eigenvalue λ_i is not real, that is $\lambda_i = a + Ib$, $b \neq 0$. $y = Y^i$ is a solution to the transport equation

$$y_t + (a + Ib)y_x = 0.$$

In Fourier space:

$$\hat{y}_t + (a + Ib)I\xi\hat{y} = 0.$$

This implies that

$$\hat{y}(\xi, t) = e^{-Ia\xi t}e^{b\xi t}\hat{y}(\xi, 0).$$

High-frequency modes are exponentially unstable...

Weak Solution

Definition: $W(X,t)$ is a weak solution of $W_t + \nabla_X \cdot Q(W) = 0$, $W(X,0) = W_0(X)$ if for any regular test function $\varphi(X,t)$ with bounded support,

$$\int_{X,t\geq 0} (W\varphi_t + Q(W)\cdot\nabla_X\varphi) = \int_X W_0\varphi(\cdot,0).$$

By integration by parts: strong $\Rightarrow$ weak and weak + regular $\Rightarrow$ strong.
What happens in the weak + discontinuous case?

Rankine-Hugoniot

Weak solution with discontinuity on a surface Σ of the space-time ("shock"). Normal vector (N, n_t) to this surface, oriented from side L to side R. We note $[a] = a_R - a_L$ the jump of the quantity a across the discontinuity.
Rankine-Hugoniot relations:

$$n_t[W] + N \cdot [Q(W)] = 0.$$

If N is a unit spatial vector then $n_t = -\sigma$ where σ is the normal speed of the discontinuity. We find

$$\sigma[W] = N \cdot [Q(W)].$$

Caution: some calculations are no longer valid for weak solutions. For example, if w is a weak solution of $w_t + (w^2/2)_x = 0$, w is not necessarily a weak solution of $(w^2/2)_t + (w^3/3)_x = 0$.

Loss of Uniqueness

There is no uniqueness of weak solutions for the Cauchy problem.
Example (with Burgers $q(w) = w^2/2$):

$$w_t + q(w)_x = 0,$$

$$w(x,0) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{otherwise.} \end{cases}$$

At least two weak solutions:

$$w_1(x,t) = \begin{cases} 0 & \text{if } x < t/2, \\ 1 & \text{otherwise.} \end{cases}$$

$$w_2(x,t) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{if } x > t, \\ x/t & \text{otherwise.} \end{cases}$$

We only keep the second solution (as it is less "discontinuous").

Lax Characteristic Criterion

There is no need to introduce a shock when the characteristics do not intersect. A shock of velocity σ satisfies the Lax characteristic criterion ($m = 1$, $d = 1$) if

$$q'(w_L) > \sigma > q'(w_R).$$

In the case $m > 1$, $d > 1$, the Lax characteristic criterion becomes: there exists an index i such that

$$\lambda_i(w_L, N) > \sigma > \lambda_i(w_R, N).$$

Here, N is the normal vector to the discontinuity surface, unitary, and oriented from L to R.

Entropy

The characteristic criterion is geometric. Not practical for numerics. We seek an integral criterion.
An entropy $s(W)$ associated with the entropy flux $G(W)$ is a function that satisfies an additional conservation law

$$s(W)_t + \sum_i \partial_i G^i(W) = 0$$

when W is a strong solution.
Then, setting $A^i(W) = D_W Q^i(W)$,

$$D_W s(W) A^i(W) = D_W G^i(W).$$

For $m = 1$ any function is an entropy. It is more complicated if $m > 1$.

Practical Calculation

As we work with strong solutions, we can change variables. If $W = W(Y)$

$$D_Y W Y_t + A^i D_Y W \partial_i Y = 0, \quad A^i = D_W Q^i,$$

which implies

$$Y_t + B^i(Y)\partial_i Y = 0, \quad B^i = P^{-1} A^i P, \quad P = D_Y W.$$

With $s(W) = u(Y)$ and $G^i(W) = H^i(Y)$, we have

$$D_Y u B^i = D_Y H^i.$$

Example: Saint-Venant

Saint-Venant equations, $m = 2$, $d = 1$, water height h, velocity u, gravity $g = 9.81\text{m/s}^2$.

$$W = \begin{pmatrix} h \\ hu \end{pmatrix}, \quad Q(W) = \begin{pmatrix} hu \\ hu^2 + gh^2/2 \end{pmatrix}.$$

By performing calculations in variables $Y = (h, u)^\top$, we find (non-unique solution)

$$s(W) = h\frac{u^2}{2} + \frac{gh^2}{2}, \quad G(W) = h\frac{u^3}{2} + ugh^2.$$

Lax Entropy

An entropy $s(W)$ is a Lax entropy if s is strictly convex with respect to W. A weak solution is a Lax solution if, in the weak sense,

$$s(W)_t + \partial_i G^i(W) \leq 0.$$

Lax entropy criterion for shocks

$$n_t[s(W)] + N \cdot [G(W)] \leq 0,$$

or with shock velocity σ

$$\sigma[s(W)] \geq N \cdot [G(W)].$$

Often, but not always, Lax entropy criterion $\Leftrightarrow$ Lax characteristic criterion [14].

Legendre Transform

An important tool: the Legendre transformation. Consider a function s from $\mathcal{R} \subset \mathbb{R}^m$ to $\mathbb{R}$. Assume that the gradient of s, $\nabla_W s(W)$ from $\mathcal{R}$ to $\mathcal{S} = \nabla s(\mathcal{C})$ is invertible.
This is the case if s is strictly convex, for example. The Legendre transformation s^* of s is defined for $V \in \mathcal{S}$ by

$$s^*(V) = V \cdot W - s(W), \quad V = \nabla s(W).$$

Examples: $s(x) = x^2/2$, $s(x) = x^3/3$, $s(x, y) = y^2/2/x + x^2/2$.
When s is strictly convex, the Legendre transformation coincides with the Fenchel transformation

$$s^*(V) = \sup_W \left(V \cdot W - s(W)\right).$$

In the general case, $\nabla s(W)$ is multivalued, it requires differential geometry...

Useful General Properties

- $V = \nabla s(W) \Leftrightarrow W = \nabla s^*(V)$.
- $s^{**} = s$
- $ds(W) = \nabla s(W) \cdot dW = V \cdot dW$. And $ds^*(V) = \nabla s^*(V) \cdot dV = W \cdot dV$. Exchange of variables and derivatives. Justifies the term conjugate or dual function. Useful in thermodynamics.

Convex Case

If s is strictly convex.

- s^* is strictly convex
- the Hessian matrices of s and s^* are symmetric and positive definite.
- The inf-convolution

$$s_1 \square s_2(W) := \inf_{W=W_1+W_2} s_1(W_1) + s_2(W_2)$$

  is changed into an addition:

$$s^*(V) = s_1^*(V) + s_2^*(V).$$

Duality and Lax Entropy

If s is a Lax entropy, we can calculate its Legendre transform s^*.
Entropic variables:

$$V = \nabla s(W) \Leftrightarrow W = \nabla s^*(V).$$

We then define the dual entropy flux:

$$G^{i,\star}(V) = V \cdot Q^i(W) - G^i(W).$$

(Note: this is not a Legendre transformation, hence the symbol "$\star$" is different from "$*$"). Property:

$$\nabla G^{i,\star}(V) = Q^i(W).$$

In other words: the gradient of the dual entropy is the conservative variables. The gradient of the dual entropy flux, is the flux of the CLS.
The scalar functions $(s^*, G^{i,\star})$ contain all the information on the CLS. It can be seen that the existence of a Lax entropy is a strong property: one reconstructs $d+1$ vectorial functions from only $d+1$ scalar functions!

Mock's Theorem

Theorem

A system is symmetrizable if and only if it admits a Lax entropy [15, 4, 10].

Proof.

$\Leftarrow$: $\partial_t W + \partial_i Q^i(W) = 0$ can also be written as $\partial_t \nabla s^*(V) + \partial_i \nabla G^{i,\star}(V) = 0$. Therefore,

$$D^2 s^*(V)\partial_t V + D^2 G^{i,\star}(V)\partial_i V = 0.$$

The Hessian matrices are symmetric and s^* is strictly convex, therefore $D^2 s^*(V)$ is positive definite.
$\Rightarrow$: if there exists a change of variables that symmetrizes the CLS, then $\partial_t W(V) + \partial_i W(V) Q^i(W) = 0$ with $W(V)$ symmetric and positive definite and $W(V)Q^i(W)$ symmetric. By Poincaré lemma, these are the Hessians of s^* and $G^{i,\star}$. Thus, $s = s^{**}$ and $G^i = G^{i,\star\star}$. □

Example: Saint-Venant

Calculate s, G^i, s^*, $G^{i,\star}$. See [9]

Vanishing Viscosity

Entropic solutions are limits of viscous solutions:

$$\partial_t W^\epsilon + \partial_x Q(W^\epsilon) - \epsilon \partial_{xx} W^\epsilon = 0.$$

The viscosity $\epsilon > 0$ ensures that W^ϵ is regular. It is assumed that $W^\epsilon \to W$ (in a suitable sense). By integration by parts and passing to the limit, W is a weak solution. Multiply by $Ds(W^\epsilon)$:

$$\partial_t s(W^\epsilon) + \partial_x g(W^\epsilon) - \epsilon \nabla s \partial_{xx} W^\epsilon = 0,$$

or, since $DsDQ = Dg$,

$$\partial_t s(W^\epsilon) + \partial_x g(W^\epsilon) = \epsilon Ds \partial_{xx} W^\epsilon = \epsilon \partial_x Ds \partial_x W - \epsilon D^2 s \partial_x W \cdot \partial_x W,$$

As s is convex $D^2 s \partial_x W \cdot \partial_x W \geq 0$. Then we multiply by a test function $\varphi \geq 0$ and we integrate by parts

$$\int_{x,t} (-s(W^\epsilon)\partial_t \varphi - g(W^\epsilon)\partial_x \varphi) \leq \epsilon \int_{x,t} W^\epsilon \partial_x Ds \partial_x \varphi.$$

Thus, when $\epsilon \to 0$, we have in the weak sense

$$\partial_t s(W) + \partial_x g(W) \leq 0.$$

Kinetic Approximation

Kinetic Representation

System of Conservation Laws (CSL)

$$\partial_t W + \partial_i Q^i(W) = 0. \tag{1}$$

Kinetic vectors F_k

$$W = \sum_{k=1}^{n_v} F_k.$$

Global kinetic vector F, made of all the F_k stacked together:

$$F = (F_1^\mathsf{T}, \dots, F_{n_{nv}}^\mathsf{T})^\mathsf{T}.$$

Or

$$W = PF,$$

with P a constant matrix, called the **projection matrix**.

BGK Model

Kinetic velocities V_k **constants**, $k = 1 \dots n_v$. Transport with BGK-type relaxation

$$\partial_t F_k + V_k \cdot \nabla F_k = \frac{1}{\varepsilon}(F_k^{eq} - F_k), \quad k = 1 \dots n_v.$$

Kinetic equilibrium $F_k^{eq} = F_k^{eq}(W)$.
Noting 1_m the identity matrix of size $m \times m$ and V^i the diagonal matrices

$$V^i = \begin{pmatrix} V_1^i 1_m & & \\ & \ddots & \\ & & V_{n_v}^i 1_m \end{pmatrix},$$

the BGK system can also be written in the full vector form

$$\partial_t F + \sum_{i=1}^{d} \partial_i \left(V^i F \right) = \frac{1}{\varepsilon}(F^{\mathrm{eq}}(W) - F).$$

Consistency

As $\varepsilon \to 0$, we expect $F_k \simeq F_k^{eq}$. The kinetic system is therefore an approximation of the CLS (1) if

$$W = \sum_k F_k^{\mathrm{eq}}(W), \quad Q^i(W) = \sum_{k=1}^{n_v} V_k^i F_k^{\mathrm{eq}}(W), \tag{2}$$

Kinetic Scheme

BGK relaxation: nonlinear coupling between all kinetic vectors F_k. To decouple, a decomposition scheme (*splitting*) is used. Each time step Δt is divided into:

- Transport: computation of $F_k(\cdot, t^-)$ from $F_k(\cdot, t-\Delta t^+)$ by solving
$$\partial_t F + \sum_{i=1}^{d} \partial_i \left(V^i F\right) = 0.$$
- Get the conservative variables
$$W(\cdot, t) = \sum_k F_k(\cdot, t^-).$$
- Relaxation: computation of $F_k(\cdot, t^+)$
$$F_k(\cdot, t^+) = \omega F_k^{eq}(W(\cdot, t)) + (1-\omega) F_k(\cdot, t^-).$$

Note: $\omega \in [1, 2]$ is the relaxation parameter. First-order scheme if $\omega = 1$, second-order scheme if $\omega = 2$ (over-relaxation). W is continuous in time, but not F_k.

Kinetic Entropy

A kinetic Lax-Mock theory can be developed. Suppose we find functions $s_k^*(V)$ such that

$$\sum_{k=1}^{n_v} s_k^* = s^*, \quad \sum_k V_k^i s_k^* = G^{i,\star}.$$

Let

$$F_k^{eq}(W(V)) = \nabla_V s_k^*(V).$$

Then, by taking the gradient:

- $\sum_k F_k^{eq} = \nabla_V s^* = W$,
- $\sum_k V_k^i F_k^{eq} = \nabla_V G^{i,\star} = Q^i$.

Moreover, if the s_k^* are convex, the equilibrium is also a minimum of the kinetic entropy:

$$s(W) = \min_{W=\sum_k F_k} \sum_k s_k(F_k) = \sum_k s_k(F_k^{eq}).$$

Entropic Stability

It then becomes easy to prove the entropic stability of the kinetic scheme. The total entropy (x is assumed to be in an infinite or periodic domain)

$$\mathcal{S}(t) = \int_x \sum_k s_k(F_k)$$

is conserved during the transport step. It is sufficient to show that

$$\sum_k s_k(F_k(\cdot, t^+)) \leq \sum_k s_k(F_k(\cdot, t^-)).$$

This is the case (proof) when $\omega = 1$ and also (diagram) for $\omega \simeq 2$.

Sub-characteristic Condition

The above proof works as long as the s_k are convex, which is equivalent to s_k^* being convex. Taking the case $d = 1$ and $n_v = 2$, we have

$$s_{1,2}^* = \frac{s^*}{2} \pm \frac{g^\star}{2\lambda}.$$

Since s^* is strictly convex, if λ is large enough, we expect s_k^* to also be strictly convex, at least locally. The condition of s_k^* being strictly convex leads to the sub-characteristic condition. Examples: transport, Burgers, Saint-Venant.

Approximate Flux

Another way to study stability: equivalent equation. The projection matrix P is a matrix with m rows and mn_v columns. It is extended to an invertible matrix

$$M = \begin{pmatrix} P \\ R \end{pmatrix},$$

called the moment matrix, such that

$$\begin{pmatrix} W \\ Z \end{pmatrix} = MF.$$

The vector $Z = RF$ is called the "approximate flux". The "flux error" is also defined as

$$Y = R(F - F^{eq}).$$

It is enlightening to find the PDE satisfied by the couple (W, Y).

Equivalent PDE Algorithm

The kinetic scheme is a functional operator that computes $F(\cdot, t+\Delta t^+)$ from $F(\cdot, t^+)$. With the previous change of variables, we have thus a well-defined operator $\mathcal{M}(\Delta t)$, such that

$$\begin{pmatrix} W \\ Y \end{pmatrix}(\cdot, t+\Delta t^+) = \mathcal{M}(\Delta t)\begin{pmatrix} W \\ Y \end{pmatrix}(\cdot, t^+).$$

To find the equivalent PDE, we perform a Taylor expansion in Δt of

$$\frac{\mathcal{M}(\Delta t/2) - \mathcal{M}(-\Delta t/2)}{\Delta t}\begin{pmatrix} W \\ Y \end{pmatrix} = \partial_t \begin{pmatrix} W \\ Y \end{pmatrix} + O(\Delta t^2).$$

This expansion can be automated with Maple or SymPy for instance.

Flux Error Oscillations

In the set of variables (W, Y), the relaxation step

$$F_k(\cdot, t^+) = \omega F_k^{eq}(W(\cdot, t)) + (1-\omega) F_k(\cdot, t^-),$$

becomes simply

$$\begin{pmatrix} W \\ Y \end{pmatrix}(\cdot, t^+) = \begin{pmatrix} W \\ (1-\omega) Y \end{pmatrix}(\cdot, t^-).$$

In particular, if $\omega = 2$, the flux error Y is changed to $-Y$. To remove this rapid oscillation of frequency $1/\Delta t$, we can replace $\mathcal{M}(\Delta t)$ by $\mathcal{M}(\Delta t/2) \circ \mathcal{M}(\Delta t/2)$ in the analysis.

Form of the Equivalent PDE

The operator $\mathcal{M}$ is composed of shifts and nonlinear relaxations. In the asymptotic development, the shifts produce partial derivatives. The result is a system of nonlinear PDEs of the form

$$\partial_t \begin{pmatrix} W \\ Y \end{pmatrix} + \frac{r(\omega)}{\Delta t} \begin{pmatrix} 0 \\ Y \end{pmatrix} + \sum_{i=1}^{d} A^i \partial_i \begin{pmatrix} W \\ Y \end{pmatrix}$$

$$+\Delta t \sum_{1 \le i,j \le d} B^{i,j} \partial_{i,j} \begin{pmatrix} W \\ Y \end{pmatrix} = O(\Delta t^2). \qquad (3)$$

Examples

Jin-Xin Model [13]

We apply the previous theory to the Xin-Jin model for $d = 1$, $n_v = 2$,

$$V^1 = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}, \quad F = \begin{pmatrix} F^+ \\ F^- \end{pmatrix}, \quad M = \begin{pmatrix} 1 & 1 \\ \lambda & -\lambda \end{pmatrix}.$$

$$F^{eq} = \begin{pmatrix} \frac{W}{2} + \frac{Q(W)}{2\lambda} \\ \frac{W}{2} - \frac{Q(W)}{2\lambda} \end{pmatrix}, \quad F = \begin{pmatrix} \frac{W}{2} + \frac{Q(W)}{2\lambda} + \frac{Y}{2\lambda} \\ \frac{W}{2} - \frac{Q(W)}{2\lambda} - \frac{Y}{2\lambda} \end{pmatrix}.$$

Jin-Xin, Equivalent System

With $\delta = \omega - 1$, we find

$$O(\Delta t^2) = \partial_t \begin{pmatrix} W \\ Y \end{pmatrix} - \frac{1}{\Delta t}\frac{\delta^4 - 1}{2\delta^2}\begin{pmatrix} 0 \\ Y \end{pmatrix}$$

$$+ \begin{pmatrix} Q'(W) & \gamma_1 \\ \gamma_1(\lambda^2 - Q'(W)^2) & -\gamma_2 Q'(W) \end{pmatrix} \partial_x \begin{pmatrix} W \\ Y \end{pmatrix}$$

$$\Delta t \frac{\delta^2 - 1}{32\delta^2} \begin{pmatrix} (\lambda^2 - v^2)(-\delta^2 + 4\delta - 1) & 3(\delta^2+1)Q'W) \\ 3(\delta^2+1)(\lambda^2 - v^2)Q'W) & \gamma_3 \end{pmatrix} \partial_{xx} \begin{pmatrix} W \\ Y \end{pmatrix}.$$

$$\gamma_1 = \frac{(\delta - 1)^2\left(\delta^2 + 1\right)}{\delta^2}, \quad \gamma_2 = \frac{\delta^4 + 1}{2\delta^2}$$

$$\gamma_3 = -(5Q'(W)^2 + 3\lambda^2)(\delta^2 + 1) + 4(\lambda^2 - Q'(W)^2)\delta$$

Jin-Xin, Equivalent Equation

Under the assumption that $Y = O(\Delta t)$, we obtain, to order 2 in Δt:

$$\partial_t W + \partial_x Q(W) = \frac{1}{2}(\frac{1}{\omega} - \frac{1}{2})\Delta t \partial_x (\lambda^2 - Q'(W)^2)\partial_x W.$$

Jin-Xin Stability

- The terms of the first order of the equivalent system are symmetrizable (thus hyperbolic) if

$$\lambda > \left|Q'(W)\right|.$$

- Under the same condition, the equivalent equation is stable.

In this case, the two stability conditions are equivalent.

D2Q4 Model [9, 2]

We apply the previous theory to the D2Q4 model for transport $(W = w,\ Q(W) \cdot N = aN^1 + bN^2)$, $d = 2$, $n_v = 4$,

$$V^1 = \begin{pmatrix} \lambda & & & \\ & -\lambda & & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \quad V^2 = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & \lambda & \\ & & & -\lambda \end{pmatrix},$$

$$M = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \lambda & -\lambda & 0 & 0 \\ 0 & 0 & \lambda & -\lambda \\ \lambda^2 & \lambda^2 & -\lambda^2 & -\lambda^2 \end{pmatrix}.$$

$$F^{eq} = \frac{1}{4} \begin{pmatrix} w + 2aw/\lambda \\ w - 2aw/\lambda \\ w + 2bw/\lambda \\ w - 2bw/\lambda \end{pmatrix}.$$

D2Q4, equivalent system

We recover the form (3)

$$\partial_t \begin{pmatrix} W \\ Y \end{pmatrix} + \frac{r(\omega)}{\Delta t} \begin{pmatrix} 0 \\ Y \end{pmatrix} + \sum_{i=1}^{d} A^i \partial_i \begin{pmatrix} W \\ Y \end{pmatrix}$$

$$+\Delta t \sum_{1 \leq i,j \leq d} B^{i,j} \partial_{i,j} \begin{pmatrix} W \\ Y \end{pmatrix} = O(\Delta t^2).$$

Details in [9].

D2Q4, equivalent equation

Under the assumption that $Y = O(\Delta t)$, we obtain to order 2 in Δt:

$$\partial_t w + a\partial_x w + b\partial_y w = \frac{\Delta t}{2}(\frac{1}{\omega} - \frac{1}{2})\nabla \cdot (D\nabla w),$$

with

$$D = \begin{pmatrix} \lambda^2/2 - a^2 & -ab \\ -ab & \lambda^2/2 - b^2 \end{pmatrix}.$$

D2Q4 stability

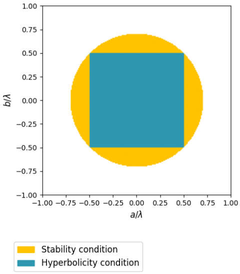
- The first order terms of the equivalent system are symmetrizable (hence hyperbolic) if and only if

$$\lambda > \sqrt{2}\sqrt{a^2 + b^2}.$$

- The equivalent equation is stable if and only if

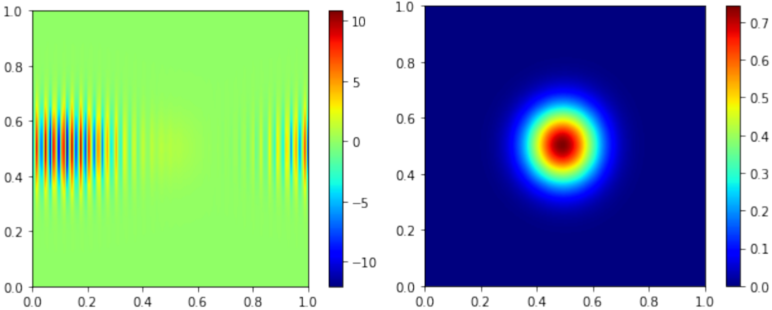
$$\lambda > 2\max(|a|, |b|).$$

The hyperbolicity condition is more restrictive than the diffusion condition.



D2Q4 Numerical Results

Transport of a Gaussian with $\omega = 1.6$, $(a, b) = (1, 0)$ on the unit square, $N_x = 200$ cells in x and in y. Left $\lambda = 1.6$ (stable diffusion), right $\lambda = 2.2$ (stable entropy)



The most constraining condition appears to be necessary.

Lattice-Boltzmann [8]

The standard D2Q9 model could be analyzed using this approach.
TODO !

Schemes without CFL

DG Approximation

In the LBM, the transport equation

$$\partial_t f + V \cdot \nabla f = 0 \tag{4}$$

is solved by shifting. It no longer works on unstructured meshes (since it is non-conservative). It can be solved with a DG (Discontinuous Galerkin) scheme. Computational domain: Ω. Triangulation of Ω: $\mathtt{T} = (L_i)$ in open cells L_i such that

$$\overline{\Omega} = \bigcup_i \overline{L_i}, \quad L_i \cap L_j = \emptyset \text{ if } i \neq j.$$

At time $t_n = n\Delta t$, on cell $L \in \mathtt{T}$, the solution is approximated by the discontinuous function f^n.

$$f(X, n\Delta t) \simeq f^n(X) = \sum_{k=1}^{p} f_L^{n,k}(t)\phi_L^k(X), \quad X \in L,$$

where the ϕ_L^k are DG basis functions on the cell L.

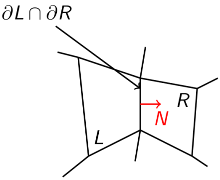
Implicit DG Scheme

A DG scheme, implicit, first-order in time, is given by:

$$\forall(L,k) \quad \int_L \frac{f^n - f^{n-1}}{\Delta t}\phi_L^k - \int_L f^n V \cdot \nabla \phi_L^k$$

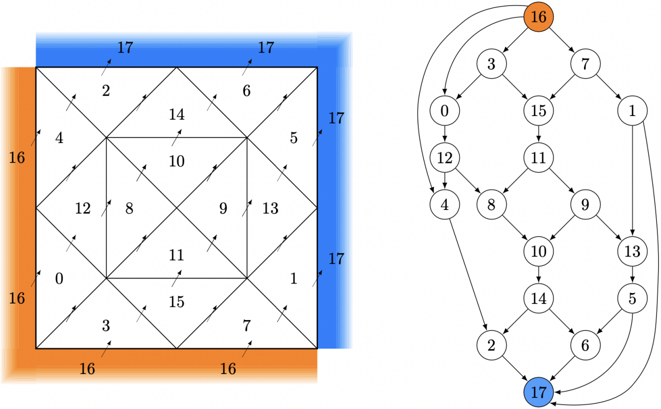
$$+ \int_{\partial L} \left(V \cdot N^+ f_L + V \cdot N^- f_R\right)\phi_L^k = 0.$$

- The outward normal to L on ∂L is noted N.
- We use the upwind flux ($a^+ = \max(a,0)$, $a^- = \min(a,0)$).
- R denotes the neighbor of L along ∂L.



Explicit Algorithm

The "implicit" scheme is actually **explicit**, thanks to the upwind flux. Cell R is "upstream" of cell L if $V \cdot N_{RL} > 0$. Construction of the dependency graph: oriented arc $R \to L$ if R is upstream of L. The time step can then be solved explicitly by traversing the graph in a topological order.



Application: Antenna Simulation

- Maxwell's equations: $W = (E^T, H^T)^T$, electric field $E \in \mathbb{R}^3$, magnetic field $H \in \mathbb{R}^3$.
- Maxwell's flux:

$$Q(W, N) = \begin{pmatrix} -N \times H \\ N \times E \end{pmatrix}.$$

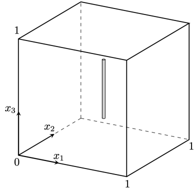
- Source term, conductivity σ, Ohm's law

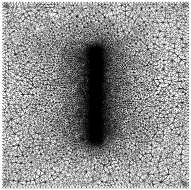
$$S(W) = \begin{pmatrix} -\sigma E \\ 0 \end{pmatrix}.$$

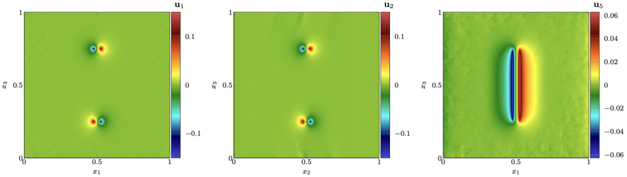
$$\partial_t W + \nabla \cdot Q(W) = S(W).$$

Numerical Results

- Unstructured mesh of an electrical wire in a cube. Sending a plane pulse.
- Second order DG-LBM solver in time (implicit Euler replaced by Crank-Nicolson).
- CFL=7.



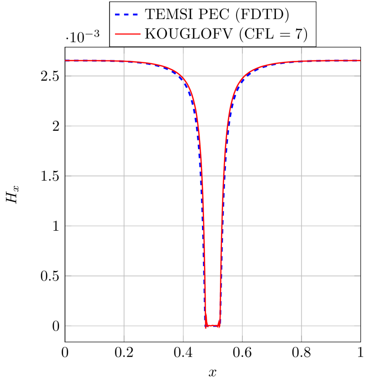




(a) Solution at time $t = 0.75$; left panel: $E_1|_{x_2=0.5}$; middle panel: $E_2|_{x_1=0.5}$; right panel: $H_2|_{x_2=0.5}$.

Comparison of FDTD and DG

It is possible to make $\sigma = +\infty$ in the scheme while remaining explicit. The source term is resolved in the relaxation step. This is equivalent to doing $E \leftarrow -E$ in this step. Comparison with a finite difference code (Yee's FDTD scheme) on a uniform mesh.



Boundary Conditions

Boundary Conditions

- A fundamental challenge with numerical schemes: stable and precise handling of boundary conditions.
- Still an open problem for LBM.
- We present an attempt for stabilizing a second order boundary condition.

Transport Equation

For $\omega = 2$, the LBM is second-order. In practice, the application of boundary conditions can reduce the order or stability.
Consider the 1D transport equation with speed $c > 0$ and a boundary condition on the left, $W = w$, $Q^1(W) = cw$,

$$\begin{aligned} \partial_t w + c\partial_x w &= 0, \quad x \in [L, R] \\ w(x, 0) &= 0, \\ w(0, t) &= w_0(x). \end{aligned}$$

- Grid points: $x_i = L + ih + h/2$, $0 \leq i < N$, with $h = (R - L)/N$.
- Time step: $\Delta t = h/\lambda$. Time $t_n = n\Delta t$.

LBM

$$F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}, \quad W = F_1 + F_2.$$

We denote $F_i^{n,-}$ the value of $F(x_i, t_n^-)$ before relaxation. In the shifting step

$$F_{1,i}^{n,-} = F_{1,i+1}^{n-1}, \quad F_{2,i}^{n,-} = F_{2,i-1}^{n-1},$$

the values $F_{2,-1}^{n-1}$ (left boundary) and $F_{1,N}^{n-1}$ (right boundary) are missing. Ghost cell method

$$F_{2,-1}^{n-1} = b_L(F_{1,0}^{n-1}, F_{2,0}^{n-1}), \quad F_{1,N}^{n-1} = b_R(F_{1,N-1}^{n-1}, F_{2,N-1}^{n-1}).$$

Entropic Stability [3, 7, 1]

The incoming kinetic entropy must be smaller than the outgoing one:

$$s_2(b_L(F_1, F_2)) \leq s_1(F_1), \quad s_1(b_R(F_1, F_2)) \leq s_2(F_2). \qquad (5)$$

Application to the D1Q2 model. We impose $W = F_1 + F_2 = 0$ on the left and $Y = 0 = \lambda(F_2 - F_1) - c(F_1 + F_2)$ on the right. Thus:

$$b_L(F_1, F_2) = -F_1, \quad b_R(F_1, F_2) = \frac{\lambda - c}{\lambda + c} F_2$$

Simple calculations show that (5) is satisfied. The scheme is stable, but even when $\omega = 2$, it is experimentally only first-order.

Scheme of Order 2

It is more accurate to apply a Neumann condition[6] $\partial_x Y = 0$ on the right. This extends the stencil of the ghost function to the right as

$$F_{1,N}^{n-1} = b_R(F_{1,N-1}^{n-1}, F_{2,N-1}^{n-1}, F_{1,N-2}^{n-1}, F_{2,N-2}^{n-1}). \tag{6}$$

To prevent an increase in entropy, the following scheme is applied:

- Calculate $F_{1,N}^{n-1}$ with (6);
- If the entropy condition is not satisfied, i.e. if $s_1(F_{1,N}^{n-1}) > s_2(F_{2,N-1}^{n-1})$ then replace $F_{1,N}^{n-1}$ with the closest value $\widetilde{F_{1,N}^{n-1}}$ such that $s_1(\widetilde{F_{1,N}^{n-1}}) = s_2(F_{2,N-1}^{n-1})$.

Extension to D2Q4

- For $d > 1$, on a boundary point, in general, the number of incoming characteristics of the kinetic model and the equivalent system are different.
- This phenomenon leads to unstable or inaccurate results when $\omega \simeq 2$.
- Entropy limiter improves the results.

Transport equation in 2D with velocity $c = (a, b)$ on the square $\Omega =]0, 1[\times]0, 1[$.

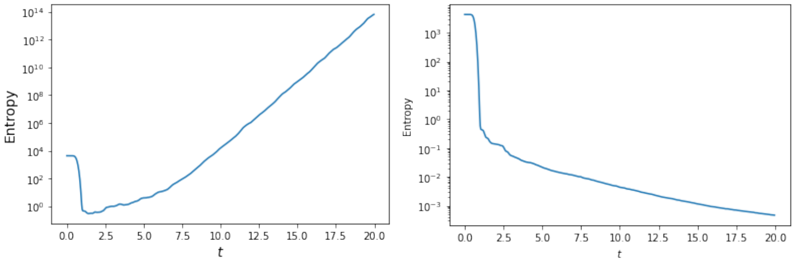
$$\partial_t W + \sum_{i=1}^{2} \partial_i Q^i(W) = 0, \quad Q^1(W) = aW, \quad Q^2(W) = bW.$$

Second Order Boundary Conditions[11, 12]

- Transport equation in 2D with velocity $c = (a, b)$ on the square $\Omega =]0, 1[\times]0, 1[$.
- Normal vector (n_1, n_2) on $\partial\Omega$.
- Test of two boundary condition strategies.

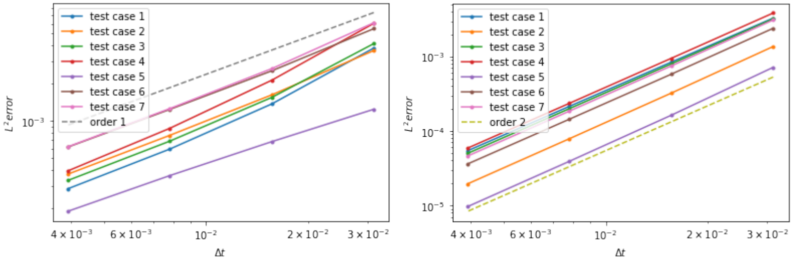
Boundary conditions	Entropy stable	Second order accurate
Inflow border	Exact solution on w $y_3 = 0$	Exact solution on w
Outflow border	$y_1 n_1 + y_2 n_2 = 0$ $y_3 = 0$	Neumann on $v_1 y_1 + v_2 y_2$
Corner inflow/inflow	Exact solution on w $y_3 = 0$	Exact solution on w $y_3 = 0$
Corner inflow/outflow	Exact solution on w $n_1 y_1 + n_2 y_2 = 0$ $y_3 = 0$	Exact solution on w Neumann on $v_1 y_1 + v_2 y_2$
Corner outflow/outflow	$y_1 = 0$ $y_2 = 0$ $y_3 = 0$	Neumann on $v_1 y_1 + v_2 y_2$ $y_3 = 0$

Entropy Evolution



Left without entropy limitation, Right with limitation.

Order



Left: First-order stable boundary condition (CL), Right: Second-order boundary condition with entropy stabilization

Conclusion

- Systems of conservation laws provide a very rich class of models for physics.
- The kinetic approach is a general and highly effective method for building numerical approximations.
- The numerical viscosity intuition is useful but not always correct.
- Entropic theory allows for the mathematical study of stability and consistence of these schemes.

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