Initialisation pour les schémas de Boltzmann sur réseau

aspects discrets et asymptotiques

Thomas Bellotti

Ecole polytechnique

Workshop “Schémas numériques de type Boltzmann”
Bordeaux - 24th November 2022

Section 1

Introduction

Arbitrariness on the initial data / initialization schemes

Consider a scalar linear Cauchy problem on $u = u(t, \boldsymbol{x})$:

$$\begin{cases} \partial_t u(t, \boldsymbol{x}) + \boldsymbol{V} \cdot \nabla_{\boldsymbol{x}} u(t, \boldsymbol{x}) = 0, & (t, \boldsymbol{x}) \in \mathbb{R}_+ \times \mathbb{R}^d, \\ u(0, \boldsymbol{x}) = u^\circ(\boldsymbol{x}), & \boldsymbol{x} \in \mathbb{R}^d. \end{cases}$$

- **Mesoscopic methods**: many variables, one time step.
  How to initialize the remaining variables?
  [*Ex.:* Kinetic schemes and Lattice Boltzmann.]

- **Multistep methods**: one variable, many time steps.
  How to initialize the scheme?
  [*Ex.:* Leap-frog scheme $\mathrm{u}_j^{n+1} = \mathrm{u}_j^{n-1} + \Delta t V / \Delta x (\mathrm{u}_{j-1}^n - \mathrm{u}_{j+1}^n)$.]

Lattice Boltzmann schemes belong to **both categories**.

Arbitrariness for the initialization of LBM schemes

Lattice Boltzmann schemes seen as

- **Mesoscopic methods**: how to devise the initial data for the non-conserved moments?

- **Multistep methods** [Bellotti *et al.*, '22]: how the choice of initial data for the non-conserved moments determines the initialization schemes on the conserved m_1 moment approximating u?

Today: structure of the talk

Tools:

- Introduce a **modified equation** analysis [Warming and Hyett, '74] for the initial conditions/starting schemes for LBM methods.
- Study the **number of initialization schemes** in connection with the notion of **observability** (dynamical systems).

Interest of the modified equation (by L.N. Trefethen)

"Finite difference approximations have a more complicated physics than the equations they are designed to simulate. The irony is no paradox, however, for finite differences are used not because the numbers they generate have simple properties, but because those numbers are simple to compute."

Goal: devise initial data guaranteeing

- **Orders of consistency** of the initialization schemes: no reduction of the order of the bulk method [Strikwerda, '04].
- **Time smoothness** of the discrete solutions: no oscillating boundary layers [Van Leemput *et al.*, '09].

Section 2

Lattice Boltzmann schemes

Lattice Boltzmann schemes

We consider multiple-relaxation-times (MRT) LBM schemes [D'Humières, '92]. The basic ingredients are:

- Time and space steps Δt and Δx. Hyperbolic scaling: $\Delta t = \Delta x / \lambda$ for a fixed lattice velocity $\lambda > 0$.
- Discrete velocities $\boldsymbol{c}_1, \dots, \boldsymbol{c}_q \in \mathbb{Z}^d$, with $q \in \mathbb{N}^*$.
  [*Ex.:* D$_1$Q$_2$: $q = 2$, $c_1 = 1$, $c_2 = -1$] [Graille, '14]
- An invertible moment matrix $\boldsymbol{M} \in \mathrm{GL}_q(\mathbb{R})$.
  [*Ex.:* D$_1$Q$_2$: $\boldsymbol{M} = \begin{pmatrix} 1 & 1 \\ \lambda & -\lambda \end{pmatrix}$]
- A relaxation matrix $\boldsymbol{S} = \mathrm{diag}(s_1, s_2, \dots, s_q)$, where $s_i \in]0, 2]$ for $i \in [\![2, q]\!]$ and $s_1 \in \mathbb{R}$.
- The equilibrium coefficients $\boldsymbol{\epsilon} \in \mathbb{R}^q$ ($\mathbf{m}^{\mathrm{eq}} = \boldsymbol{\epsilon} \mathrm{m}_1$) such that $\epsilon_1 = 1$: the first moment is **conserved**. Thus $\mathrm{m}_1 \approx u$.

Lattice Boltzmann schemes

The algorithm

- Given $\mathbf{m}(0, \boldsymbol{x}) \in \mathbb{R}^q$ for every $\boldsymbol{x} \in \Delta x \mathbb{Z}^d$.
- For $k \in \mathbb{N}$
  - **Collision**. Using the collision matrix $\boldsymbol{K} := \boldsymbol{I} - \boldsymbol{S}(\boldsymbol{I} - \boldsymbol{\epsilon} \otimes \boldsymbol{e}_1)$:

    $$\mathbf{m}^{\star}(k\Delta t, \boldsymbol{x}) = \boldsymbol{K}\mathbf{m}(k\Delta t, \boldsymbol{x}), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d.$$

    The post-collision distribution densities $\mathbf{f}^{\star}(k\Delta t, \boldsymbol{x}) = \boldsymbol{M}^{-1}\mathbf{m}^{\star}(k\Delta t, \boldsymbol{x})$.
  - **Transport**:

    $$\mathrm{f}_j((k+1)\Delta t, \boldsymbol{x}) = \mathrm{f}_j^{\star}(k\Delta t, \boldsymbol{x} - \Delta x \boldsymbol{c}_j), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d, \quad j \in [\![1, q]\!].$$

    The moments at the new time $\mathbf{m}((k+1)\Delta t, \boldsymbol{x}) = \boldsymbol{M}\mathbf{f}((k+1)\Delta t, \boldsymbol{x})$.

We define the number of moments relaxing **away from the equilibrium**

$$Q := \mathrm{card}\{s_i \neq 1 \ : \ i \in [\![2, q]\!]\}.$$

Section 3

Corresponding Finite Difference scheme

Corresponding Finite Difference scheme in the bulk

The evolution matrix of the scheme ($\mathbf{m}(t+\Delta t) = \mathbf{E}\mathbf{m}(t)$)

$$\mathbf{E} := \boldsymbol{M}\mathrm{diag}(\mathsf{x}^{\boldsymbol{c}_1}, \dots, \mathsf{x}^{\boldsymbol{c}_q})\boldsymbol{M}^{-1}\boldsymbol{K} \in \mathcal{M}_q(\mathbb{R}[\mathsf{x}_1, \mathsf{x}_1^{-1}, \dots, \mathsf{x}_d, \mathsf{x}_d^{-1}]),$$

where $\mathsf{x} = (\mathsf{x}_1, \dots, \mathsf{x}_d)$ and thus $\mathsf{x}^{\boldsymbol{c}} = \mathsf{x}_1^{c_1} \cdots \mathsf{x}_d^{c_d}$ for any $\boldsymbol{c} \in \mathbb{Z}^d$. Here, the upwind space shift operators x_ℓ for $\ell \in [\![1, d]\!]$ such that

$$(\mathsf{x}_\ell \phi)(\boldsymbol{x}) = \phi(\boldsymbol{x} - \Delta x \boldsymbol{e}_\ell), \qquad \boldsymbol{x} \in \mathbb{R}^d.$$

Considering also the forward time shift operator z such that

$$(\mathsf{z}\phi)(t) = \phi(t + \Delta t), \qquad t \in \mathbb{R}.$$

The conserved moment m_1 of the LBM scheme fulfills

$$\mathsf{z}\mathsf{m}_1(t, \boldsymbol{x}) = -\sum_{k=q-Q-1}^{q-1} \mathsf{c}_k \mathsf{z}^{k+1-q} \mathsf{m}_1(t, \boldsymbol{x}), \qquad (t, \boldsymbol{x}) \in \Delta t[\![Q, +\infty]\!] \times \Delta x \mathbb{Z}^d,$$

where $\det(\mathsf{z}\boldsymbol{I} - \mathbf{E}) = \sum_{k=0}^{k=q} \mathsf{c}_k \mathsf{z}^k$. Easily $\mathsf{c}_k = 0$ for $k \in [\![0, q-Q-2]\!]$.
We call this scheme corresponding bulk Finite Difference scheme: multi-step with $Q+2$ stages, thus need for **initialization** through Q initialization schemes.

Corresponding Finite Difference scheme

- Given $\mathbf{m}(0, \boldsymbol{x})$ for every $\boldsymbol{x} \in \Delta x \mathbb{Z}^d$.
- **Initialization schemes**. For $k \in [\![1, Q]\!]$

$$\mathrm{m}_1(k\Delta t, \boldsymbol{x}) = (\mathbf{E}^k \mathbf{m})_1(0, \boldsymbol{x}), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d. \tag{1}$$

- **Corresponding bulk Finite Difference scheme**. For $k \in [\![Q, +\infty]\!]$

$$\mathrm{m}_1((k+1)\Delta t, \boldsymbol{x}) = -\sum_{\ell=q-Q-1}^{q-1} \mathrm{c}_\ell \mathrm{m}_1((k+\ell+1-q)\Delta t, \boldsymbol{x}), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d.$$

Nomenclature:

- **initialization schemes**, to indicate (1) for $k \in [\![1, Q]\!]$;
- **starting schemes**, to indicate (1) for any $k \in \mathbb{N}^*$.

Corresponding Finite Difference scheme: an easy example

Consider the D_1Q_2. For the initialization

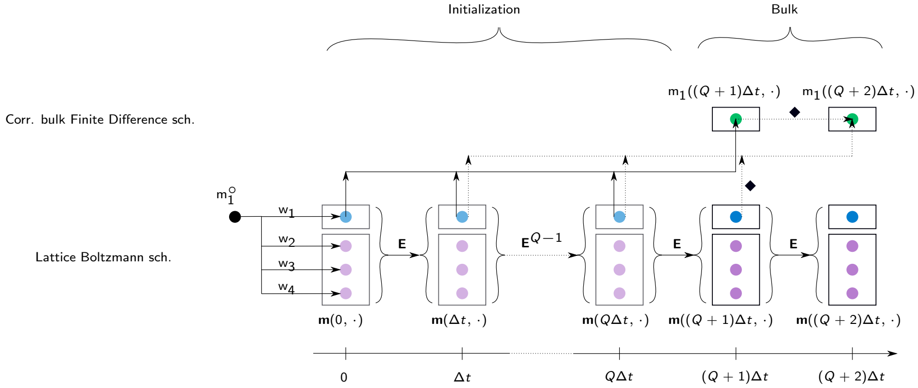
$$\mathrm{m}_1(\Delta t, x) = \Big(\Big(\mathrm{S}(\mathrm{x}_1) + \frac{s_2\epsilon_2}{\lambda}\mathrm{A}(\mathrm{x}_1)\Big)\mathrm{m}_1\Big)(0,x) + \frac{(1-s_2)\epsilon_2}{\lambda}(\mathrm{A}(\mathrm{x}_1)\mathrm{m}_2)(0,x),$$

where $\mathrm{S}(\mathrm{x}_1) = (\mathrm{x}_1 + \mathrm{x}_1^{-1})/2$ and $\mathrm{A}(\mathrm{x}_1) = (\mathrm{x}_1 - \mathrm{x}_1^{-1})/2$ are the symmetric and anti-symmetric parts of operators.

$$\mathrm{m}_1((k+1)\Delta t, x) = \Big((2-s_2)\mathrm{S}(\mathrm{x}_1) + \frac{s_2\epsilon_2}{\lambda}\mathrm{A}(\mathrm{x}_1)\Big)\mathrm{m}_1(k\Delta t, x) \\ -(1-s_2)\mathrm{m}_1((k-1)\Delta t, x).$$

- $s_2 = 0$: scheme for the wave equation with velocities $\pm\lambda$.
$$\underbrace{\mathrm{m}_1((k+1)\Delta t, x) - 2\mathrm{m}_1(k\Delta t, x) + \mathrm{m}_1((k-1)\Delta t, x)}_{\simeq \Delta t^2 \partial_{tt} u(t^k, x) + O(\Delta t^4)} = \underbrace{2(\mathrm{S}(\mathrm{x}_1) - 1)\mathrm{m}_1(k\Delta t, x)}_{\simeq \Delta x^2 \partial_{xx} u(t^k, x) + O(\Delta x^4)}$$
- $s_2 = 1$: Lax-Friedrichs scheme:
$$\mathrm{m}_1((k+1)\Delta t, x) = \Big(\mathrm{S}(\mathrm{x}_1) + \frac{\epsilon_2}{\lambda}\mathrm{A}(\mathrm{x}_1)\Big)\mathrm{m}_1(k\Delta t, x).$$
- $s_2 = 2$: leap-frog scheme:
$$\mathrm{m}_1((k+1)\Delta t, x) = \mathrm{m}_1((k-1)\Delta t, x) + \frac{2\epsilon_2}{\lambda}\mathrm{A}(\mathrm{x}_1)\mathrm{m}_1(k\Delta t, x).$$

Recap of the situation



Section 4

Modified equation analysis

Initialization

Let m_1° such that $\mathrm{m}_1^\circ(\boldsymbol{x}) = u^\circ(\boldsymbol{x})$ for $\boldsymbol{x} \in \Delta x \mathbb{Z}^d$. Since linear problem and the equilibria of the non-conserved moments are functions of the conserved one:

$$\mathbf{m}(0, \boldsymbol{x}) = \mathbf{w}\mathrm{m}_1^\circ(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d,$$

where we have

- a **local initialization**, if $\mathbf{w} \in \mathbb{R}^q$, or
- a **prepared initialization**, if $\mathbf{w} \in (\mathbb{R}[\mathrm{x}_1, \mathrm{x}_1^{-1}, \dots, \mathrm{x}_d, \mathrm{x}_d^{-1}])^q$.

  [*Ex.:* Let $d = 1$ and $\mathrm{w}_1 = \mathrm{S}(\mathrm{x}_1)$, so

$$\mathrm{m}_1(0, x) = \mathrm{w}_1 \mathrm{m}_1^\circ(x) = \frac{1}{2}(\mathrm{m}_1^\circ(x - \Delta x) + \mathrm{m}_1^\circ(x + \Delta x)) = \frac{1}{2}(u^\circ(x - \Delta x) + u^\circ(x + \Delta x)), \qquad x \in \Delta x \mathbb{Z},$$

  is an example of prepared initialization of the conserved moment.]

Modified equation of the bulk scheme

Assumptions from now on: $\boldsymbol{M}$, $\boldsymbol{S}$ and ϵ_i for $i \in [\![1, q]\!]$ are independent of Δx.
From [Dubois, '19]

$$\boldsymbol{\mathcal{G}} = \lambda \boldsymbol{M} \sum_{|\mathfrak{n}|=1} \text{diag}(\boldsymbol{c}_1^{\mathfrak{n}}, \dots, \boldsymbol{c}_q^{\mathfrak{n}}) \partial^{\mathfrak{n}} \boldsymbol{M}^{-1} \in \mathcal{M}_q(\mathbb{R}[\partial_t, \partial_{x_1}, \dots, \partial_{x_d}]),$$

$$[\textit{Ex.:} \quad \mathrm{D}_1\mathrm{Q}_2\text{: } \boldsymbol{\mathcal{G}} = \begin{pmatrix} 0 & \partial_x \\ \lambda \partial_x & 0 \end{pmatrix}]$$

Theorem ([Bellotti, '22])

The **modified equation for the bulk Finite Difference scheme** *is given by*

$$\partial_t \phi(t, \boldsymbol{x}) + \Big(\mathcal{G}_{11} + \sum_{r=2}^{q} \mathcal{G}_{1r} \epsilon_r\Big) \phi(t, \boldsymbol{x})$$

$$+ \frac{\Delta x}{\lambda} \sum_{i=2}^{q} \Big(\frac{1}{s_i} - \frac{1}{2}\Big) \mathcal{G}_{1i} \Big(\Big(\mathcal{G}_{11} + \sum_{r=2}^{q} \mathcal{G}_{1r}\epsilon_r\Big)\epsilon_i - \mathcal{G}_{i1} - \sum_{r=2}^{q} \mathcal{G}_{ir}\epsilon_r\Big) \phi(t, \boldsymbol{x}) = O(\Delta x^2).$$

To solve the right equation: $\mathcal{G}_{11} + \sum_{r=2}^{r=q} \mathcal{G}_{1r}\epsilon_r = \boldsymbol{V} \cdot \nabla_{\boldsymbol{x}}$.

Modified equations of the starting schemes: principles

Discrete time-space operator $\mathrm{d} \in \mathbb{R}[\mathrm{z}, \mathrm{x}_1, \mathrm{x}_1^{-1}, \dots, \mathrm{x}_d, \mathrm{x}_d^{-1}]$, we indicate $\mathrm{d} \asymp \delta$ where $\delta \in (\mathbb{R}[\partial_t, \partial_{x_1}, \dots, \partial_{x_d}])[\![\Delta x]\!]$ if for any smooth $\phi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$

$$\mathrm{d}\phi(t, \boldsymbol{x}) = \sum_{h=0}^{+\infty} \Delta x^h \delta^{(h)} \phi(t, \boldsymbol{x}), \qquad (t, \boldsymbol{x}) \in \mathbb{R} \times \mathbb{R}^d.$$

The starting schemes read

$$\mathrm{z}^k \mathrm{m}_1(0, \boldsymbol{x}) = (\mathbf{E}^k \mathbf{w})_1 \mathrm{m}_1^{\circ}(\boldsymbol{x}), \qquad k \in \mathbb{N}^*, \quad \boldsymbol{x} \in \Delta x \mathbb{Z}^d.$$

Consistency analysis in practice: use schemes on smooth fcts. of $\mathbb{R} \times \mathbb{R}^d$ instead than grid fcts. over $\Delta t \mathbb{N} \times \Delta x \mathbb{Z}^d$, then truncated asymptotic equivalents.

$$\zeta^k \phi(0, \boldsymbol{x}) = (\boldsymbol{\mathcal{E}}^k \boldsymbol{\omega})_1 \phi(0, \boldsymbol{x}), \qquad k \in \mathbb{N}^*, \quad \boldsymbol{x} \in \mathbb{R}^d,$$

where $\mathrm{z}^k \asymp \zeta^k = e^{k\Delta x/\lambda \partial_t} = 1 + k\Delta x/\lambda \partial_t + O(\Delta x^2)$ and $\mathbf{E} \asymp \boldsymbol{\mathcal{E}} = e^{-\Delta x/\lambda \boldsymbol{\mathcal{G}}} \boldsymbol{K}$ and $\mathrm{w} \asymp \omega$. Most involved part

$$\begin{aligned} \boldsymbol{\mathcal{E}}^k &= (\boldsymbol{\mathcal{E}}^{(0)} + \Delta x \boldsymbol{\mathcal{E}}^{(1)} + O(\Delta x^2))^k \\ &= (\boldsymbol{\mathcal{E}}^{(0)})^k + \Delta x \sum_{\ell=0}^{\ell=k-1} (\boldsymbol{\mathcal{E}}^{(0)})^{\ell} \boldsymbol{\mathcal{E}}^{(1)} (\boldsymbol{\mathcal{E}}^{(0)})^{k-1-\ell} + O(\Delta x^2). \end{aligned}$$

Conditions for consistent starting schemes - local init.

Proposition

Consider a local initialization, i.e. $\mathbf{w} \in \mathbb{R}^q$*, then under the conditions*

$$\begin{aligned} & & & & & \mathrm{w}_1 = 1, \\ \text{for} \quad & r \in [\![2, q]\!], & \text{if} \quad & \mathcal{G}_{1r} \neq 0, & \text{then} \quad & \mathrm{w}_r = \epsilon_r, \end{aligned}$$

the **starting schemes are consistent** *with the modified equation of the bulk Finite Difference scheme at order* $O(\Delta x)$*. Moreover, the initial datum feeding the bulk Finite Difference scheme and the starting schemes is consistent with the initial datum of the Cauchy problem.*

[*Ex.:* D_1Q_2: The initialization scheme: Lax-Friedrichs scheme

$$\mathrm{m}_1(\Delta t, x) = \left(\mathrm{S}(\mathrm{x}_1) + \frac{\epsilon_2}{\lambda}\mathrm{A}(\mathrm{x}_1)\right)\mathrm{m}_1^{\circ}(x), \quad \text{or}$$

$$\mathrm{m}_{1,j}^1 = \frac{1}{2}(\mathrm{m}_{1,j-1}^{\circ} + \mathrm{m}_{1,j+1}^{\circ}) + \frac{\epsilon_2}{2\lambda}(\mathrm{m}_{1,j-1}^{\circ} - \mathrm{m}_{1,j+1}^{\circ}), \quad \text{known to be consistent.}$$

]

Conditions for consistent starting schemes - prepared init.

Proposition

Consider a prepared initialization, i.e. $\mathbf{w} \in (\mathbb{R}[\mathsf{x}_1, \mathsf{x}_1^{-1}, \dots, \mathsf{x}_d, \mathsf{x}_d^{-1}])^q$*, with*

$$\mathsf{w}_i = \sum\nolimits_{\mathfrak{e}} w_{i,\mathfrak{e}} \mathbf{x}^{\mathfrak{e}}, \qquad i \in [\![1, q]\!].$$

Then under the conditions

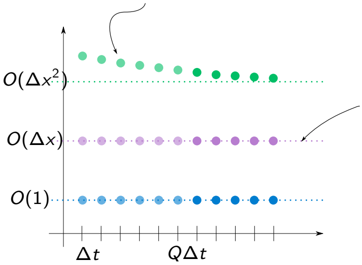
$$\omega_1^{(0)} = \sum_{\mathfrak{e}} w_{1,\mathfrak{e}} = 1,$$

for every $|\mathfrak{n}| = 1$, $\sum_{\mathfrak{e}} w_{1,\mathfrak{e}} \mathfrak{e}^{\mathfrak{n}} = 0$, $\Big[$Rem.: $\omega_1^{(1)} = -\sum_{|\mathfrak{n}|=1} \Big(\sum_{\mathfrak{e}} w_{i,\mathfrak{e}} \mathfrak{e}^{\mathfrak{n}}\Big) \partial^{\mathfrak{n}}\Big]$

for $r \in [\![2, q]\!]$, if $\mathcal{G}_{1r} \neq 0$, then $\omega_r^{(0)} = \sum_{\mathfrak{e}} w_{r,\mathfrak{e}} = \epsilon_r$,

the **starting schemes are consistent** *with the modified equation of the bulk Finite Difference scheme at order* $O(\Delta x)$*. Moreover, the initial datum feeding the bulk Finite Difference scheme and the starting schemes is consistent with the initial datum of the Cauchy problem.*

Initialization schemes *versus* starting schemes



Proposition

Let $H \in \mathbb{N}^*$. Assume that

- $\omega_1^{(0)} = 1$ *and* $\omega_1^{(h)} = 0$ *for* $h \in [\![1, H]\!]$.
- *The modified equations of the Q* **initialization schemes** *match the one of the bulk Finite Difference scheme for any order $h \in [\![1, H]\!]$.*

Then, the modified equations of the ∞ **starting schemes** *match the one of the bulk Finite Difference scheme for any order $h \in [\![1, H]\!]$.*

Stop! Wrap up

1. Proposed **modified equation** analysis of the initial condition: can be extended above $O(\Delta x)$ (sequel).

2. Conditions to have **consistency** of the initialization schemes: no order reduction.

3. Controlling the behavior **inside the initialization layer** implies a control **eventually in time**.

Section 5

Example D_1Q_2

D_1Q_2

The modified equation of the bulk Finite Difference scheme:

$$\partial_t \phi(t,x) + \epsilon_2 \partial_x \phi(t,x) - \lambda \Delta x \left(\frac{1}{s_2} - \frac{1}{2}\right)\left(1 - \frac{\epsilon_2^2}{\lambda^2}\right)\partial_{xx}\phi(t,x) = O(\Delta x^2).$$

Initializations to test:

- **Lax-Friedrichs**: $\mathrm{w}_1 = 1$, $\mathrm{w}_2 = \epsilon_2$. Satisfies the Proposition.

$$\mathrm{m}_{1,j}^{1} = \frac{1}{2}(\mathrm{m}_{1,j-1}^{\circ} + \mathrm{m}_{1,j+1}^{\circ}) + \frac{\epsilon_2}{2\lambda}(\mathrm{m}_{1,j-1}^{\circ} - \mathrm{m}_{1,j+1}^{\circ}).$$

- **Centered** (good): $w_{1,\pm 1} = \frac{1}{2}$, $w_{2,\pm 1} = \mp \frac{\lambda \pm s_2 \epsilon_2}{2(1-s_2)}$, $w_{2,0} = \frac{\epsilon_2}{1-s_2}$. Satisfies the Proposition.

$$\mathrm{m}_{1,j}^{1} = \mathrm{m}_{1,j}^{\circ} + \frac{\epsilon_2}{2\lambda}(\mathrm{m}_{1,j-1}^{\circ} - \mathrm{m}_{1,j+1}^{\circ}).$$

- **Centered** (bad): $w_{1,\pm 2} = \pm \frac{\epsilon_2}{2\lambda}$, $w_{1,\pm 1} = \frac{1}{2}$, $w_{2,\pm 2} = -\frac{\epsilon_2(1 \pm s_2 \epsilon_2/\lambda)}{2(1-s_2)}$, $w_{2,\pm 1} = \mp \frac{\lambda \pm s_2 \epsilon_2}{2(1-s_2)}$. **Does not satisfy the Proposition**, indeed

$$\mathrm{m}_1(0) \simeq u^{\circ} + \Delta x \underbrace{2\epsilon_2/\lambda \partial_x}_{\omega_1^{(1)}} u^{\circ} + O(\Delta x^2).$$

D_1Q_2

- **Lax-Wendroff**. The coefficients are $w_{1,\pm 1} = \frac{1-\epsilon_2^2/\lambda^2}{2}$, $w_{1,0} = \frac{\epsilon_2^2}{\lambda^2}$, $w_{2,\pm 1} = \mp\frac{(\lambda \pm s_2\epsilon_2)(1-\epsilon_2^2/\lambda^2)}{2(1-s_2)}$ and $w_{2,0} = \frac{\epsilon_2(1-s_2\epsilon_2^2/\lambda^2)}{1-s_2}$. It fulfills the Proposition.

$$\mathrm{m}_{1,j}^{1} = \mathrm{m}_{1,j}^{\circ} + \frac{\epsilon_2}{2\lambda}(\mathrm{m}_{1,j-1}^{\circ} - \mathrm{m}_{1,j+1}^{\circ}) + \frac{\epsilon_2^2}{2\lambda^2}(\mathrm{m}_{1,j-1}^{\circ} - 2\mathrm{m}_{1,j}^{\circ} + \mathrm{m}_{1,j+1}^{\circ}).$$

- **Smooth initialization**, inspired by [Van Leemput *et al.*, '09]. $\mathrm{w}_1 = 1$, $w_{2,\pm 1} = \pm\frac{\lambda(1-\epsilon_2^2/\lambda^2)}{2s_2}$, $w_{2,0} = \epsilon_2$ and fulfilling the Proposition.

$$\begin{aligned}\mathrm{m}_{1,j}^{1} =& \frac{1}{2}(\mathrm{m}_{1,j-1}^{\circ} + \mathrm{m}_{1,j+1}^{\circ}) + \frac{(1-s_2)\epsilon_2^2}{2\lambda}(\mathrm{m}_{1,j-1}^{\circ} - \mathrm{m}_{1,j+1}^{\circ}) \\ &+ \frac{(1-s_2)\lambda\epsilon_2(1-\epsilon_2^2/\lambda^2)}{4s_2}(\mathrm{m}_{1,j-2}^{\circ} - 2\mathrm{m}_{1,j}^{\circ} + \mathrm{m}_{1,j+2}^{\circ}).\end{aligned}$$

Order of convergence

Initial data for the Cauchy problem:

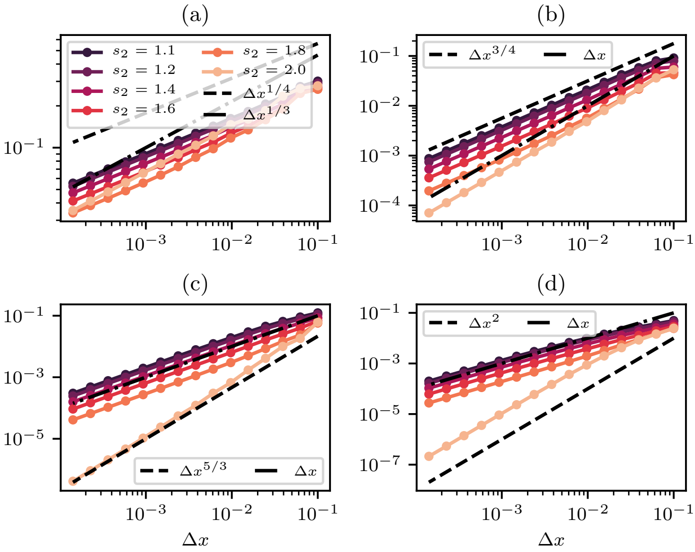
$$
\begin{aligned}
&\text{(a)} \quad u^\circ(x) = \chi_{|x|\leq 1/2}(x) \in H^\sigma, \quad \text{for any} \quad \sigma < \sigma_0 = 1/2.\\
&\text{(b)} \quad u^\circ(x) = (1-2|x|)\chi_{|x|\leq 1/2}(x) \in H^\sigma, \quad \text{for any} \quad \sigma < \sigma_0 = 3/2.\\
&\text{(c)} \quad u^\circ(x) = \cos^2(\pi x)\chi_{|x|\leq 1/2}(x) \in H^\sigma, \quad \text{for any} \quad \sigma < \sigma_0 = 5/2.\\
&\text{(d)} \quad u^\circ(x) = \exp\left(-1/(1-|2x|^2)\right)\chi_{|x|\leq 1/2}(x) \in C_c^\infty,
\end{aligned}
$$

For initialization schemes which are **consistent** with the transport equation, the convergence rates [Strikwerda, '04] are:

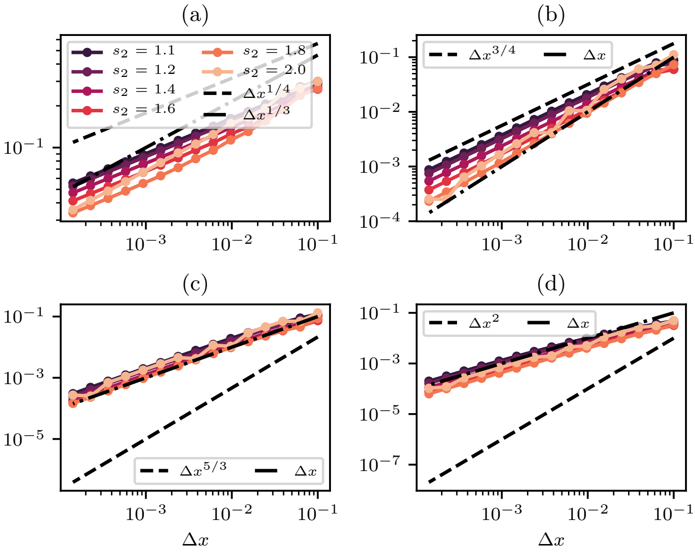
Test	Bulk scheme 1st order ($s_2 < 2$)	Bulk scheme 2nd order ($s_2 = 2$)
(a)	order 1/4	order 1/4
(b)	order 3/4	order 3/4
(c)	order 1	order 5/3
(d)	order 1	order 2

Caveat: these rates are the right ones if: 1. the initialization scheme is consistent; 2. we perturb the initial datum from order two: $\omega_1^{(1)} = 0$.

Order of convergence: good centered

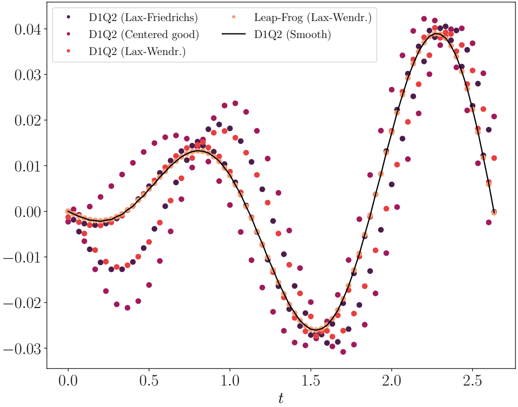


Order of convergence: bad centered



Time smoothness

Following [Van Leemput *et al.*, '09], the simulation is carried on the periodic domain $[0, 1]$ discretized with $\Delta x = 1/30$, $s_2 = 2$, $\lambda = 1$ and $\epsilon_2 = V = 0.66$ with $u^{\circ}(x) = \cos(2\pi x)$.



We measure the error at the eigth cell in time.

Time smoothness: explanation

We give the example for the **Lax-Friedrichs** initialization. For $k \in \mathbb{N}^*$, the modified equation for the starting schemes are

$$\partial_t \phi(0, x) + \epsilon_2 \partial_x \phi(0, x) - \lambda \Delta x \left(\frac{1}{2} + \sum_{\ell=1}^{k-1} \left(1 - \frac{\ell}{k}\right)(1 - s_2)^{\ell} \right) \left(1 - \frac{\epsilon_2^2}{\lambda^2}\right) \partial_{xx} \phi(0, x) = O(\Delta x^2).$$

- **Asymptotic match** of the bulk scheme dissipation:

$$\lim_{k \to +\infty} \underbrace{\left(\frac{1}{2} + \sum_{\ell=1}^{k-1} \left(1 - \frac{\ell}{k}\right)(1 - s_2)^{\ell} \right)}_{\text{diss. starting schemes}} = \underbrace{\frac{1}{s_2} - \frac{1}{2}}_{\text{diss. bulk scheme}} \qquad \textbf{Caveat!}$$

- **Behavior for** $s_2 = 2$

$$\left[\frac{1}{2} + \sum_{\ell=1}^{k-1} \left(1 - \frac{\ell}{k}\right)(1 - s_2)^{\ell} \right]_{s_2=2} = \frac{1 - (-1)^k}{4k} = \begin{cases} 0, & \text{for } k \text{ even}, \\ 1/(2k), & \text{for } k \text{ odd}. \end{cases}$$

Similar conclusions for the **good centered** and the **Lax-Wendroff**.

Time smoothness: explanation

For the **smooth initialization**, the modified equations for the starting schemes are

$$\partial_t \phi(0,x) + \epsilon_2 \partial_x \phi(0,x) + O(\Delta x^2) - \lambda \Delta x \underbrace{\left(\frac{1}{2} - \sum_{\ell=1}^{k-1} \Big(1 - \frac{\ell}{k}\Big)(1-s_2)^{\ell} + \frac{1}{k s_2} \sum_{\ell=1}^{k} (1-s_2)^{\ell} \right)}_{=\frac{1}{s_2}-\frac{1}{2} \quad \text{(dissipation bulk scheme)}} \Big(1 - \frac{\epsilon_2^2}{\lambda^2}\Big) \partial_{xx}\phi(0,x) = 0,$$

for $k \in \mathbb{N}^*$. Unsurprising if we apply the Proposition with $H = 2$.

For the **bad centered** scheme, the modified equations are

$$\partial_t \phi(0,x) + \epsilon_2 \left(1 + \frac{2}{k} \left(1 - \sum_{\ell=0}^{k-1} (1-s_2)^{\ell} \right) \right) \partial_x \phi(0,x) = O(\Delta x), \qquad k \in \mathbb{N}^*.$$

Stop! Wrap up

What does this example teach us?

1. **Careful** when **preparing the conserved moment** $\mathrm{m}_1(0)$: multistep bulk Finite Difference scheme.
2. **Consistent** schemes **preserve** the **convergence order** provided that $\mathrm{m}_1(0)$ is at least second-order accurate w.r.t. u°.
3. **Time smoothness** thanks to **matched numerical dissipation** at $O(\Delta x^2)$.
4. The **modified equations** for the starting schemes at order $O(\Delta x^2)$ provide a valuable tool to **quantitatively** investigate the behavior **close to the initial time**.

Section 6

Observability

Towards observability: D_1Q_3

Richer D_1Q_3 scheme [Dubois *et al.*, '20]: $d = 1$, $q = 3$, $c_1 = 0$, $c_2 = 1$, $c_3 = -1$ and

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

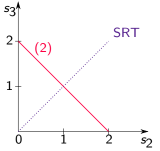
Look for: conditions under which $\mathrm{w}_1, \mathrm{w}_2, \mathrm{w}_3 \in \mathbb{R}$ yield initialization schemes **matching the dissipation** at $O(\Delta x^2)$ of the bulk Finite Difference scheme.

If $s_2, s_3 \neq 1$, then $Q = 2$ and we have the non-linear system (initialization, bulk)

$$\begin{cases} \frac{1}{3} - \frac{\epsilon_2^2}{2\lambda^2} + \frac{s_3\epsilon_3}{6\lambda^2} + \frac{(1-s_3)\mathrm{w}_3}{6\lambda^2} &= \left(\frac{1}{s_2} - \frac{1}{2}\right)\left(\frac{2}{3} - \frac{\epsilon_2^2}{\lambda^2} + \frac{\epsilon_3}{3\lambda^2}\right), \\ \frac{(2-s_2)}{3} - \frac{(2-s_2)\epsilon_2^2}{2\lambda^2} + \frac{s_3(5-2s_2-s_3)\epsilon_3}{12\lambda^2} + \frac{(1-s_3)(4-2s_2-s_3)\mathrm{w}_3}{12\lambda^2} &= \left(\frac{1}{s_2} - \frac{1}{2}\right)\left(\frac{2}{3} - \frac{\epsilon_2^2}{\lambda^2} + \frac{\epsilon_3}{3\lambda^2}\right). \end{cases}$$

This is enough by Proposition for $H = 2$.
Between many conditions, one is remarkable

$$s_3 = 2 - s_2. \qquad (2)$$



Towards observability

In [Bellotti *et al.*, '22]: the choice $s_3 = 2 - s_2$ could yield a bulk Finite Difference scheme with **three stages instead of four**, see [D'Humières and Ginzburg, '09].

LBM : **linear time-invariant discrete-time** system

$$\begin{aligned} \mathsf{z}\mathbf{m}(t, \boldsymbol{x}) = \mathbf{E}\mathbf{m}(t, \boldsymbol{x}), &\qquad (t, \boldsymbol{x}) \in \Delta t \mathbb{N} \times \Delta x \mathbb{Z}^d, \\ \mathbf{m}(0, \boldsymbol{x}) &\qquad \text{given for } \boldsymbol{x} \in \Delta x \mathbb{Z}^d, \\ \mathbf{y} = \boldsymbol{C}\mathbf{m} &\qquad \text{(output).} \end{aligned}$$

We are solely interested in the conserved moment m_1, then $\boldsymbol{C} = \boldsymbol{e}_1^{\mathsf{T}} \in \mathbb{R}^q$.

We introduce the **observability matrix** of the system

$$\boldsymbol{\Omega} := \begin{bmatrix} \boldsymbol{C} \\ \boldsymbol{C}\mathbf{E} \\ \vdots \\ \boldsymbol{C}\mathbf{E}^{q-1} \end{bmatrix} \in \mathcal{M}_q(\mathbb{R}[\mathsf{x}_1, \mathsf{x}_1^{-1}, \dots, \mathsf{x}_d, \mathsf{x}_d^{-1}]).$$

Observability

- Systems on **fields**

$$\text{Observable} \quad \iff \quad \text{rank}(\boldsymbol{\Omega}) = q.$$

A.k.a. can $\boldsymbol{m}(0)$ be reconstructed from $m_1(0), m_1(\Delta t), \dots, m_1((q-1)\Delta t)$?

- Systems on **rings**. **Several notions** (not equivalent):
  - According to [Brewer *et al.*, '86]

$$\text{Observable} \quad \iff \quad \text{Left action of } \boldsymbol{\Omega} \text{ injective.}$$

  - [Fliess and Mounier, '98], *etc.*..

We define the **observability index** $o \leq Q+1$ mimicking the definition for systems over fields as

$$o := \max_{\ell \in \mathbb{N}} \text{rank}(\boldsymbol{\Omega}_\ell), \quad \text{where} \quad \boldsymbol{\Omega}_\ell := \begin{bmatrix} \boldsymbol{C} \\ \boldsymbol{CE} \\ \vdots \\ \boldsymbol{CE}^{\ell-1} \end{bmatrix} \in \mathcal{M}_{\ell \times q}(\mathbb{R}[\mathsf{x}_1, \mathsf{x}_1^{-1}, \dots, \mathsf{x}_d, \mathsf{x}_d^{-1}]).$$

Trivial example: D_1Q_2

- **Observable** according to [Brewer *et al.*, '86] for $s_2 \neq 1$ (*e.g.* $Q = 1$. Check $\det(\boldsymbol{\Omega})$ for this).
- **Observability index**:

$$o = Q + 1 = \begin{cases} 1, & s_2 = 1, \\ 2, & s_2 \neq 1. \end{cases}$$

- **Unobservable space**:

$$\ker(\boldsymbol{\Omega}) = \begin{cases} \{(0, \mathrm{m}_2)^{\mathsf{T}} \ : \ \forall \mathrm{m}_2 = \mathrm{m}_2(\boldsymbol{x}) \text{ latt. fct.}\}, & s_2 = 1, \\ \{(0, \mathrm{m}_2)^{\mathsf{T}} \ : \ \forall \mathrm{m}_2 = \mathrm{m}_2(\boldsymbol{x}) \text{ latt. fct. s.t. } \mathsf{A}(\mathrm{x}_1)\mathrm{m}_2 = 0\}, & s_2 \neq 1. \end{cases}$$

For example

$$\mathrm{m}_1(0, \cdot) = 0, \qquad \mathrm{m}_2(0, j\Delta x) = (-1)^j,$$

belongs to $\ker(\boldsymbol{\Omega})$: the solution will remain zero forever.

Observability and number of stages of the bulk scheme

We introduce the coefficients $\mathbf{p}_o \in (\mathbb{R}[\mathsf{x}_1, \mathsf{x}_1^{-1}, \dots, \mathsf{x}_d, \mathsf{x}_d^{-1}])^o$ such that

$$\mathbf{p}_o \boldsymbol{\Omega}_o = -\boldsymbol{C}\mathbf{E}^o.$$

The solution of this problem exists thanks to the definition of o. We then introduce the monic polynomial

$$\Psi_o(\mathsf{z}) := \mathsf{z}^o + \sum_{k=1}^{o} \mathsf{p}_{o,k} \mathsf{z}^{k-1}.$$

By construction ($\boldsymbol{C} = \boldsymbol{e}_1^{\mathsf{T}}$)

$$\Psi_o(\mathbf{E}) = \mathbf{E}^o + \sum_{k=1}^{o} \mathsf{p}_{o,k} \mathbf{E}^{k-1} = \begin{pmatrix} 0 & \dots & 0 \\ \star & \cdots & \star \\ \vdots & \ddots & \vdots \\ \star & \cdots & \star \end{pmatrix}.$$

Indeed, see [Bellotti *et al.*, '22], $\Psi_o(\mathsf{z})$ divides $\det(\mathsf{z}\boldsymbol{I} - \mathbf{E})$, whence if $o = Q + 1$, we naturally have $\Psi_o(\mathsf{z}) = \mathsf{z}^{Q+1-q} \det(\mathsf{z}\boldsymbol{I} - \mathbf{E})$.

Corresponding Finite Difference scheme revisited

Now, $\Psi_o(\mathrm{z})$ does the trick that $\det(\mathrm{z}\boldsymbol{I} - \mathbf{E})$, the characteristic polynomial of $\mathbf{E}$ did before.

- Given $\mathbf{m}(0, \boldsymbol{x})$ for every $\boldsymbol{x} \in \Delta x \mathbb{Z}^d$.
- **Initialization schemes**. For $k \in [\![1, o-1]\!]$

$$\mathrm{m}_1(k\Delta t, \boldsymbol{x}) = \boldsymbol{C}\mathbf{E}^k \mathbf{m}(0, \boldsymbol{x}), \qquad \boldsymbol{x} \in \Delta x \mathbb{Z}^d.$$

- **Corresponding bulk Finite Difference scheme**. For $k \in [\![o-1, +\infty]\!]$

$$\mathrm{m}_1((k+1)\Delta t, \boldsymbol{x}) = -\left(\sum_{\ell=q-o}^{q-1} \mathrm{p}_{o,o+\ell+1-q} \mathrm{m}_1((k+\ell+1-q)\Delta t, \cdot) \right)(\boldsymbol{x}),$$

for $\boldsymbol{x} \in \Delta x \mathbb{Z}^d$.

Changing Q into $o-1$, all the previous Propositions for initialization (now for $k \leq o-1$) and starting schemes are **still valid**.

Back to the D_1Q_3: a less trivial example

We select $s_2 + s_3 = 2$ with $s_2 \neq 1$.

- **Non observable**: it can be seen that $o = 2 < 3$, whereas $Q + 1 = 3$.
- We can compute $\Psi_2(\mathsf{z})$:

$$\det(\mathsf{z}\boldsymbol{I} - \mathbf{E}) = (\mathsf{z} + (1 - s_2))\Psi_2(\mathsf{z}), \qquad \text{with}$$

$$\Psi_2(\mathsf{z}) = \mathsf{z}^2 + \Big(-\frac{s_2\epsilon_2}{\lambda}\mathsf{A}(\mathsf{x}_1) - \frac{\epsilon_3}{\lambda^2}(2 - s_2)(\mathsf{S}(\mathsf{x}_1) - 1) - (2 - s_2)\Big)\mathsf{z} + (1 - s_2).$$

- **Unobservable space**

$$\ker(\boldsymbol{\Omega}) = \{(0, \mathsf{m}_2, \mathsf{m}_3)^{\mathsf{T}} \ : \ \forall \mathsf{m}_2 = \mathsf{m}_2(\boldsymbol{x}), \ \mathsf{m}_3 = \mathsf{m}_3(\boldsymbol{x}) \text{ latt. fct. s.t.}$$
$$\mathsf{A}(\mathsf{x}_1)\mathsf{m}_2 = 1/3\lambda \underbrace{(\mathsf{S}(\mathsf{x}_1) - 1)}_{\substack{\text{three-points} \\ \text{discrete Laplacian}}} \mathsf{m}_3\}.$$

Link $\mathrm{D}_d\mathrm{Q}_{1+2W}$ TRT with magic parameters equal to 1/4

Consider any spatial dimension d and $1+2W$ velocities with $W \in \mathbb{N}^*$, which is the number of so-called **links**. The velocities should be such that

$$\boldsymbol{c}_1 = \boldsymbol{0}, \qquad \boldsymbol{c}_{2j} = -\boldsymbol{c}_{2j+1} \in \mathbb{Z}^d, \qquad j \in [\![1, W]\!],$$

and the moment matrix

$$\boldsymbol{M} = \left(\begin{array}{c|cc|c|cc} 1 & 1 & 1 & \cdots & 1 & 1 \\ \hline 0 & \multicolumn{2}{c|}{\multirow{2}{*}{$\tilde{\boldsymbol{M}}$}} & & & \\ 0 & & & & & \\ \hline \vdots & & & \ddots & & \\ \hline 0 & & & & \multicolumn{2}{c}{\multirow{2}{*}{$\tilde{\boldsymbol{M}}$}} \\ 0 & & & & & \end{array}\right) \in \mathcal{M}_{1+2W}(\mathbb{R}), \quad \text{with} \quad \tilde{\boldsymbol{M}} = \begin{pmatrix} \lambda & -\lambda \\ \lambda^2 & \lambda^2 \end{pmatrix}.$$

The relaxation parameters should be such that

$$s_{2\ell} = s \in]0, 2], \qquad s_{2\ell+1} = 2 - s, \qquad \ell \in [\![1, W]\!].$$

Link D_dQ_{1+2W} TRT with magic parameters equal to 1/4

Proposition

The **characteristic polynomial** *of the scheme matrix* **E** *for the previously described schemes is given by*

$$\det(z\boldsymbol{I} - \mathbf{E}) = (z + (1-s))\left(z^2 - (1-s)^2\right)^{W-1}\Psi_2(z),$$

where

$$\Psi_2(z) = z^2 - (2-s)z + (1-s) - z\frac{s}{\lambda}\sum_{\ell=1}^{W} A(\mathbf{x}^{\boldsymbol{c}_{2\ell}})\epsilon_{2\ell} - z\frac{(2-s)}{\lambda^2}\sum_{\ell=1}^{W}(S(\mathbf{x}^{\boldsymbol{c}_{2\ell}}) - 1)\epsilon_{2\ell+1},$$

annihilates the first row of the matrix **E**. *Thus,* $o = 2$ *if* $s \neq 1$ *and* $o = 1$ *if* $s = 1$.

Moral: these class of scheme is quite easy to master in terms of **smooth initialization**: only one **initialization scheme** to consider.

Link $\text{D}_d\text{Q}_{1+2W}$ TRT with magic parameters equal to 1/4

Proposition (Modified equations)

The **modified equation** *for the* **bulk Finite Difference scheme** *is*

$$\partial_t \phi(t, \boldsymbol{x}) + \sum_{\ell=1}^{W} \epsilon_{2\ell} \sum_{|\mathfrak{n}|=1} \boldsymbol{c}_{\ell}^{\mathfrak{n}} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \phi(t, \boldsymbol{x}) + O(\Delta x^2)$$

$$- \frac{\Delta x}{\lambda} \Big(\frac{1}{s} - \frac{1}{2} \Big) \Bigg(2 \sum_{\ell=1}^{W} \epsilon_{2\ell+1} \sum_{|\mathfrak{n}|=2} \frac{\boldsymbol{c}_{2\ell}^{\mathfrak{n}}}{\mathfrak{n}!} \partial_{\boldsymbol{x}}^{\mathfrak{n}} - \Bigg(\sum_{\ell=1}^{W} \epsilon_{2\ell} \sum_{|\mathfrak{n}|=1} \boldsymbol{c}_{2\ell}^{\mathfrak{n}} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \Bigg)^2 \Bigg) \phi(t, \boldsymbol{x}) = 0.$$

For local initializations $\mathbf{w} \in \mathbb{R}^q$ *with* $\text{w}_1 = 1$ *and* $\text{w}_{2\ell} = \epsilon_{2\ell}$ *for* $\ell \in [\![1, W]\!]$*, the* **modified equation** *for the* **unique initialization scheme** *is*

$$\partial_t \phi(0, \boldsymbol{x}) + \sum_{\ell=1}^{W} \epsilon_{2\ell} \sum_{|\mathfrak{n}|=1} \boldsymbol{c}_{\ell}^{\mathfrak{n}} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \phi(0, \boldsymbol{x}) + O(\Delta x^2)$$

$$= \frac{\Delta x}{2\lambda} \Big(2 \sum_{\ell=1}^{W} ((2-s)\epsilon_{2\ell+1} - (1-s)\text{w}_{2\ell+1}) \sum_{|\mathfrak{n}|=2} \frac{\boldsymbol{c}_{2\ell}^{\mathfrak{n}}}{\mathfrak{n}!} \partial_{\boldsymbol{x}}^{\mathfrak{n}} - \Big(\sum_{\ell=1}^{W} \epsilon_{2\ell} \sum_{|\mathfrak{n}|=1} \boldsymbol{c}_{2\ell}^{\mathfrak{n}} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \Big)^2 \Big) \phi(0, \boldsymbol{x}).$$

Link D_dQ_{1+2W} TRT with magic parameters equal to 1/4

Smooth initialization (*i.e.* match in the numerical dissipation): **differential constraint**

$$\sum_{\ell=1}^{W} \mathrm{w}_{2\ell+1} \sum_{|\mathfrak{n}|=2} \frac{\boldsymbol{c}_{2\ell}^{\mathfrak{n}}}{\mathfrak{n}!} \partial_{\boldsymbol{x}}^{\mathfrak{n}} = \frac{1}{s} \left(\left(\sum_{\ell=1}^{W} \epsilon_{2\ell} \sum_{|\mathfrak{n}|=1} \boldsymbol{c}_{2\ell}^{\mathfrak{n}} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \right)^2 - (2-s) \sum_{\ell=1}^{W} \epsilon_{2\ell+1} \sum_{|\mathfrak{n}|=2} \frac{\boldsymbol{c}_{2\ell}^{\mathfrak{n}}}{\mathfrak{n}!} \partial_{\boldsymbol{x}}^{\mathfrak{n}} \right).$$

For some schemes it is possible to satisfy (D_1Q_3, D_2Q_9, ...), for other (D_2Q_5) ... no.

Stop! Wrap up

Strong lack of observability (huge $\ker(\mathbf{\Omega}) \leftrightsquigarrow \det(z\boldsymbol{I} - \mathbf{E})/\Psi_o(z)$, small $\mathrm{Im}(\mathbf{\Omega}) \leftrightsquigarrow \Psi_o(z)$, see previous $\mathrm{D}_d\mathrm{Q}_{1+2W}$ TRT):

the multi-step **constraint** on m_1 has **very little steps**

or equivalently

the **corresponding bulk Finite Difference scheme** has **very little time steps**.

Consequences on the design on the initialization:

Few constraints to study to **match orders** above $O(\Delta x)$.

Conclusions

Tools we have introduced:

1. **Modified equation** analysis for the initial condition for LBM methods.
2. Notion of **observability** determining the **number of initialization schemes** (difficult to characterize).

Results:

1. **Modified equation**:
   - **Consistency** of the initialization schemes.
   - **Time smoothness** of the discrete solutions *via* numerical dissipation.
2. **Observability**:
   - **Reduced number of constraints** to match orders in the expansions between initialization and bulk schemes.

Thank you for your attention!

Section 7

Backup slides

Structure of the collision matrix K

Upper-triangular matrix with

$$\boldsymbol{K}^{\ell} = \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ \pi_{\ell}(s_2)\epsilon_2 & (1-s_2)^{\ell} & 0 & & & \vdots \\ \pi_{\ell}(s_3)\epsilon_3 & 0 & (1-s_3)^{\ell} & \ddots & & \vdots \\ \pi_{\ell}(s_4)\epsilon_4 & 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ \pi_{\ell}(s_q)\epsilon_q & 0 & 0 & \cdots & 0 & (1-s_q)^{\ell} \end{pmatrix}, \qquad \ell \in \mathbb{N}^*,$$

with polynomials π_ℓ are defined recursively as $\pi_0(X) := 0$ and $\pi_{\ell+1}(X) := X + (1-X)\pi_\ell(X)$ for $\ell \in \mathbb{N}$.

How to devise the forward centered scheme

We first try $\mathrm{w}_1 = 1$ and prepared initialization of the non-conserved one, thus $\mathrm{w}_2 \in \mathbb{R}[\mathrm{x}_1, \mathrm{x}_1^{-1}, \dots, \mathrm{x}_d, \mathrm{x}_d^{-1}]$. We look for a compactly supported solution of the following infinite system

$$\dots, \quad w_{2,1} - w_{2,3} = 0, \quad w_{2,0} - w_{2,2} = -\frac{\lambda(1 - \epsilon_2/\lambda + s_2\epsilon_2/\lambda)}{1 - s_2},$$
$$w_{2,-1} - w_{2,1} = \frac{2\lambda}{1 - s_2}, \quad w_{2,-2} - w_{2,0} = -\frac{\lambda(1 + \epsilon_2/\lambda - s_2\epsilon_2/\lambda)}{1 - s_2},$$
$$w_{2,-3} - w_{2,-1} = 0, \quad \dots$$

This problem cannot be solved by a compactly supported sequence. We are indeed trying to perform a deconvolution in the ring of Finite Difference operators, which is not solvable because the operator $\mathrm{x}_1 - \mathrm{x}_1^{-1}$ is not a unit. Even on a bounded domain, where the problem is the one of inverting a circulant matrix, this circulant matrix is not invertible.

How to devise the forward centered scheme

Considering a prepared initialization for both moments, thus $\mathrm{w}_1, \mathrm{w}_2 \in \mathbb{R}[\mathrm{x}_1, \mathrm{x}_1^{-1}, \ldots, \mathrm{x}_d, \mathrm{x}_d^{-1}]$, several choices are possible to recover this scheme. The infinite system to solve reads

$$
\begin{aligned}
&\ldots \\
\frac{1+s_2\epsilon_2/\lambda}{2} w_{1,1} + \frac{1-s_2}{2\lambda} w_{2,1} + \frac{1-s_2\epsilon_2/\lambda}{2} w_{1,3} - \frac{1-s_2}{2\lambda} w_{2,3} &= 0, \\
\frac{1+s_2\epsilon_2/\lambda}{2} w_{1,0} + \frac{1-s_2}{2\lambda} w_{2,0} + \frac{1-s_2\epsilon_2/\lambda}{2} w_{1,2} - \frac{1-s_2}{2\lambda} w_{2,2} &= \frac{\epsilon_2}{2\lambda}, \\
\frac{1+s_2\epsilon_2/\lambda}{2} w_{1,-1} + \frac{1-s_2}{2\lambda} w_{2,-1} + \frac{1-s_2\epsilon_2/\lambda}{2} w_{1,1} - \frac{1-s_2}{2\lambda} w_{2,1} &= 1, \\
\frac{1+s_2\epsilon_2/\lambda}{2} w_{1,-2} + \frac{1-s_2}{2\lambda} w_{2,-2} + \frac{1-s_2\epsilon_2/\lambda}{2} w_{1,0} - \frac{1-s_2}{2\lambda} w_{2,0} &= -\frac{\epsilon_2}{2\lambda}, \\
\frac{1+s_2\epsilon_2/\lambda}{2} w_{1,-3} + \frac{1-s_2}{2\lambda} w_{2,-3} + \frac{1-s_2\epsilon_2/\lambda}{2} w_{1,-1} - \frac{1-s_2}{2\lambda} w_{2,-1} &= 0, \\
&\ldots
\end{aligned}
$$

In order to construct a (non-unique) solution, we first enforce the compactness: $w_{1,\ell} = w_{2,\ell} = 0$ for $|\ell| \geq 2$.

How to devise the forward centered scheme

From this, we obtain the finite system

$$\begin{aligned}
\Big(1 + \frac{s_2\epsilon_2}{\lambda}\Big) w_{1,1} + \frac{1-s_2}{\lambda} w_{2,1} &= 0, \\
\Big(1 + \frac{s_2\epsilon_2}{\lambda}\Big) w_{1,0} + \frac{1-s_2}{\lambda} w_{2,0} &= \frac{\epsilon_2}{\lambda}, \\
\Big(1 + \frac{s_2\epsilon_2}{\lambda}\Big) w_{1,-1} + \frac{1-s_2}{\lambda} w_{2,-1} + (1 - s_2\epsilon_2/\lambda) w_{1,1} - \frac{(1-s_2)}{\lambda} w_{2,1} &= 2, \\
\Big(1 - \frac{s_2\epsilon_2}{\lambda}\Big) w_{1,0} - \frac{1-s_2}{\lambda} w_{2,0} &= -\frac{\epsilon_2}{\lambda}, \\
\Big(1 - \frac{s_2\epsilon_2}{\lambda}\Big) w_{1,-1} - \frac{1-s_2}{\lambda} w_{2,-1} &= 0.
\end{aligned}$$

We then split the central equation using a parameter $\theta \in \mathbb{R}$, having $(1 + s_2\epsilon_2/\lambda)w_{1,-1} + (1 - s_2)/\lambda w_{2,-1} = \theta$ and $(1 - s_2\epsilon_2/\lambda)w_{1,1} - (1 - s_2)/\lambda w_{2,1} = 2 - \theta$.

How to devise the forward centered scheme

Introducing the matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 + \frac{s_2 \epsilon_2}{\lambda} & \frac{1-s_2}{\lambda} \\ 1 - \frac{s_2 \epsilon_2}{\lambda} & -\frac{1-s_2}{\lambda} \end{pmatrix},$$

we solve the systems $\boldsymbol{A}(w_{1,1}, w_{2,1})^{\mathsf{T}} = (0, 2-\theta)^{\mathsf{T}}$, $\boldsymbol{A}(w_{1,0}, w_{2,0})^{\mathsf{T}} = (\epsilon_2/\lambda, -\epsilon_2/\lambda)^{\mathsf{T}}$ and $\boldsymbol{A}(w_{1,-1}, w_{2,-1})^{\mathsf{T}} = (\theta, 0)^{\mathsf{T}}$, yielding

$$w_{1,1} = \frac{2-\theta}{2}, \qquad w_{2,1} = -\frac{\lambda(1 + s_2\epsilon_2/\lambda)(2-\theta)}{2(1-s_2)}, \qquad w_{1,0} = 0, \qquad w_{2,0} = \frac{\epsilon_2}{1-s_2},$$

$$w_{1,-1} = \frac{\theta}{2}, \qquad w_{2,-1} = \frac{\lambda(1 - s_2\epsilon_2/\lambda)\theta}{2(1-s_2)}.$$

Unsurprisingly these coefficients are defined for $s_2 \neq 1$, since otherwise there is no initialization scheme to devise. The only way to fulfill the Proposition is to take $\theta = 1$, giving

$$w_{1,\pm 1} = \frac{1}{2}, \qquad w_{2,\pm 1} = \mp \frac{\lambda \pm s_2 \epsilon_2}{2(1-s_2)}, \qquad w_{2,0} = \frac{\epsilon_2}{1-s_2}.$$

Hints on the analysis at $O(\Delta x^2)$ for the $\mathrm{D}_1\mathrm{Q}_2$

We are left to consider

$$
\begin{aligned}
(\boldsymbol{\mathcal{E}}^k)^{(2)} &= \sum \{\text{perm. of } \boldsymbol{\mathcal{E}}^{(0)} \ (k-1 \text{ times}) \text{ and } \boldsymbol{\mathcal{E}}^{(2)} \ (\text{once})\} \\
&+ \sum \{\text{perm. of } \boldsymbol{\mathcal{E}}^{(0)} \ (k-2 \text{ times}) \text{ and } \boldsymbol{\mathcal{E}}^{(1)} \ (\text{twice})\} \\
&= \sum_{\ell=0}^{\ell=k-1} (\boldsymbol{\mathcal{E}}^{(0)})^{\ell} \boldsymbol{\mathcal{E}}^{(2)} (\boldsymbol{\mathcal{E}}^{(0)})^{k-1-\ell} \\
&+ \sum_{\ell=0}^{\ell=k-2} \sum_{p=0}^{p=k-2-\ell} (\boldsymbol{\mathcal{E}}^{(0)})^{\ell} \boldsymbol{\mathcal{E}}^{(1)} (\boldsymbol{\mathcal{E}}^{(0)})^{p} \boldsymbol{\mathcal{E}}^{(1)} (\boldsymbol{\mathcal{E}}^{(0)})^{k-2-\ell-p}.
\end{aligned}
$$

$$
\begin{aligned}
(\boldsymbol{\mathcal{E}}^k)^{(2)}_{11} = \Bigg(\frac{k}{2} &+ \sum_{\ell=0}^{\ell=k-2} \sum_{p=1}^{p=k-1-\ell} (1-s_2)^p \\
&+ \frac{\epsilon_2^2}{\lambda^2} \sum_{\ell=0}^{\ell=k-2} \sum_{p=0}^{p=k-2-\ell} \Big(s_2^2 + s_2(1-s_2)\pi_{k-2-\ell-p}(s_2) \\
&+ (1-s_2)\pi_p(s_2)\pi_{k-1-\ell-p}(s_2) \Big) \Bigg) \partial_{xx}.
\end{aligned}
$$

Hints on the analysis at $O(\Delta x^2)$ for the D_1Q_2

$$(\boldsymbol{\mathcal{E}}^k)_{12}^{(2)} = \frac{\epsilon_2}{\lambda^2} \sum_{\ell=0}^{k-2} \sum_{p=0}^{k-2-\ell} (1 - s_2)^{k-1-\ell-p} \pi_{p+1}(s_2) \partial_{xx}.$$

Analysis at $O(\Delta x^2)$: good forward centered scheme

Consider the **good forward centered** initialization. For $k \in \mathbb{N}^*$, the modified equation for the starting schemes are

$$\partial_t \phi(0,x) + \epsilon_2 \partial_x \phi(0,x) + O(\Delta x^2)$$
$$= \lambda \Delta x \underbrace{\left(\left(\frac{1}{2} + \sum_{\ell=1}^{k-1} \left(1 - \frac{\ell}{k}\right)(1-s_2)^{\ell} \right) \left(1 - \frac{\epsilon_2^2}{\lambda^2}\right) + \frac{1}{2k}\left(1 - 2\sum_{\ell=0}^{k-1}(1-s_2)^{\ell}\right)\right)}_{=D(k,s_2,\epsilon_2,\lambda)} \partial_{xx}\phi(0,x).$$

- **Asymptotic match** of the bulk scheme dissipation:

$$\lim_{k\to+\infty} D(k, s_2, \epsilon_2, \lambda) = \underbrace{\left(\frac{1}{s_2} - \frac{1}{2}\right)\left(1 - \frac{\epsilon_2^2}{\lambda^2}\right)}_{\text{diss. bulk scheme}}.$$

- **Behavior for** $s_2 = 2$

$$D(k, s_2, \epsilon_2 = 2, \lambda) = \begin{cases} 1/(2k), & \text{for } k \text{ even}, \\ -\epsilon_2^2/(2\lambda^2 k), & \text{for } k \text{ odd}, \end{cases}$$

Analysis at $O(\Delta x^2)$: Lax-Wendroff scheme

Consider the **Lax-Wendroff** initialization. For $k \in \mathbb{N}^*$, the modified equation for the starting schemes are

$$\partial_t \phi(0,x) + \epsilon_2 \partial_x \phi(0,x) + O(\Delta x^2)$$
$$= \lambda \Delta x \underbrace{\left(\frac{1}{2} + \sum_{\ell=1}^{k-1} \left(1 - \frac{\ell}{k}\right)(1-s_2)^{\ell} + \frac{1}{2k}\left(1 - 2\sum_{\ell=0}^{k-1}(1-s_2)^{\ell}\right)\right)}_{=D(k,s_2)} \left(1 - \frac{\epsilon_2^2}{\lambda^2}\right) \partial_{xx}\phi(0,x).$$

- **Asymptotic match** of the bulk scheme dissipation:

$$\lim_{k \to +\infty} D(k, s_2) = \underbrace{\left(\frac{1}{s_2} - \frac{1}{2}\right)}_{\text{diss. bulk scheme}}.$$

- **Behavior for** $s_2 = 2$

$$D(k, s_2 = 2) = \frac{1 + (-1)^k}{4k} = \begin{cases} 1/(2k), & \text{for } k \text{ even}, \\ 0, & \text{for } k \text{ odd}, \end{cases}$$

Analysis at $O(\Delta x^2)$: D_1Q_3

The modified equation of the bulk Finite Difference scheme reads

$$\partial_t \phi(t,x) + \epsilon_2 \partial_x \phi(t,x) - \lambda \Delta x \left(\frac{1}{s_2} - \frac{1}{2} \right) \left(\frac{2}{3} - \frac{\epsilon_2^2}{\lambda^2} + \frac{\epsilon_3}{3\lambda^2} \right) \partial_{xx} \phi(t,x) = O(\Delta x^2).$$

To have compatible numerical dissipation:

Factors controlling dissipation		Leverages to have compatible dissipation
$s_2 = 1$	$\epsilon_3 \geq -2\lambda^2 + 3\epsilon_2^2$	$s_3 = 1$, any w_3 $s_3 \neq 1$, $w_3 = \epsilon_3$
$s_2 \neq 1$	$\epsilon_3 > -2\lambda^2 + 3\epsilon_2^2$	$s_3 = 2 - s_2$, $w_3 = (2(-2\lambda^2 + 3\epsilon_2^2) - (2 - s_2)\epsilon_3)/s_2$
	$\epsilon_3 = -2\lambda^2 + 3\epsilon_2^2$	$s_3 = 1$, any w_3 $s_3 \neq 1$, $w_3 = \epsilon_3$

Numerical experiences unobservable subspaces

Consider the D_1Q_2. Two sets of initial data

$$\text{(a)} \qquad m_1(0,\cdot) = 0, \qquad m_2(0, j\Delta x) = (1 + 3(-1)^j)/8,$$

$$\text{(b)} \qquad m_1(0,\cdot) = 0, \qquad m_2(0, j\Delta x) = 0.1\exp(-1/(1-(4(j\Delta x - 0.5))^2)).$$

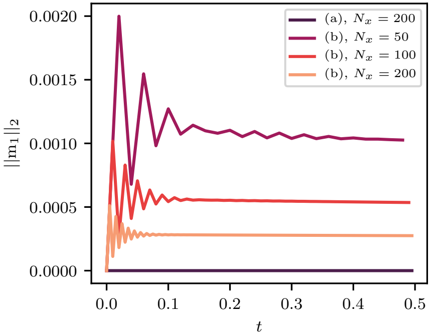


Figure: L^2 norm of the conserved moment as function of the time for the D_1Q_2 scheme choosing $\lambda = 1$, $\epsilon_2 = 0.5$ and $s_2 = 1.8$.

Numerical experiences unobservable subspaces

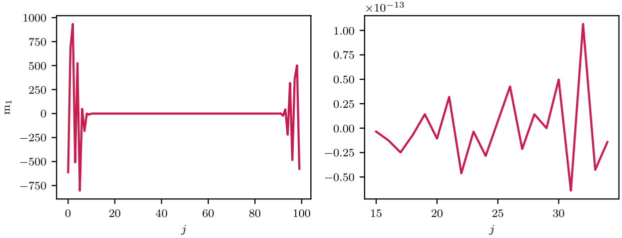
We now conside the $\mathrm{D}_1\mathrm{Q}_3$. We select

$$\mathrm{m}_1(0, \cdot) = 0, \qquad \mathrm{m}_2(0, j\Delta x) = j, \qquad \mathrm{m}_3(0, j\Delta x) = -3\lambda j^2,$$

which thus belongs to $\ker(\boldsymbol{\Omega})$ when $s_2 + s_3 = 2$. We discretize using periodic boundary conditions. These boundary conditions are incompatible with the data, but we shall observe the outcome way inside the computational domain.

Numerical experiences unobservable subspaces

$$s_2 = 1.8, \qquad s_3 = 2 - s_2$$



$$s_2 = 1.8, \qquad s_3 = 1.2$$