Equivalent systems of kinetic relaxation schemes

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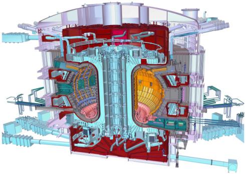
Tokamak and fusion

Tokamak: Toroidal chamber containing hydrogen plasma confined with a magnetic field and heated to high temperatures, to create energy.



The drift of the plasma inside a tokamak can be modelized by the **Vlasov-Poisson system**

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + (E + v \times B) \cdot \nabla_v f = 0, \\ E = -\nabla \phi, \\ -\Delta \phi = \rho - \rho_0, \end{cases}$$

with

- $f(x,t,v)$ the distribution of ions,
- $E(x,t)$ the electric field,
- $\rho(x,t) = \int f(x,t,v)dv$ the density,
- $\phi(x,t)$ the potential,
- $B(x,t)$ the imposed magnetic field.

Challenges

- Capture the small structures, without imposing small time steps,
- Achieve stability at high order,
- Build boundary conditions which are both stable and accurate.

▶ We consider a **relaxation kinetic scheme**, which approximates a hyperbolic equation by a set of transport equations with constant velocities.

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Kinetic approximation

We consider the conservation law in d dimensions

$$\partial_t \bar{w} + \nabla \cdot \boldsymbol{q}(\bar{w}) = 0, \qquad (\mathcal{E})$$

with $\bar{w}(\boldsymbol{x}, t) \in \mathbb{R}$, $\boldsymbol{x} \in \mathbb{R}^d$, $\boldsymbol{q}(\bar{w}) \in \mathbb{R}^d$.

We consider the BGK kinetic model

$$\partial_t f_i + \nabla \cdot (\boldsymbol{\lambda}_i f_i) = \frac{1}{\varepsilon}\left(f_i^{eq}(w) - f_i\right), \qquad \text{for } i = 1, \ldots, n_v, \qquad (\mathcal{K})$$

where

- $\boldsymbol{\lambda}_i$ are the kinetic velocities,
- $\boldsymbol{f} = (f_i)$ is the kinetic unknown such as $w = \sum_{i=1}^{n_v} f_i$,
- $\boldsymbol{f}^{eq}(w) = (f_i^{eq}(w))$ is the equilibrium kinetic vector which satisfies the **consistency relations**

$$w = \sum_{i=1}^{n_v} f_i^{eq}(w) \quad \text{and} \quad \boldsymbol{q}(w) = \sum_{i=1}^{n_v} \boldsymbol{\lambda_i} f_i^{eq}(w).$$

In the limit $\varepsilon \to 0$, $w = \sum_{i=1}^{n_v} f_i$ tends to the solution $\bar{w}$.

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Indeed, as

$$\varepsilon \left(\partial_t f_i + \nabla \cdot (\boldsymbol{\lambda}_i f_i) \right) = f_i^{eq} - f_i,$$

when $\varepsilon \to 0$, we have $f_i \to f_i^{eq}$.
By summing the n_v kinetic equations $(\mathcal{K})$, we obtain

$$\sum_{i=1}^{n_v} \partial_t f_i + \sum_{i=1}^{n_v} \boldsymbol{\lambda}_i \cdot \boldsymbol{\nabla} f_i = \frac{1}{\varepsilon} \left(\sum_{i=1}^{n_v} f_i^{eq} - \sum_{i=1}^{n_v} f_i \right) = 0.$$

We took the limit when $\varepsilon \to 0$, we have

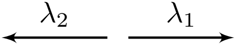
$$\partial_t \left(\sum_{i=1}^{n_v} f_i^{eq} \right) + \boldsymbol{\nabla} \cdot \left(\sum_{i=1}^{n_v} \boldsymbol{\lambda}_i f_i^{eq} \right) = 0.$$

Using the consistency conditions, we finally retrieve the initial equation $(\mathcal{E})$

$$\partial_t w + \nabla \cdot (\boldsymbol{q}(w)) = 0.$$

Example: The $D1Q2$ model

- In the $D1Q2$ model, we have $n_v = 2$ opposite kinetic velocities:



$$\boldsymbol{\lambda}_1 = (\lambda), \quad \boldsymbol{\lambda}_2 = (-\lambda).$$

The consistency conditions

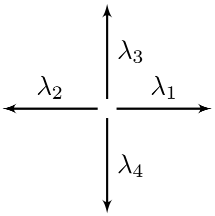
$$w = \sum_{i=1}^{n_v} f_i^{eq} \quad \text{and} \quad q(w) = \sum_{i=1}^{n_v} \boldsymbol{\lambda_i} f_i^{eq},$$

impose the equilibrium kinetic vector

$$f_i^{eq}(w) = \frac{w}{2} + \frac{\boldsymbol{\lambda}_i \cdot q(w)}{2\lambda^2}.$$

Example: The $D2Q4$ model

- In the $D2Q4$ model, we have $n_v = 4$ velocities along the Cartesian axes:



$$\boldsymbol{\lambda}_1 = \begin{pmatrix} \lambda \\ 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_2 = \begin{pmatrix} -\lambda \\ 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_3 = \begin{pmatrix} 0 \\ \lambda \end{pmatrix}, \quad \boldsymbol{\lambda}_4 = \begin{pmatrix} 0 \\ -\lambda \end{pmatrix}.$$

The 3 consistency equations let us one **degree of freedom**. We choose the equilibrium kinetic vector

$$f_i^{eq}(w) = \frac{w}{4} + \frac{\boldsymbol{\lambda}_i \cdot \boldsymbol{q}(w)}{2\lambda^2} + \frac{m^3(\boldsymbol{\lambda}_i) z_3^{eq}(w)}{4\lambda^4},$$

with

$$m^3(\boldsymbol{\lambda}_i) = (\lambda_{i,1})^2 - (\lambda_{i,2})^2,$$

and

$$z_3^{eq} = 0.$$

Splitting method

To solve in time the kinetic model

$$\partial_t f_i + \boldsymbol{\lambda}_i \cdot \boldsymbol{\nabla} f_i = \frac{1}{\varepsilon}(f_i^{eq} - f_i), \qquad (\mathcal{K})$$

we apply a splitting method:

- **Transport step** :

$$\partial_t f_i + \boldsymbol{\lambda}_i \cdot \boldsymbol{\nabla} f_i = 0. \qquad (\mathcal{T})$$

  On a structured and adapted mesh, we can solve exactly these transport equations with the characteristic method

$$f_i^*(\boldsymbol{x}, t + \Delta t) = f_i(\boldsymbol{x} - \Delta t \boldsymbol{\lambda_i}, t),$$

  or we can approximate the solution on an unstructured mesh.

- **Relaxation step** :

$$\partial_t f_i = \frac{1}{\varepsilon}(f_i^{eq} - f_i). \qquad (\mathcal{R}_\omega)$$

  We approximate it by the relaxation

$$f_i^{n+1} = f_i^* + \omega\left(f_i^{*,eq} - f_i^*\right), \quad \text{with } \omega \in [1, 2].$$

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Application to a plasma model

Before some theoretical results, let us see an example of application of this model.

We consider the model in 3 dimensions which describes the drift of the plasma inside a tokamak

$$\begin{cases} \partial_t \rho + \nabla \cdot (v\rho) = 0, \\ -\Delta_{x,y}\phi = \rho, \\ E = -\nabla_{x,y}\phi, \end{cases}$$

where

- ρ is the **density**,
- $v = E \times e_z + B$ is the **velocity**,
- E is the **electric field**,
- $B = (-\sin(\theta)e_x + \cos(\theta)e_y)B_\theta + B_z e_z$ a divergence-free **magnetic field**.

We consider a cylinder

$$\Omega = \{(r\cos(\theta), r\sin(\theta), z) \mid r_{min} \leqslant r \leqslant r_{max}, 0 \leqslant \theta \leqslant 2\pi,\ 0 \leqslant z \leqslant L = 1\},$$

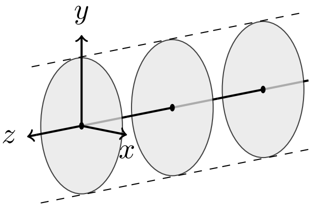
with homogeneous Dirichlet boundary conditions for the potential ϕ.

Dimensional splitting

As we have different behaviors according to the direction, we split the transport between the poloidal planes and the toroidal direction.

- In the (x, y) planes, we use a $D2Q4$ model for solving $\partial_t \rho + \nabla_{(x,y)} \cdot \left(\begin{pmatrix} v_x \\ v_y \end{pmatrix} \rho \right) = 0$:

$$\boldsymbol{\lambda}_0 = \begin{pmatrix} \lambda_p \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{\lambda}_1 = \begin{pmatrix} -\lambda_p \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{\lambda}_2 = \begin{pmatrix} 0 \\ \lambda_p \\ 0 \end{pmatrix}, \ \boldsymbol{\lambda}_3 = \begin{pmatrix} 0 \\ -\lambda_p \\ 0 \end{pmatrix}.$$



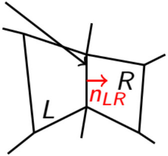
- In the z direction, we use a $D1Q2$ model for solving $\partial_t \rho + \partial_z (v_z \rho) = 0$:

$$\boldsymbol{\lambda}_4 = \begin{pmatrix} 0 \\ 0 \\ \lambda_z \end{pmatrix}, \quad \boldsymbol{\lambda}_5 = \begin{pmatrix} 0 \\ 0 \\ -\lambda_z \end{pmatrix}.$$

	In the (x, y) planes	In the z direction
Transport equations	Discontinuous Galerkin	Lattice Boltzmann
Mesh	Unstructured	Periodic structured
Parallelization	OpenMP	MPI
Condition	CFL-less	$\Delta t = \Delta z / \lambda_t$

Transport equation in the poloidal plan

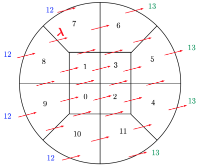
- **Implicit Discontinuous Galerkin** scheme

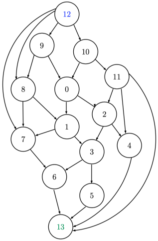


$$\int_L \frac{f_L^n - f_L^{n-1}}{\Delta t}\psi_i^L - \int_L \boldsymbol{\lambda}\cdot\boldsymbol{\nabla}\psi_i^L f_L^n$$
$$+ \int_{\partial L}\left((\boldsymbol{\lambda}\cdot\boldsymbol{n}_{LR})^+ f_L^n + (\boldsymbol{\lambda}\cdot\boldsymbol{n}_{LR})^- f_R^n\right)\psi_i^L = 0,$$

$\forall L, \forall i$, with ψ_i^L the basis function.

- As the transport equation are at **constant velocity**, we can use a **downwind algorithm**, which makes the resolution **explicit**.





  - ▶ We extend to the second order time accuracy with the same approach.

3D Diocotron testcase

We initialize the density with

$$\rho(r,\theta,z,0) = e^{-\frac{(r-r_0)^2}{2\sigma^2}} \left(1 + \varepsilon \cos\left(k\theta + lz\frac{2\pi}{L}\right)\right).$$

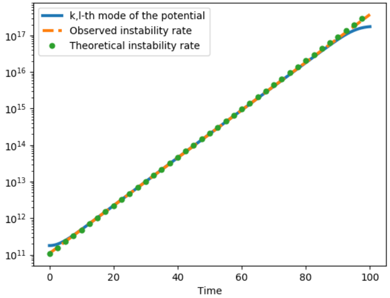


Figure: Instability rate observed compared to the theoretical one, with $\Delta t = 0.0026$, $n_t = 38400$, $\omega = 1.99$, $n_p = 128$, $\lambda_p = 7$, $\lambda_z = 3$, $B_\theta = 0.1$, $B_z = 1$, $k = 2$, $l = 1$ and a poloidal mesh of size 80×50.

3D view of the Diocotron testcase

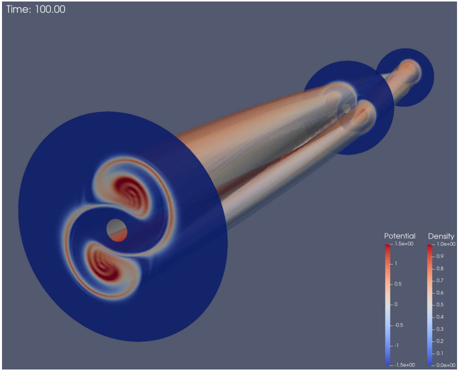


Figure: Evolution of the density in three poloidal planes.

- Execution time $\simeq 17,6$ hours
- $n_{\text{CFL}} \approx 33$
  - It would have taken 33 times longer with an explicit scheme with CFL !

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Equivalent equations analysis

- To analyze the solution given by a $DdQn_v$ kinetic model, it is classical to consider the **equivalent equation on w**, see for example [Dub08,Gra14].

- As the $DdQn_v$ model approximates an equation with n_v equations and n_v variables f_i, we propose to compute an **equivalent system** on n_v variables: w and $n_v - 1$ equilibrium deviation variables.

- We will compare the **subcharacteristic stability condition** given by the analysis of the equivalent equation and the **hyperbolicity condition** given by the equivalent system.

- To simplify, we consider the transport equation

$$\partial_t w + \sum_{k=1}^{d} v_i \partial_i w = 0,$$

but we could extend these computations to a variable velocity $v(x,t)$.

Flux errors

We define the **approximated fluxes** as

$$z_k = \sum_{i=1}^{n_v} \lambda_{i,k} f_i, \qquad \text{for } 1 \leqslant k \leqslant d,$$

and the **flux errors** as

$$y_k = z_k - q_k(w) \approx 0, \qquad \text{for } 1 \leqslant k \leqslant d.$$

For the $D2Q4$ model, we add a fourth variable

$$z_3 = \sum_{i=1}^{n_v} (\lambda_{i,1}^2 - \lambda_{i,2}^2) f_i \approx 0.$$

We will compute the equivalent system in the

$$(w, \boldsymbol{y}) = \Big(w, y_1, y_2, z_3\Big)$$

variables.

Operators

We consider the following operators on $(w, \boldsymbol{y})$:

- $\mathcal{T}(\Delta t)$ the exact **transport operator**,
- $\mathcal{R}_\omega$ the **relaxation operator** of parameter $\omega \in [1, 2]$.

As each time step, the solution is given by

$$\begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} (t + \Delta t) = \mathcal{S}(\Delta t) \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} (t)$$

with

$$\mathcal{S}(\Delta t) = \mathcal{T}\left(\frac{\Delta t}{4}\right) \circ \mathcal{R}_\omega \circ \mathcal{T}\left(\frac{\Delta t}{2}\right) \circ \mathcal{R}_\omega \circ \mathcal{T}\left(\frac{\Delta t}{4}\right).$$

- When $\omega = 2$, this operator is time-symmetric, and therefore second-order accurate.

The equivalent system

Taylor expansion with a Computer Algebra System:

$$\partial_t \begin{pmatrix} w(t) \\ \boldsymbol{y}(t) \end{pmatrix} = \frac{\begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix}(t+\Delta t) - \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix}(t-\Delta t)}{2\Delta t} + O(\Delta t^2),$$
$$= \frac{\mathcal{S}(\Delta t) - \mathcal{S}^{-1}(\Delta t)}{2\Delta t} \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix}(t) + O(\Delta t^2).$$

We obtain an **equivalent system on** $(w, \boldsymbol{y})$ of the form

$$\partial_t \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} - \frac{a}{\Delta t} \begin{pmatrix} 0 \\ \boldsymbol{y} \end{pmatrix} + \sum_{i=1}^{d} B_i \partial_i \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} + \Delta t \sum_{i,j=1}^{d} C_{ij} \partial_{ij} \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} = O(\Delta t^2).$$

The equivalent equation

$$\partial_t \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} - \frac{a}{\Delta t} \begin{pmatrix} 0 \\ \boldsymbol{y} \end{pmatrix} + \sum_{i=1}^{d} B_i \partial_i \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} + \Delta t \sum_{i,j=1}^{d} C_{ij} \partial_{ij} \begin{pmatrix} w \\ \boldsymbol{y} \end{pmatrix} = O(\Delta t^2).$$

We assume that $\boldsymbol{y} = O(\Delta t)$. Inserting this hypothesis in the equivalent system, we obtain

$$\boldsymbol{y} = \frac{\Delta t}{a} \sum_{i=1}^{d} B_i[:,1] \partial_i w + O(\Delta t^2).$$

Then, by replacing $\boldsymbol{y}$ in the first equation of the equivalent system, we retrieve **the equivalent equation on w** given in [Dub08,Gra14], of the form

$$\partial_t w + \sum_{i=1}^{d} b_i \partial_i w + \Delta t \sum_{i,j=1}^{d} c_{ij} \partial_{ij}^2 w = O(\Delta t^2).$$

Hyperbolicity condition

We consider a system of the form

$$\partial_t \begin{pmatrix} w \\ y \end{pmatrix} + \sum_{k=1}^{d} \partial_k B_k \begin{pmatrix} w \\ y \end{pmatrix} = 0.$$

- This system is **hyperbolic** if for all unit vector $\boldsymbol{n} \in \mathbb{R}^d$, the matrix $\sum_{k=1}^{d} n_k B_k$ is diagonalizable in $\mathbb{R}$.

- This system is **symmetrizable** if it exists a symmetric positive definite matrix P such as for all unit vector $\boldsymbol{n} \in \mathbb{R}^d$, the matrix $P\left(\sum_{k=1}^{d} n_k B_k\right)$ is symmetric, or, more simply, such as PB_k is symmetric for all $k = 1, \ldots, d$.

A symmetrizable system is hyperbolic.

Entropy

A system is symmetrizable if and only if it exists an entropy.

For the transport equation, the entropy is

- a **quadratic** form on $(w, \boldsymbol{y})$,
- a **diagonal quadratic** form on the kinetic variable $\boldsymbol{f}$, meaning we have

$$\Sigma(\boldsymbol{f}) = \sum_{i=1}^{n_v} \alpha_i f_i^2, \qquad \text{with } \alpha_k > 0.$$

General methodology

$(\mathcal{E})$		$DdQn_v$		Equivalent system		Equivalent equation
w	$\rightsquigarrow$	$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}$	$\leftrightarrow$	$\begin{pmatrix} w \\ y_1 \\ y_2 \\ z_3 \end{pmatrix}$	$\xrightarrow[\boldsymbol{y}=O(\Delta t)]{}$	w
				$\downarrow$		$\downarrow$
				Hyperbolic stability condition		Diffusive stability condition

Application to the $D1Q2$ model

$$\partial_t w + v\partial_x w = 0$$

Entropy

$$\Sigma(\boldsymbol{f}) = \frac{2\lambda}{\lambda+v} f_1^2 + \frac{2\lambda}{\lambda-v} f_2^2.$$

Equivalent system	**Hyperbolicity condition**
$\partial_t \begin{pmatrix} w \\ y \end{pmatrix} - \frac{1}{\Delta t}\frac{\omega(2-\omega)(\omega^2-2\omega+2)}{2(\omega-1)^2}\begin{pmatrix} 0 \\ y \end{pmatrix} + \begin{pmatrix} v & \gamma_1 \\ (\lambda^2-v^2)\gamma_1 & -v\gamma_2 \end{pmatrix}\partial_x \begin{pmatrix} w \\ y \end{pmatrix} = O(\Delta t),$ **with** $\gamma_1 = \frac{(\omega-2)^2(\omega^2-2\omega+2)}{8(\omega-1)^2}$ **and** $\gamma_2 = \frac{\omega^4-4\omega^3+6\omega^2-4\omega+2}{2(\omega-1)^2}.$	$\lambda > \lvert v\rvert$
Equivalent equation	**Diffusive stability condition**
$\partial_t w + v\partial_x w + \Delta t \frac{2-\omega}{4\omega}(\lambda^2-v^2)\partial_{xx} w = O(\Delta t^2).$	$\lambda > \lvert v\rvert$

Numerical verification

We consider monochromatic exact solutions

$$\begin{pmatrix} \tilde{w} \\ \tilde{y} \end{pmatrix} = \begin{pmatrix} w_0 \\ y_0 \end{pmatrix} e^{ikx+\gamma t}, \qquad \text{with } k \in \mathbb{N} \text{ and } \gamma \in \mathbb{C}.$$

We obtain the following dispersion relation by injecting this solution

- in the equivalent equation on w

$$\left(\gamma_{eq} + vik_{eq} - \Delta t c k_{eq}^2\right) \tilde{w} = 0,$$

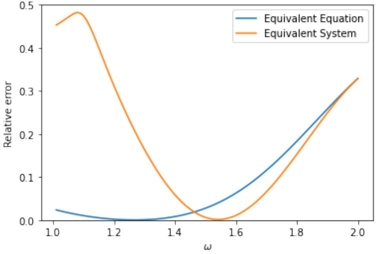
- in the equivalent system on (w, y)

$$\left(\gamma_{sys} I_2 - \frac{a}{\Delta t} + Bik_{sys} - \Delta t C k_{sys}^2\right) \begin{pmatrix} \tilde{w} \\ \tilde{y} \end{pmatrix} = 0.$$

For the equivalent system, we obtain two γ_{sys}. We choose the one that makes the solution w decrease slowly.

Comparison of the equivalent system and the equivalent equation

We compute the relative errors $\dfrac{\sum_{i=0}^{Nx}\sum_{n=0}^{Nt}(w^{i,n}-\tilde{w}^{i,n})^2}{\sum_{i=0}^{Nx}\sum_{n=0}^{Nt}(w^{i,n})^2}$ according to ω:



- For little values of ω, the equivalent equation appears to be the most accurate.
- For greater values of ω, the equivalent system is more relevant.

Equivalent system for the $D2Q4$ model

$$\partial_t w + v_1 \partial_1 w + v_2 \partial_2 w = 0$$

Equivalent system:

$$\partial_t \begin{pmatrix} w \\ y_1 \\ y_2 \\ z_3 \end{pmatrix} - \frac{1}{\Delta t} \frac{\omega(\omega-2)(\omega^2-2\omega+2)}{4(\omega-1)^2} \begin{pmatrix} 0 \\ y_1 \\ y_2 \\ z_3 \end{pmatrix}$$

$$+ \begin{pmatrix} v_1 & 2\gamma_1 & 0 & 0 \\ \gamma_1(\lambda^2 - 2v_1) & -v_1\gamma_2 & 0 & \frac{\gamma_2}{2} \\ -2v_1v_2\gamma_1 & -v_2\gamma_2 & 0 & 0 \\ 2\lambda^2 v_1 \gamma_1 & \lambda^2\gamma_2 & 0 & 0 \end{pmatrix} \partial_1 \begin{pmatrix} w \\ y_1 \\ y_2 \\ z_3 \end{pmatrix}$$

$$+ \begin{pmatrix} v_2 & 0 & 2\gamma_1 & 0 \\ -2v_1v_2\gamma_1 & 0 & -v_1\gamma_2 & 0 \\ \gamma_1(\lambda^2 - 2v_2^2) & 0 & -v_2\gamma_2 & -\frac{\gamma_2}{2} \\ -2\lambda^2 v_2\gamma_1 & 0 & -\lambda^2\gamma_2 & 0 \end{pmatrix} \partial_2 \begin{pmatrix} w \\ y_1 \\ y_2 \\ z_3 \end{pmatrix} = O(\Delta t),$$

with $\gamma_1 = \frac{(\omega-2)^2(\omega^2-2\omega+2)}{16(\omega-1)^2}$ and $\gamma_2 = \frac{\omega^4-4\omega^3+6\omega^2-4\omega+2}{2(\omega-1)^2}$.

Numerical validation of the equivalent system when $\omega = 2$

We want to verify that the equivalent system is a good approximation of the solution given by the $D2Q4$ model.

We can compare

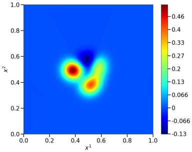
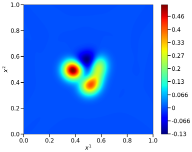
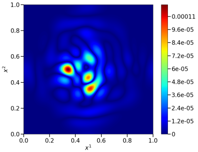
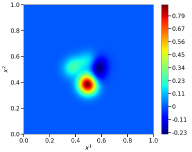
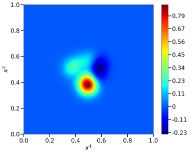
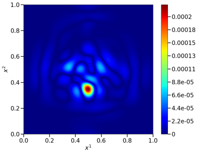
- $\boldsymbol{y}^{vf}$: solution of the equivalent equation with a finite volume method,
- $\boldsymbol{y}^{kin} = \sum_{i=1}^{n_v} \boldsymbol{\lambda_i} f_i - \boldsymbol{q}(\sum_{i=1}^{n_v} f_i)$, with $\boldsymbol{f}$ the solution of $(\mathcal{E})$ with the $D2Q4$ model.

We choose $\Omega = [0,1] \times [0,1]$ with a mesh of size 800×800, $\boldsymbol{q}'(w) = (1,1)$, $\lambda = 3$, $T_f = 0.06$ and a Gaussian initialization

$$w(\boldsymbol{x}, 0) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}_0^w\|^2}{2\sigma^2}\right) \quad \text{and} \quad y_k(\boldsymbol{x}, 0) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}_0^y\|^2}{2\sigma^2}\right),$$

with $\sigma = 0.05$, $\boldsymbol{x}_0^w = (0.25, 0.25)$ and $\boldsymbol{x}_0^y = (0.5, 0.5)$.

Numerical validation of the equivalent system when $\omega = 2$

	$\boldsymbol{y}^{kin}$	$\boldsymbol{y}^{vf}$	$\lVert \boldsymbol{y}^{kin} - \boldsymbol{y}^{vf} \rVert$
y_1			
y_2			

- The equivalent system is a good approximation of the scheme, and therefore it gives useful information about its behavior.

Equivalent equation on w

If we assume that $\boldsymbol{y} = O(\Delta t)$, then we retrieve the **equivalent equation on w**

$$\partial_t w + \nabla \cdot \boldsymbol{q}(w) = \frac{\Delta t}{2}\left(\frac{1}{\omega} - \frac{1}{2}\right) \nabla \cdot (\mathcal{D}_4 \nabla w) + O(\Delta t^2),$$

with the diffusion matrix

$$\mathcal{D}_4 = \begin{pmatrix} \frac{\lambda^2}{2} - v_1^2 & -v_1 v_2 \\ -v_1 v_2 & \frac{\lambda^2}{2} - v_2^2 \end{pmatrix}.$$

Stability conditions

see [Bou05]

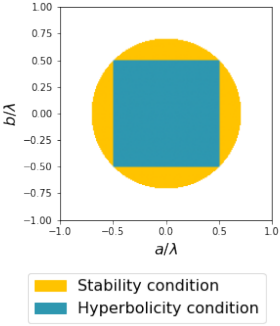
The equivalent system is **hyperbolic** if

$$\max(|v_1|, |v_2|) < \frac{\lambda}{2}.$$

When $\omega \neq 2$, the equivalent equation is **diffusive** iff

$$v_1^2 + v_2^2 \leqslant \frac{\lambda^2}{2}.$$

- The diffusive stability condition is less restrictive than the hyperbolicity condition.

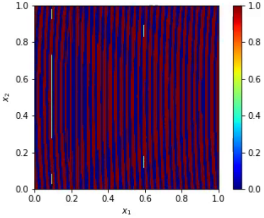
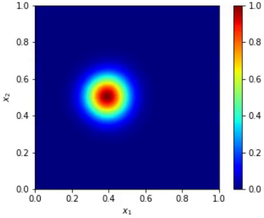


What happens if the diffusive stability condition is satisfied but not the hyperbolicity condition ?

$\omega = 2$

We choose the velocity $\boldsymbol{v} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Diffusion condition:	$\lambda > \sqrt{2(v_1^2 + v_2^2)} = \sqrt{2}$
Hyperbolic stability condition:	$\lambda > 2\max(\lvert v_1\rvert, \lvert v_2\rvert) = 2$

<table>
<tr><th>$\lambda = 1.6$</th><th>$\lambda = 2.2$</th></tr>
<tr><td>
</td><td>
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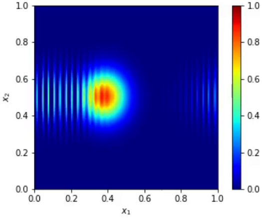
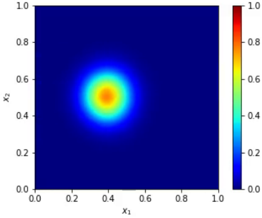
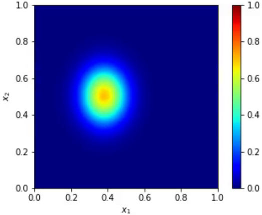
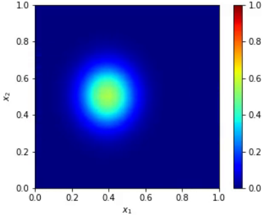
	

$\omega = 1.2$

We choose the velocity $\boldsymbol{v} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Diffusion condition:	$\lambda > \sqrt{2(v_1^2 + v_2^2)} = \sqrt{2}$
Hyperbolic stability condition:	$\lambda > 2\max(\lvert v_1 \rvert, \lvert v_2 \rvert) = 2$

$\lambda = 1.6$	$\lambda = 2.2$
	

Plan

Boundary conditions

In theory, the over-relaxation kinetic scheme gives us a second order accuracy. But in practice, it is achieved only if the boundary conditions are well adapted.

We want to find boundary conditions that ensures

- **stability**,
- **second order accuracy**.

We study the simplified case of **transport** at constant velocity:

$$\partial_t w + v \partial_x w = 0.$$

Moreover, we are only supposed to know the solution w on the **inflow border**, namely when $vn \leqslant 0$, with n an outward normal vector.

Boundary conditions for the $D1Q2$ model

We approximate the k^{th} kinetic unknown at point $x_i = i\Delta x$ and at time $t_n = n\Delta t$ by

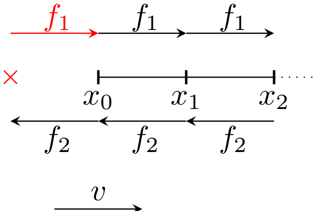
$$f_k(x_i, t_n) \approx (f_k)_i^n.$$

We solve the transport step with a Lattice-Boltzmann method. We denote

$$(f_1)_i^{n+1,*} = (f_1)_{i-1}^n \qquad \text{and} \qquad (f_2)_i^{n+1,*} = (f_2)_{i+1}^n.$$

- On the left border, we need to define f_1.
- On the right border, we need to define f_2.

We assume that $v > 0$.



Decreasing of the entropy

The entropy of the $D1Q2$ model is

$$\Sigma(\boldsymbol{f}) = \frac{2\lambda}{\lambda + v} f_1^2 + \frac{2\lambda}{\lambda - v} f_2^2.$$

To be stable, we need the entropy to decrease with time. In other words, we do not want the quantity which is entering into the geometry to be greater than the one which is leaving it.

The entropy decreases if

$$\begin{cases} |f_1| \leqslant \sqrt{\frac{\lambda+v}{\lambda-v}} |f_2| & \text{on the left border,} \\ |f_2| \leqslant \sqrt{\frac{\lambda-v}{\lambda+v}} |f_1| & \text{on the right border.} \end{cases} \qquad (\mathcal{C})$$

Let us verify that imposing

- the exact solution on w on the inflow border,
- $y = 0$ on the outflow border,

satisfy the decrease of the entropy.

At the left inflow border

We have

$$f_1 = \frac{\lambda + v}{2\lambda} w + \frac{y}{2\lambda} \qquad \text{and} \qquad f_2 = \frac{\lambda - v}{2\lambda} w - \frac{y}{2\lambda}.$$

A **Dirichlet boundary condition** $w = 0$, gives us

$$f_1 = -f_2.$$

By inserting this expression in the entropy condition of the left border

$$|f_1| \leqslant \sqrt{\frac{\lambda + v}{\lambda - v}} |f_2|,$$

we obtain

$$1 \leqslant \sqrt{\frac{\lambda + v}{\lambda - v}},$$

which is true, as we have $v > 0$ and $\lambda > v$ (subcharacteristic condition).

At the right outflow border

We have

$$f_1 = \frac{\lambda + v}{2\lambda} w + \frac{y}{2\lambda} \qquad \text{and} \qquad f_2 = \frac{\lambda - v}{2\lambda} w - \frac{y}{2\lambda}.$$

A **Dirichlet boundary condition on the flux error** $y = 0$, gives us

$$f_1 = \frac{\lambda + v}{\lambda - v} f_2.$$

By inserting this expression in the entropy condition of the right border

$$|f_2| \leqslant \sqrt{\frac{\lambda - v}{\lambda + v}} |f_1|$$

we obtain

$$1 \leqslant \sqrt{\frac{\lambda + v}{\lambda - v}},$$

which is true, as we have $v > 0$ and $\lambda > v$ (subcharacteristic condition).

Boundary conditions for the $D2Q4$ model

- By the same approach of decreasing entropy, we can find stable boundary conditions in 2 dimensions. We just have to be careful with the corners.
- We also propose boundary conditions of second order accuracy, but for which the stability is not satisfied.

	Entropy decreasing BC	Order 2 BC
Inflow border	Exact solution on w $z_3 = 0$	Exact solution on w
Outflow border	$\boldsymbol{\lambda}_b \cdot \boldsymbol{y} = 0$ $z_3 = 0$	Neumann on $\boldsymbol{v} \cdot \boldsymbol{y}$
Corner inflow/inflow	Exact solution on w $z_3 = 0$	Exact solution on w $z_3 = 0$
Corner inflow/outflow	Exact solution on w $\boldsymbol{\lambda}_b \cdot \boldsymbol{y} = 0, z_3 = 0$	Neumann on $\boldsymbol{v} \cdot \boldsymbol{y}$ $z_3 = 0$
Corner outflow/outflow	$y_1 = 0, y_2 = 0$ $z_3 = 0$	Exact solution on w Neumann on $\boldsymbol{v} \cdot \boldsymbol{y}$

Test-cases

We choose a square geometry $\Omega = [0,1] \times [0,1]$.
We initialize w with a **function with compact support**

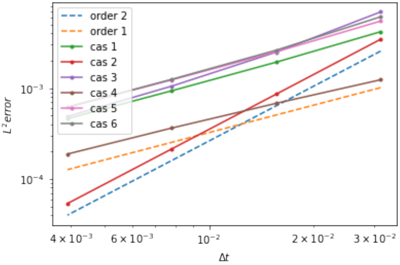
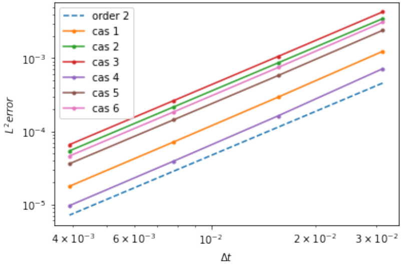
$$w(\boldsymbol{x}, t) = \begin{cases} 0 & \text{if } r(\boldsymbol{x}) > 1, \\ (1 - r(\boldsymbol{x})^2)^5 & \text{otherwise.} \end{cases}$$

with $r(\boldsymbol{x}) = \frac{\sqrt{(x_1 - x_1^0)^2 + (x_2 - x_2^0)^2}}{0.4}$, with different centers and velocities:

Test case	x_1^0	x_2^0	v_1	v_2
1	-0.5	0.5	1	0
2	0.5	0.5	-1	0
3	0	0.5	1	0
4	$-\sqrt{2}/4$	$-\sqrt{2}/4$	$\sqrt{2}/2$	$\sqrt{2}/2$
5	$\sqrt{2}/4$	$\sqrt{2}/4$	$-\sqrt{2}/2$	$-\sqrt{2}/2$
4	0	0	$\sqrt{2}/2$	$\sqrt{2}/2$

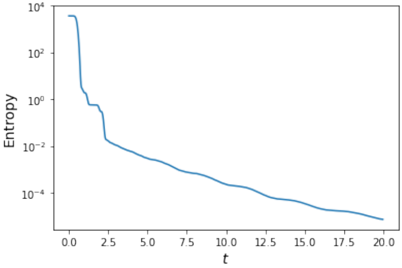
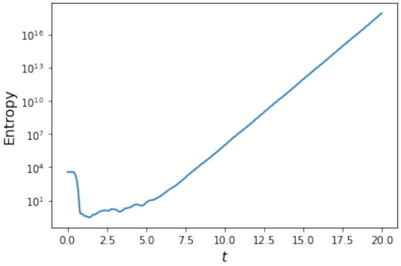
We take $\lambda = 2$, $T = 0.5$, and $Nt = 16, 32, 64, 128$.

Order of convergence

Entropy decreasing BC	Order 2 BC
	

- The entropy decreasing boundary conditions leads to first order accuracy.
- The second boundary conditions give a second order accuracy.

Evolution of the entropy

Entropy decreasing BC	Order 2 BC
	

- As expected, the first boundary conditions respect the decrease of the entropy.
- The second boundary conditions are not stable in large time. The entropy increases with time.
  Work in progress: make them stable !

Conclusion and perspectives

- We have built stable boundary conditions and second order accuracy boundary conditions. We could combine them to verify the both properties.
  - Work in progress: make the second order boundary conditions stable.
- We have proposed an equivalent system for the equation transport. We could extend this theory to any hyperbolic system.
- In the application part, we could use poloidal meshes and consider more realistic physical models with transport in curved torus.

Thank you for your attention !

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