LBM method as kinetic relaxation schemes. High-order methods and low-mach viscous problems

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Workshop LBM, CMAP, May 2018

Thanks to: M. Boileau², F. Drui², M. Mehrenberger², L. Thanhuser³, C. Klingenberg ³

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Outline

Physical and mathematical context

LBM as implicit relaxation method

High-order CFL free schemes and unstructured meshes

Kinetic representation for multi-scale problems

Kinetic relaxation method for diffusion problems





Physical and mathematical context



Applications considered

- Steady or quasi-steady flows (long time limit).
- Multi-scale problem: capture the slow scale and filter the fast one (ex: low mach).
 - Fusion DT: At sufficiently high energies, deuterium and tritium (plasmas) can fuse to Helium. Free energy is released.
- Tokamak: toroïdal chamber where the plasma is confined using magnetic fields.
- Difficulty: plasma instabilities. Important topic for ITER.



Simulation of MHD instabilities

Simulation: slow flow around plasmas equilibrium (in green):



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Implicit method and general grids

Classical solution

- Explicit scheme: CFL given by the high frequency discretized of the waves.
- **Solution**: implicit scheme to filter the frequencies not considered.
- Solution for implicit schemes:
 - □ Direct solver. CPU cost and consumption memory too large in 3D.
 - □ Iterative solver. Problem of conditioning.

Problem of conditioning

- Multi-scale PDE (low Mach regime) ==> huge ratio between discrete eigenvalues.
- High order scheme for transport: small/high frequencies and anisotropy ==> huge ratio between discrete eigenvalues.
- Storage the matrix and perhaps the preconditioning: large memory consumption.

Mesh and geometry

- **Geometry**: toroidal geometry. Poloidal section: circle or D-shape.
- Meshes: curved meshes, unstructured meshes, Multi-Patch + mapping.

Current work

LBM-type algorithm: CFL free and matrix-free on complex geometries.



LBM as implicit relaxation method



LBM

- We consider the following system $\partial_t U + \partial_x F(U) = 0$.
- We consider the new variable Mf = U and the velocities set $V = [v_1, ..., v_n]$.

Time loop

- At the time t^n , we have f^n .
- We apply the transport step:

$$f_i^*(x) = f_i^n(x - v_i \Delta t) \quad \forall i \le N$$

Relaxation step:

$$\boldsymbol{f}^{n+1} = \boldsymbol{f}^* + \Omega(\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^*)$$

with $\Omega = M^{-1}SM$ with S a diagonal matrix with $s_k \in \{0, 2\}$

To write the first substep we choose $v_i = k\lambda \frac{\Delta t}{\Delta x}$ with k an integer (in general: 0, 1, 2). Consistency :

 $\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \Delta t \partial_x (\boldsymbol{A}(\boldsymbol{U}, \lambda, S) \partial_x \boldsymbol{U}) + \Delta t^2 \partial_x \boldsymbol{B}(\boldsymbol{U}, \partial_x \boldsymbol{U}, \partial_{xx} \boldsymbol{U}, \lambda, S)$

We can increase the order with the good parameters.

- Advantages: very very simple algorithm.
- Drawbacks: complicate to manage with large Δt and complex grids.



Rewritting: transport step

Transport step:

$$f_i^*(x) = f_i^n(x - v_i \Delta t) \quad \forall i \leq N$$

- We solve $\partial_t f_i + v_i \partial_x f_i = 0$ with the characteristic method.
- Possible since we choose the velocity $v_i = k\lambda \frac{\Delta t}{\Delta x}$.
- Avoiding this constrains, $x v_i \Delta t$ in not a mesh node but inside a cell. Natural solution: Backward or Forward Semi-Lagrangian method.

SL methods

- BSL: we compute the origin of the characteristic curve and interpolate (high-order) the value obtained.
- **FSL**: we follow of the characteristic curve and project (high-order) the value obtained.
- B-splines, Lagrange interpolation. Nodal or average projection. etc
- The transport step can be rewrite as advection equation:

$$\partial_t f_i + v_i \partial_x f_i = 0, \quad \forall i \leq N$$

solved with BSL (or FSL) with exact interpolation (projection).

Natural extension

Relax assumption on the velocities and use full BSL solver for advection (or other solver like FV or DG).



Relaxation step:

$$\boldsymbol{f}^{n+1} = \boldsymbol{f}^* + \Omega(\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^*)$$

- We recognize an operator closed to BGK operator.
- BGK operator:

$$\partial_t \boldsymbol{f} = rac{R}{arepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f})$$

Dicretizating the previous scheme with a θ scheme you obtain:

$$\frac{\boldsymbol{f}^{n+1}-\boldsymbol{f}^n}{\Delta t} = \frac{\theta R}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}^{n+1})-\boldsymbol{f}^{n+1}) + \frac{(1-\theta)R}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}^n)-\boldsymbol{f}^n)$$

- The equilibrium is construct such that $U^{n+1} = U^n$.
- Consequently

$$\frac{\boldsymbol{f}^{n+1}-\boldsymbol{f}^n}{\Delta t}=\frac{\theta R}{\varepsilon}(\boldsymbol{f}^{eq}(\boldsymbol{U}^n)-\boldsymbol{f}^{n+1})+\frac{(1-\theta)R}{\varepsilon}(\boldsymbol{f}^{eq}(\boldsymbol{U}^n)-\boldsymbol{f}^n)$$

Conclusion

• The relaxation can be write as a θ -scheme for a generalized BGK operator.

Remark: $\Omega = I_D$ is equivalent to $\varepsilon = 0$, $R = I_d$ and $\theta = 1$ (first order scheme). $\Omega = 2I_D$ is equivalent to $\varepsilon = 0$, $R = I_d$ and $\theta = 0.5$ (second order scheme).

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$$\left(I_d + \frac{\theta \Delta tR}{\varepsilon}\right) \boldsymbol{f}^{n+1} = \left(I_d - \frac{(1-\theta)\Delta tR}{\varepsilon}\right) \boldsymbol{f}^n + \frac{\Delta R}{\varepsilon} \boldsymbol{f}^{eq}(\boldsymbol{U}^n)$$

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Consequently

$$\boldsymbol{f}^{n+1} = \boldsymbol{f}^n + \underbrace{\left(\boldsymbol{I}_d + \frac{\theta \Delta tR}{\varepsilon}\right)^{-1} \frac{\Delta R}{\varepsilon}}_{\Omega} (\boldsymbol{f}^{eq}(\boldsymbol{U}^n) - \boldsymbol{f}^n)$$

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Rewritting: algorithm

On one time step, the first step (T) is a discretization of

$$\partial_t \boldsymbol{f} + \Lambda \partial_x \boldsymbol{f} = 0$$

The second step (C) is a discretization of

$$\partial_t \boldsymbol{f} = rac{R}{arepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f})$$

The algorithm can be view as a first order Lie splitting scheme in time:

$$\boldsymbol{f}^n = [T(\Delta t) \circ (\Delta t)]^n \boldsymbol{f}^0$$

Natural extension: Second order strang splitting scheme in time:

$$f^n = \left[T\left(\frac{1}{2}\Delta t\right)\circ(\Delta t)\circ T\left(\frac{1}{2}\Delta t\right)\right]^n f^0.$$

However T (¹/₂Δt) ο T (¹/₂Δt) = T(Δt).
 So the second order splitting is given by

$$f^n = T\left(\frac{1}{2}\Delta t\right) \circ [T(\Delta t) \circ (\Delta t)]^n \circ T\left(\frac{1}{2}\Delta t\right) f^0$$

Conclusion

The algorithm can be view as a first order splitting or a second order splitting if we add a beginning and final transport step.



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Rewritting: advantages and drawbacks

Conclusion

A LBM method can be view the discretization of the model

$$\partial_t \boldsymbol{f} + \Lambda \partial_x \boldsymbol{f} = \frac{R}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f})$$

which gives at the limit

$$\partial_t oldsymbol{U} + \partial_x oldsymbol{F}(oldsymbol{U}) = O(arepsilon)$$

- obtained with
 - □ A time Lie splitting scheme,
 - \Box A θ -scheme for the relaxation step (unconditionnaly stable)==> AP scheme.
 - □ A BSL scheme for the transport with exact interpolation (choice of velocities).
- Idea: use this other formulation to use different schemes in space and time.
- To treat complex geometries and large time steps. We propose
 - □ Use a high order BSL scheme (without exact interpolation) or implicit DG schemes.
 - □ Use another time scheme for relaxation (not studied).
 - $\hfill\square$ Increase the time order of the full algorithm.
- General model: $[D1Q2]^n$. One D1Q2 by equation (B. Graille, S. Jin):

$$\begin{cases} \partial_t \mathbf{f}_+ + \lambda \partial_x \mathbf{f}_+ = \frac{1}{\varepsilon} (\mathbf{f}_+^{eq} - \mathbf{f}_+) \\ \partial_t \mathbf{f}_- - \lambda \partial_x \mathbf{f}_- = \frac{1}{\varepsilon} (\mathbf{f}_-^{eq} - \mathbf{f}_-) \end{cases}$$

with
$$m{f}^{eq}_{\pm}=rac{1}{2}m{U}\pmrac{m{F}(m{U})}{2\lambda}$$



High-order CFL free schemes and unstructured meshes





Inia

Consistency

Consistency space

- **Exact transport**: the choice of the velocities link time and space discretization.
- Semi- Lagrangian: Interpolation 2q + 1 gives a consistency error $O(\frac{\hbar^{2d+2}}{\Delta t})$.

Consistency in time

We define the two operators for each step :

$$T_{\Delta t}: e^{\Delta t \wedge \partial_x} \boldsymbol{f}^{n+1} = \boldsymbol{f}^n$$

$$R_{\Delta t}: \boldsymbol{f}^{n+1} + \theta \frac{\Delta t}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^{n+1}) = \boldsymbol{f}^n - (1-\theta) \frac{\Delta t}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^n)$$

Final scheme: $T_{\Delta t} \circ R_{\Delta t}$ is consistent with

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \left(\frac{(2-\omega)\Delta t}{2\omega}\right) \partial_x \left(D(\boldsymbol{U})\partial_x \boldsymbol{U}\right) + O(\Delta t^2)$$

• with
$$\omega = \frac{\Delta t}{\varepsilon + \theta \Delta t}$$
 and $D(\boldsymbol{U}) = (P \Lambda^2 \partial_{\boldsymbol{U}} \boldsymbol{f}^{eq} - A(\boldsymbol{U})^2).$

Drawback

For $[D1Q2]^2$ scheme we have a large error: $D(U) = (\lambda^2 I_d - A(U)^2)$



High-Order time schemes

Second-order scheme

- □ Scheme for transport step $T(\Delta t)$: Crank Nicolson or exact time scheme.
- Classical full second order scheme:

$$\Psi(\Delta t) = T\left(\frac{\Delta t}{2}\right) \circ R(\Delta t) \circ T\left(\frac{\Delta t}{2}\right).$$

□ Numerical test: first and second order splitting: converge at second order.

- □ Second order: probably only for the macroscopic variables.
- AP full second order scheme:

$$\Psi_{ap}(\Delta t) = T\left(\frac{\Delta t}{4}\right) \circ R\left(\frac{\Delta t}{2}\right) \circ T\left(\frac{\Delta t}{2}\right) \circ R\left(\frac{\Delta t}{2}\right) \circ T\left(\frac{\Delta t}{4}\right).$$

 \Box Ψ and Ψ_{ap} symmetric in time. $\Psi_{ap}(0) = I_d$.

High order scheme

Using composition method

$$M_{p}(\Delta t) = \Psi_{ap}(\gamma_{1}\Delta t) \circ \Psi_{ap}(\gamma_{2}\Delta t).... \circ \Psi_{ap}(\gamma_{s}\Delta t)$$

□ with $\gamma_i \in [-1, 1]$, we obtain a *p*-order schemes.

- Susuki scheme : s = 5, p = 4. Kahan-Li scheme: s = 9, p = 6.
- ^{\Box} Splitting non AP for $\varepsilon = 0$ converge with high-order for macroscopic variables.

Space discretization

Semi Lagrangian methods

- Forward or Backward methods. Mass or nodes interpolation/projection.
- Advantages:
 - $\hfill\square$ Possible on unstructured meshes. High order in space.
 - □ Exact in time and Matrix-free.
- Drawbacks:
 - No dissipation and difficult on very unstructured grids.

Implicit FV- DG methods

- Implicit Crank Nicolson scheme + FV DG scheme
- Advantages:
 - $\hfill\square$ Very general meshes. High order in space. Dissipation to stabilize.
 - \Box Upwind fluxes ==> triangular block matrices.
- Drawbacks:
 - $\hfill\square$ Second order in time: numerical time dispersion.
- Current choice 1D: SL-scheme.
- Current choice in 2D-3D: DG schemes.
 - Block triangular matrix solved avoiding storage.
 - □ Solve the problem in the topological order given by connectivity graph.





Burgers: convergence results

Model: Burgers equation

$$\partial_t \rho + \partial_x \left(\frac{\rho^2}{2}\right) = 0$$

- Spatial discretization: SL-scheme, 2000 cells, degree 11.
- Test: $\rho(t = 0, x) = sin(2\pi x)$. $T_f = 0.14$ (before the shock) and no viscosity.
- Scheme: splitting schemes and Suzuki composition + splitting.

	SPL 1, $\theta = 1$		SPL 1, $\theta = 0.5$		SPL 2, $\theta = 0.5$		Suzuki	
Δt	Error	order	Error	order	Error	order	Error	order
0.005	$2.6E^{-2}$	-	$1.3E^{-3}$	-	$7.6E^{-4}$	-	$4.0E^{-4}$	-
0.0025	$1.4E^{-2}$	0.91	$3.4E^{-4}$	1.90	$1.9E^{-4}$	2.0	$3.3E^{-5}$	3.61
0.00125	$7.1E^{-3}$	0.93	$8.7E^{-5}$	1.96	$4.7E^{-5}$	2.0	$2.4E^{-6}$	3.77
0.000625	$3.7E^{-3}$	0.95	$2.2E^{-5}$	1.99	$1.2E^{-5}$	2.0	$1.6E^{-7}$	3.89

- Scheme: second order splitting scheme.
- Same test after the shock:



1D isothermal Euler : Convergence

Model: isothermal Euler equation

$$\left(\begin{array}{c} \partial_t \rho + \partial_x (\rho u) = 0 \\ \partial_t \rho u + \partial_x (\rho u^2 + c^2 \rho) = 0 \end{array} \right.$$

- **Lattice**: $(D1 Q2)^n$ Lattice scheme.
- For the transport (and relaxations step) we use 6-order DG scheme in space.
- **Time step**: $\Delta t = \beta \frac{\Delta x}{\lambda}$ with λ the lattice velocity. $\beta = 1$ explicit time step.
- First test: acoustic wave with $\beta = 50$ and $T_f = 0.4$, Second test: smooth contact wave with $\beta = 100$ and $T_f = 20$.



Figure: convergence rates for the first test (left) and for the second test (right).

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- Model : compressible ideal MHD.
- **Kinetic model** : $(D2 Q4)^n$. Symmetric Lattice.
- Transport scheme : 2nd order Implicit DG scheme. 4th order ins space. CFL around 20.
- Test case : advection of the vortex (steady state without drift).
- Parameters : $\rho = 1.0$, $p_0 = 1$, $u_0 = b_0 = 0.5$, $\mathbf{u}_{drift} = [1, 1]^t$, $h(r) = exp[(1 r^2)/2]$





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E. Franck

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Velocity



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- Parameters : $\rho = 1.0$, $p_0 = 1$, $u_0 = b_0 = 0.5$, $\mathbf{u}_{drift} = [1, 1]^t$, $h(r) = exp[(1 r^2)/2]$



Magnetic field



- Model : compressible ideal MHD.
- Kinetic model : (D2 Q4)ⁿ. Symmetric Lattice.
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Magnetic field

Velocity

Numerical results: 2D-3D fluid models

- Model : liquid-gas Euler model with gravity.
- Kinetic model : $(D2 Q4)^n$. Symmetric Lattice.
- **Transport scheme** : 2 order Implicit DG scheme. 3th order in space. CFL around 6.
- **Test case** : Rayleigh-Taylor instability.

2D case in annulus

3D case in cylinder





Figure: Plot of the mass fraction of gas

Figure: Plot of the mass fraction of gas



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2D case in annulus

2D cut of the 3D case





Figure: Plot of the mass fraction of gas

Figure: Plot of the mass fraction of gas



Limitation

High-order extension allows to correct the main default of relaxation: large error.

In two situations the High-order extension is not sufficient:

- □ For discontinuous solutions like shocks.
- For strongly multi-scale problem like low-Mach problem.
- Euler equation: Sod problem.
- Second order time scheme + SL scheme:



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Left: density $\Delta t = 1.0^{-4}$. Right: density $\Delta t = 4.0^{-4}$

Conclusion: shock and high order time scheme needs limiting methods.



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 - □ For strongly multi-scale problem like low-Mach problem.

Euler equation: smooth contact (u =cts, p=cts).
 First/Second order time scheme + SL scheme. T_f = ²/_M and 100 time step.



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• Order 1 Left: M = 0.1. Right: M = 0.01

• **Conclusion**: First order method too much dissipative for low Mach flow (dissipation with acoustic coefficient).



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• Order 1 Left: M = 0.1. Right: M = 0.01

Conclusion: Second order method too much dispersive for low Mach flow (dispersion with acoustic coefficient).



Kinetic representation for multi-scale problems





Inia

"Physic" kinetic representations

Kinetic model mimics the moment model of Boltzmann equation. Euler isothermal

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0\\ \partial_t \rho u + \partial_x (\rho u^2 + c^2 \rho) = 0 \end{cases}$$

D1Q3 model: three velocities $\{-\lambda, 0, \lambda\}$. Equilibrium: quadrature of Maxwellian.

$$\rho = f_{-} + f_{0} + f_{+}, \quad q = \rho u = -\lambda * f_{-} + 0 * f_{0} + \lambda * f_{+}, \quad f_{eq} = \begin{pmatrix} \frac{1}{2}(\rho u(u - \lambda) + c^{2}\rho) \\ \rho(\lambda^{2} - u^{2} - c^{2}) \\ \frac{1}{2}(\rho u(u + \lambda) + c^{2}\rho) \end{pmatrix}$$

- Limit model : $\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0\\ \partial_t \rho u + \partial_x (\rho u^2 + c^2 \rho) = \varepsilon \left(\partial_{xx} u + u^3 \partial_{xx} \rho \right) \end{cases}$
- Good point: no diffusion on ρ equation. Bad point: stable only for low mach. No natural extension for more complex pde.

Vectorial kinetic representations

- Vectorial kinetic model (B. Graille 14): $[D1Q2]^2$ one relaxation model $\{-\lambda, \lambda\}$.
- **Good point**: stable on sub-characteristic condition $\lambda > \lambda_{max}$.
- Bad point: Wave structure approximated by transport at maximal velocity. The idea of D1Q2 equivalent to Rusanov scheme idea. Very bad accuracy for equilibrium or multi-scale problems (low mach).



Generic vectorial D1Q3

Idea

- Keep the vectorial structure: more stable since we can diffuse on all the variables.
- Add a central velocity (equal or close to zero) to capture the slow dynamics.
- Consistency condition:

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$$\begin{cases} f_{-}^{k} + f_{0}^{k} + f_{+}^{k} = U^{k}, & \forall k \in \{1..N_{c}\} \\ \lambda_{-} f_{-}^{k} + \lambda_{0} f_{0}^{k} + \lambda_{+} f_{+}^{k} = F^{k}(\boldsymbol{U}), & \forall k \in \{1..N_{c}\} \end{cases}$$
$$f_{-}^{k} + f_{0}^{k} + f_{+}^{k} = U^{k}, & \forall k \in \{1..N_{c}\} \end{cases}$$

$$\begin{cases} \lambda_{-} + \lambda_{0} + \lambda_{+} \\ (\lambda_{-} - \lambda_{0})f_{-}^{k} + (\lambda_{+} - \lambda_{0})f_{+}^{k} = \mathcal{F}^{k}(\boldsymbol{U}) - \lambda_{0}f_{0}^{k}, \quad \forall k \in \{1..N_{c}\} \end{cases}$$

We assume a decomposition of the flux (Bouchut 03)

$$F^{k}(\boldsymbol{U}) = F_{0}^{k,-}(\boldsymbol{U}) + F_{0}^{k,+}(\boldsymbol{U}) + \lambda_{0}I_{d}$$

We obtain the following equation for the equilibrium

$$\left\{ \begin{array}{l} f_{-}^{k} + f_{0}^{k} + f_{+}^{k} = U^{k}, \quad \forall k \in \{1..N_{c}\} \\ (\lambda_{-} - \lambda_{0})f_{-}^{k} + (\lambda_{+} - \lambda_{0})f_{+}^{k} = F_{0}^{k,-}(\boldsymbol{U}) + F_{0}^{k,+}(\boldsymbol{U}), \quad \forall k \in \{1..N_{c}\} \end{array} \right.$$

By analogy of the kinetic theory and kinetic flux splitting scheme we propose the following decomposition $\sum_{v>0} vf^k = F_0^{k,+}(U)$ and $\sum_{v<0} vf^k = F_0^{k,-}(U)$.



Generic vectorial D1Q3

Idea

- Keep the vectorial structure: more stable since we can diffuse on all the variables.
- Add a central velocity (equal or close to zero) to capture the slow dynamics.

The lattice $[D1Q3]^N$ is defined by the velocity set $V = [\lambda_-, \lambda_0, \lambda_+]$ and

$$\left\{ egin{array}{l} oldsymbol{f}_{-}^{eq}(oldsymbol{U}) = -rac{1}{(\lambda_0 - \lambda_-)}oldsymbol{F}_0^-(oldsymbol{U}) \ oldsymbol{f}_0^{eq}(oldsymbol{U}) = \left(oldsymbol{U} - \left(rac{oldsymbol{F}_0^+(oldsymbol{U})}{(\lambda_+ - \lambda_0)} - rac{oldsymbol{F}_0^-(oldsymbol{U})}{(\lambda_0 - \lambda_-)}
ight)
ight) \ oldsymbol{f}_{+}^{eq}(oldsymbol{U}) = rac{1}{(\lambda_+ - \lambda_0)}oldsymbol{F}_0^+(oldsymbol{U}) \end{array}$$

Stability

- Entropy stability: F_0^+ and F_0^- is an entropy decomposition of the flux $+ \partial F_0^+$, $-\partial F_0^$ and $1 - \frac{\partial F_0^+ - \partial F_0^-}{\lambda}$ are positive.
- Optimal condition for L^2 stability in linear case not clear.



D1Q3 for scalar case

First choice: D1Q3 Rusanov ($\lambda_0 = 0$)

$$F_0^-(\rho) = -\lambda_- \frac{(F(\rho) - \lambda_+ \rho)}{\lambda_+ - \lambda_-}, \quad F_0^+(\rho) = \lambda_+ \frac{(F(\rho) - \lambda_- \rho)}{\lambda_+ - \lambda_-}$$

Consistency (for $\lambda_{-} = -\lambda_{+}$): $\partial_{t}\rho + \partial_{x}F(\rho) = \sigma\Delta t\partial_{x}\left(\lambda^{2} - |\partial F(\rho)|^{2}\right)\partial_{x}\rho + O(\Delta t^{2})$

Second choice: D1Q3 Upwind

$$F_0^-(\rho) = \chi_{\{\partial F(\rho) < \lambda_0\}} \left(F(\rho) - \lambda_0 \rho \right) \quad F_0^+(\rho) = \chi_{\{\partial F(\rho) > \lambda_0\}} \left(F(\rho) - \lambda_0 \rho \right)$$

• with χ the indicatrice function.

Consistency: $\partial_t \rho + \partial_x F(\rho) = \sigma \Delta t \partial_x \left(\lambda \mid \partial F(\rho) \mid - \mid \partial F(\rho) \mid^2 \right) \partial_x \rho + O(\Delta t^2)$

Third choice: D1Q3 Lax-Wendroff ($\lambda_0 = 0$)

$$F_0^-(\rho) = \frac{1}{2} \left(F(\rho) + \frac{\alpha}{\lambda} \int^{\rho} (\partial F(u))^2 \right) \quad F_0^+(\rho) = \frac{1}{2} \left(F(\rho) + \frac{\alpha}{\lambda} \int^{\rho} (\partial F(u))^2 \right)$$

- with $\lambda_0 = 0$ and $\lambda_- = -\lambda_+$ and $\alpha \ge 1$.
- Consistency: $\partial_t \rho + \partial_x F(\rho) = \sigma \Delta t \partial_x \left((\alpha 1) | \partial F(\rho) |^2 \right) \partial_x \rho + O(\Delta t^2).$
- The last one is not entropy stable and does not satisfy the sufficient L² stability condition.



D1Q3 for Euler equation I

- **Euler equation**. Two regimes where the classical method is not optimal.
 - High-Mach regime: we use a negative and positive transport for purely positive or negative flows.
 - $\hfill\square$ Low-Mach regime: λ is closed to the sound speed so we have viscosity too large for density equation for example.
- First possibility: use classical flux vector splitting for Euler equation.
 - □ Stegel-Warming: $F^{\pm} = A^{\pm}(U)U$ with A^{\pm} positive/negative part of the Jacobian.
 - □ Van-Leer:

$$\boldsymbol{F}^{\pm}(\boldsymbol{U}) = \pm \frac{1}{4} \rho c (M \pm 1)^2 \begin{pmatrix} 1 \\ \frac{(\gamma-1)u \pm 2c}{\gamma} \\ \frac{((\gamma-1)u \pm 2c)^2}{2(\gamma+1)(\gamma-1)} \end{pmatrix}$$

- **AUSM method**: convection of ρ , q and H as Van-Leer and separated reconstruction of the pressure.
- □ Approximate Osher-Solomon: $F^{\pm}(U) = F(U) \pm |F(U)|$

$$\mid \boldsymbol{F}(\boldsymbol{U}) \mid \approx \int_{\boldsymbol{U}_0}^{\boldsymbol{U}} \mid A(\boldsymbol{U}) \mid = \int_0^1 \mid A(\boldsymbol{U}_0 + t(\boldsymbol{U} - \boldsymbol{U}_0)) \mid (\boldsymbol{U} - \boldsymbol{U}_0) dt$$

- Integral is approximated by a quadrature formula along the path (E. Toro , M Dumbser)
- □ Approximate of |A| using Halley approximation (M. J. Castro) and U_0 is the average flow.



D1Q3 for Euler equation II

Low Mach case:

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0 \\ \partial_t \rho u + \partial_x \left(\rho u^2 + \frac{p}{M} \right) = 0 \\ \partial_t E + \partial_x (Eu + pu) = 0 \end{cases}$$

We want to preserve as possible the limit:

$$p = cts, \quad u = cts, \quad \partial_t \rho + u \partial_x \rho = 0$$

Idea: Splitting of the flux (Zha-Bilgen, Toro-Vasquez):

$$\boldsymbol{F}(\boldsymbol{U}) = \begin{pmatrix} (\rho)\boldsymbol{u} \\ (\rho\boldsymbol{u})\boldsymbol{u} + \boldsymbol{p} \\ (\boldsymbol{E})\boldsymbol{u} + \boldsymbol{p}\boldsymbol{u} \end{pmatrix}$$

- Idea: Lax-Wendroff Flux splitting for convection and AUSM-type for the pressure term.
- Use only u, p and $\lambda \ (\approx c)$ to reconstruct pressure. Important to preserve the low mach limit.
- We obtain

$$\mathbf{F}^{\pm}(\mathbf{U}) = \frac{1}{2} \begin{pmatrix} (\rho u \pm \alpha \frac{u^2}{\lambda} \rho) + p \\ (\rho u^2 \pm \alpha \frac{u^2}{\lambda} q) + p(1 \pm \gamma \frac{u}{\lambda}) \\ (E u \pm \frac{u^2}{\lambda} E) + (p u \pm \alpha \frac{1}{\lambda} \gamma (u^2 + \lambda^2) p) \end{pmatrix}$$

Preserve contact.

The scheme is construct to have diffusion error on rho homogeneous $((\alpha - 1)u^2)$ (lax wendroff scheme).



Advection equation

Equation

$$\partial_t \rho + \partial_x (a(x)\rho) = 0$$

- with a(x) > 0 and $\partial_x a(x) > 0$. Dissipative equation.
- **Test case 1**: a(x) = x. 10000 cells. Order 17. $\theta = 1$ (first order).

	Rusanov		Upw	ind	Lax Wendroff	
	Error	Order	Error	Order	Error	Order
$\Delta t = 0.05$	$6.4E^{-2}$	-	$2.7E^{-2}$	-	$2.7E^{-2}$	-
$\Delta t = 0.025$	$3.8E^{-2}$	0.75	$1.2E^{-2}$	1.17	$5.7E^{-3}$	2.24
$\Delta t = 0.0125$	$1.9E^{-2}$	1.0	$4.2E^{-3}$	1.5	$5.5E^{-4}$	3.37
$\Delta t = 0.00625$	$7.9E^{-3}$	1.25	$1.3E^{-3}$	1.7	$5.3E^{-5}$	3.38

• Test case 2: $a(x) = 1 + 0.01(x - x_0)^2$. 10000 cells. Order 17. Second order time scheme.



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Left $\Delta t = 0.01$. Right $\Delta t = 0.1$. Reference (black), Rusanov (violet), Upwind (green), Lax-Wendroff $\alpha = 1$ (blue), Lax-Wendroff $\alpha = 2$ (Yellow).



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$$\partial_t \rho + \partial_x (a(x)\rho) = 0$$

with a(x) > 0 and $\partial_x a(x) > 0$. Dissipative equation.

Test case 1: a(x) = x. 10000 cells. Order 17. $\theta = 0.5$ (second order).

	Rusanov		Upw	ind	Lax Wendroff	
	Error	Order	Error	Order	Error	Order
$\Delta t = 0.05$	$3.8E^{-2}$	-	$1.2E^{-4}$	-	$1.2E^{-0}$	-
$\Delta t = 0.025$	$5.3E^{-3}$	2.84	$8.1E^{-6}$	3.8	$4.1E^{-1}$	1.55
$\Delta t = 0.0125$	$3.7E^{-4}$	3.84	$5.3E^{-7}$	3.84	$1.1E^{-4}$	11.5
$\Delta t = 0.00625$	$2.3E^{-5}$	3.88	$3.3E^{-8}$	4	$6.2E^{-6}$	4.15

Test case 2: $a(x) = 1 + 0.01(x - x_0)^2$. 10000 cells. Order 17. Second order time scheme.



Left $\Delta t = 0.01$. Right $\Delta t = 0.1$. Reference (black), Rusanov (violet), Upwind (green), Lax-Wendroff $\alpha = 2$ (Yellow) = 1 unstable.



Burgers

Model: Viscous Burgers equations

$$\partial_t \rho + \partial_x \left(\frac{\rho^2}{2}\right) = 0$$

Test case 1: $\rho(t = 0, x) = sin(2\pi x)$. 10000 cells. Order 17. First order time scheme.

	Rusanov		Upw	Upwind		Lax Wendroff $\alpha = 1$	
	Error	Order	Error	Order	Error	Order	
$\Delta t = 0.01$	$3.9E^{-2}$	-	$1.1E^{-2}$	-	$2.3E^{-3}$	-	
$\Delta t = 0.005$	$2.1E^{-2}$	0.89	$6.4E^{-3}$	0.78	$6.0E^{-4}$	1.94	
$\Delta t = 0.0025$	$1.1E^{-2}$	0.93	$3.5E^{-3}$	0.87	$1.5E^{-4}$	2.00	
$\Delta t = 0.00125$	$5.4E^{-3}$	1.03	$1.8E^{-3}$	0.96	$3.9E^{-5}$	1.95	

Shock wave. First order scheme in time.



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Left $\Delta t = 0.002$. Right $\Delta t = 0.01$. Reference (black), Rusanov (yellow), Upwind (violet), Lax-Wendroff (green), Lax-Wendroff $\alpha = 1.5$ (blue).



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	Rusanov		Upw	ind	Lax Wendroff $\alpha = 1$		
	Error	Order	Error	Order	Error	Order	
$\Delta t = 0.01$	$3.9E^{-2}$	-	$1.1E^{-2}$	-	$2.3E^{-3}$	-	
$\Delta t = 0.005$	$2.1E^{-2}$	0.89	$6.4E^{-3}$	0.78	$6.0E^{-4}$	1.94	
$\Delta t = 0.0025$	$1.1E^{-2}$	0.93	$3.5E^{-3}$	0.87	$1.5E^{-4}$	2.00	
$\Delta t = 0.00125$	$5.4E^{-3}$	1.03	$1.8E^{-3}$	0.96	$3.9E^{-5}$	1.95	

Rarefaction wave. First order scheme in time.



Left $\Delta t = 0.002$. Right $\Delta t = 0.01$. Reference (black), Rusanov (violet), Upwind (green), Lax-Wendroff $\alpha = 1$ (blue), Lax-Wendroff $\alpha = 2$ (Yellow).



1D Euler equations

Model: Euler equation

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0\\ \partial_t \rho u + \partial_x (\rho u^2 + p) = 0\\ \partial_t E + \partial_x (Eu + pu) = 0 \end{cases}$$

Test case: acoustic wave. $\rho = 1 + 0.1e^{-\frac{x^2}{\sigma}}$, u = 0 and $p = \rho$.

The domain is $\Omega = [-2, 2]$. 4000 cells and 11-order SL. $\theta = 1$ (relaxation).



Left $\Delta t = 0.002$. Right $\Delta t = 0.005$. Reference (black), Rusanov (yellow), Van-Leer (green), Osher (violet), AUSM (red).

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Conclusion: Osher and Van-Leer more accurate that Rusanov. Low-Mach less accurate for acoustic that the two other, but very accurate on the material wave.

1D Euler equations

Model: Euler equation

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

Test case: acoustic wave. $\rho = 1 + 0.1e^{-\frac{\chi^2}{\sigma}}$, u = 0 and $p = \rho$.

The domain is $\Omega = [-2, 2]$. 4000 cells and 11-order SL. $\theta = 0.666$ (relaxation).



Left $\Delta t = 0.002$. Right $\Delta t = 0.005$. Reference (black), Rusanov (yellow), Van-Leer (green), Osher (violet), AUSM (red).

39

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1D Euler equations

Model: Euler equation

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

Test case: acoustic wave. $\rho = 1 + 0.1e^{-\frac{x^2}{\sigma}}$, u = 0 and $p = \rho$.

The domain is $\Omega = [-2, 2]$. 4000 cells and 11-order SL. $\theta = 0.666$ (relaxation).



- Same test case for the low-mach scheme with $\omega = 1$. $\Delta t = 0.002$ (yellow), $\Delta t = 0.005$ (green), $\Delta t = 0.01$ (violet).
- Conclusion: Osher and Van-Leer more accurate that Rusanov. Low-Mach less accurate for acoustic that the two other, but very accurate on the material wave.



1D Euler equations II

- **Test case**: Smooth contact. We take p = 1 and u is also constant.
- **Final aim**: Where $T_f = O(\frac{1}{u})$ we want take $\Delta t = O(\frac{1}{u})$ and preserve the same error when *u* decrease.
- We choose $\Delta t = 0.02$ and $T_f = 2$. 4000 cells. We choose $\omega = 1$:

	Schemes	Rusanov	VL	Osher	LM
	$\rho(t,x)$	0.26	$1.0E^{-1}$	$8.4E^{-2}$	$1.0E^{-3}$
$u = 10^{-2}$	u(t, x)	0	$3.4E^{-3}$	$6.0E^{-7}$	0
	p(t, x)	0	$5.0E^{-4}$	$4.3E^{-8}$	0
	$\rho(t,x)$	0.26	$1.0E^{-1}$	$8.4E^{-2}$	$1.0E^{-5}$
$u = 10^{-4}$	u(t, x)	0	$3.4E^{-3}$	$6.0E^{-7}$	0
	p(t,x)	0	$5.0E^{-4}$	$4.3E^{-8}$	0
	$\rho(t,x)$	0.26	$1.0E^{-1}$	$4.8E^{-2}$	0.0
u = 0	u(t, x)	0	$3.4E^{-3}$	$6.0E^{-7}$	0
	p(t,x)	0	$5.0E^{-4}$	$4.3E^{-8}$	0

- **Drawback**: When the time step is too large we have dispersive effect.
- Possible explanation: the error would be homogeneous to

$$|
ho^n(x) -
ho(t,x)| \approx \left[O((lpha - 1)\Delta t u^2) + O(\Delta t^2 u \lambda^q)
ight] T_f.$$

- with λ closed to the sound speed.
- **Problem**: At the second order, we recover partially the problem since λ is closed to the sound speed.



1D Euler equations III

- **Possible solution**: decrease λ for the density equation.
- We propose two-scale kinetic model.
- We consider the following $[D1Q5]^3$ based on the following velocities:

$$\underbrace{V = [-\lambda_f, -\lambda_s, 0, \lambda_s, \lambda_f]}_{\text{slow scale}}$$

- The convective part associated at the slow scale. The acoustic part associated at the fast scale.
- Smooth contact: We take 200 time step and $\Delta t = \frac{0.001}{u}$:

Error	$u = 10^{-1}$	$u = 10^{-2}$	$u = 10^{-3}$	$u = 10^{-4}$
$\alpha = 1$	$2.5E^{-3}$	$2.5E^{-3}$	$2.5E^{-3}$	2.5 <i>E</i> -3
λ_s	2	0.2	0.02	0.002
λ_f	2	20	200	2000

Conclusion

Conclusion: the error <u>would be</u> homogeneous to

 $\mid \rho^n(x) - \rho(t,x) \mid \approx \left[O((\alpha - 1)\Delta t u^2) + O(\Delta t^2 u \lambda_s^q) \right] T_f.$

- with λ_s which can be taken as O(u).
- Drawback: For the stability it seems necessary to have

 $\lambda_s \lambda_f \geq C \max(u+c)$



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$\alpha = 1$	$2.5E^{-3}$	$2.5E^{-3}$	$2.5E^{-3}$	2.5 <i>E</i> -3
λ_s	2	0.2	0.02	0.002
λ_f	2	20	200	2000

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 $\mid \rho^n(x) - \rho(t,x) \mid \approx \left[O((\alpha - 1)\Delta t u^2) + O(\Delta t^2 u \lambda_s^q) \right] T_f.$

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- We consider the following $[D1Q5]^3$ based on the following velocities:

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- The convective part associated at the slow scale. The acoustic part associated at the fast scale.
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Error	$u = 10^{-1}$	$u = 10^{-2}$	$u = 10^{-3}$	$u = 10^{-4}$
$\alpha = 1$	$2.5E^{-3}$	$2.5E^{-3}$	$2.5E^{-3}$	2.5 <i>E</i> -3
λ_s	2	0.2	0.02	0.002
λ_f	2	20	200	2000

Conclusion

Conclusion: the error would be homogeneous to

 $\mid \rho^n(x) - \rho(t,x) \mid \approx \left[O((\alpha - 1)\Delta t u^2) + O(\Delta t^2 u \lambda_s^q) \right] T_f.$

- with λ_s which can be taken as O(u).
- Drawback: For the stability it seems necessary to have

 $\lambda_s \lambda_f \geq C \max(u+c)$



1D Euler equations IV

- Test case: Sod problem. 4000 cells, First order is space and time.
- Comparison of schemes:



- Reference (black), Rusanov (orange), Van-Leer (green), Osher (violet), Low-Mach with $\alpha = 1$ (red).
- Comparison of low-mach scheme for different values of α:



Kinetic relaxation method for Diffusion problem







Applications

Main parabolic problem

Coupling anisotropic diffusion + resistivity.

$$\partial_t T - \nabla \cdot ((\boldsymbol{B} \otimes \boldsymbol{B}) \nabla T + \varepsilon \nabla T) = 0$$

$$\partial_t \boldsymbol{B} - \eta \nabla \times (T^{-\frac{5}{2}} \nabla \times \boldsymbol{B}) = 0$$

$$\nabla \cdot \boldsymbol{B} = 0$$



The temperature T for the case $\eta = 0$ and B given by magnetic equilibrium.

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Kinetic model and scheme for diffusion I

- We solve the equation: $\partial_t \rho + \partial_x (u\rho) = D \partial_{xx} \rho$
- D1Q2 Kinetic system proposed (S. Jin, F. Bouchut):

$$\begin{cases} \partial_t f_- - \frac{\lambda}{\varepsilon} \partial_x f_- = \frac{1}{\varepsilon^2} (f_{eq}^- - f_-) \\ \partial_t f_+ + \frac{\lambda}{\varepsilon} \partial_x f_+ = \frac{1}{\varepsilon^2} (f_{eq}^+ - f_+) \end{cases}$$

• with $f_{eq}^{\pm} = \frac{\rho}{2} \pm \frac{\varepsilon(u\rho)}{2\lambda}$. The limit is given by:

 $\partial_t \rho + \partial_x(u\rho) = \partial_x((\lambda^2 - \varepsilon^2 \mid u \mid^2)\partial_x \rho) + \lambda^2 \varepsilon^2 \partial_x(\partial_{xx}(u\rho) + u\partial_{xx}\rho) - \lambda^2 \varepsilon^2 \partial_{xxxx}\rho$

• We introduce $\alpha > \mid u \mid$. Choosing $D = \lambda^2 - \varepsilon^2 \alpha^2$ we obtain

$$\partial_t \rho + \partial_x (u\rho) = \partial_x (D\partial_x \rho) + O(\varepsilon^2)$$

• We can choose $\varepsilon = \Delta t^{\gamma}$ and $\omega = 2$.

	$\gamma = \frac{1}{2}$		$\gamma =$	= 1	$\gamma = 2$	
	Error	order	Error	order	Error	order
$\Delta t = 0.04$	$1.87E^{-2}$	-	1.43	-	1.43	-
$\Delta t = 0.02$	$6.57E^{-3}$	1.50	0.2	0	0.23	0
$\Delta t = 0.01$	$1.85E^{-3}$	1.82	0.2	0	0.23	0
$\Delta t = 0.005$	$3.6E^{-4}$	2.36	0.2	0	0.23	0
$\Delta t = 0.0025$	$7.3E^{-5}$	2.30	0.2	0	0.23	0

The splitting scheme is not AP.



Kinetic model and scheme for diffusion II

Consistency analysis

- We consider $\partial_t \rho D \partial_{xx} \rho = 0$.
- We define the two operators for each step:

$$T_{\Delta t}: e^{\Delta t \frac{\Lambda}{\varepsilon} \partial_x} \boldsymbol{f}^{n+1} = \boldsymbol{f}^n$$

$$R_{\Delta t}: \boldsymbol{f}^{n+1} + \theta \frac{\Delta t}{\varepsilon^2} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^{n+1}) = \boldsymbol{f}^n - (1-\theta) \frac{\Delta t}{\varepsilon^2} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f}^n)$$

Final scheme: $T_{\Delta t} \circ R_{\Delta t}$ is consistent with

$$\partial_t
ho = \Delta t \partial_x \left(\left(rac{1-\omega}{\omega} + rac{1}{2}
ight) rac{\lambda^2}{arepsilon^2} \partial_x
ho
ight) + O(\Delta t^2)$$

Taking $D = \lambda^2$, $\theta = 0.5$ and $\varepsilon = \sqrt{\Delta t}$ we obtain the diffusion equation.

Question: what is the error term is this case ?

- First results (for these choices of parameters):
 - $\hfill\square$ Second order at the numerical level.
 - $\hfill\square$ At the minimum the first order theoretically.
- Problem: For a large time step, the scheme oscillate. How reduce this ?


Kinetic scheme for anisotropic/nonlinear diffusion

We consider the diffusion equation with ∂_tρ - ∂_x(A(ρ, x)∂_xρ) = 0 with D(ρ, x) > 0.
We consider a kinetic system

$$\partial_t \boldsymbol{f} + \frac{\Lambda}{\varepsilon} \partial_x \boldsymbol{f} = \frac{\boldsymbol{R}(x,\rho)}{\varepsilon^2} (\boldsymbol{f}^{eq} - \boldsymbol{f})$$

• We define $Pf = \sum_{i}^{N} f_{i} = \rho$ and $Qf = \frac{1}{\varepsilon} \sum_{i}^{N} v_{i} f_{i} = u$. • If

$$Pf_{eq} = \rho, \quad Qf^{eq} = 0, \quad \sum_{i}^{N} v_i^2 f_i^{eq} = \alpha \rho$$

and

$$P[R(x,\rho)(\mathbf{f}^{eq}-\mathbf{f})]=0, \quad Q[R(x,\rho)(\mathbf{f}^{eq}-\mathbf{f})]=-\alpha D^{-1}Q\mathbf{f}$$

• We obtain the equivalence with the following model (which gives at the limit the diffusion model)

$$\begin{cases} \partial_t \rho + \partial_x v = 0\\ \partial_t v + \frac{\alpha}{\varepsilon^2} \partial_x \rho = -\frac{\alpha}{D(x, \rho)\varepsilon^2} v \end{cases}$$

Example: D1Q2

$$\partial_t f_+ + \frac{1}{\varepsilon} \partial_x f_+ = \frac{1}{D(x,\rho)\varepsilon^2} (f_+^{eq} - f_+)$$
$$\partial_t f_- - \frac{1}{\varepsilon} \partial_x f_- = \frac{1}{D(x,\rho)\varepsilon^2} (f_-^{eq} - f_-)$$

with	f_{\pm}^{eq}	$=\frac{1}{2}\rho.$	
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Results for anisotropic/nonlinear diffusion

- We want solve the equation: $\partial_t \rho \partial_{xx} D(\rho) = 0$
- p = 1 (green) p = 2 (blue). Left $\Delta t = 0.001$. Right $\Delta t = 0.005$.



The second kinetic scheme allows to treat also nonlinear diffusion.

We want solve the equation: $\partial_t \rho = \partial_x (A(x)\partial_x \rho).$





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Results for anisotropic/nonlinear diffusion

- We want solve the equation: $\partial_t \rho \partial_{xx} D(\rho) = 0$
- p = 1 (green) p = 3 (blue). Left $\Delta t = 0.001$. Right $\Delta t = 0.005$.



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Conclusion

LBM as relaxation scheme

- **LBM** method can be rewritten as a specific scheme for BGK model.
- Using this, we propose high-order scheme with large time step algorithm (SL method).
- This algorithm is very competitive against implicit scheme (no matrices, no solvers).

D1Q3/5 schemes

- The $[D1Q3]^n$ schemes allows to reduce the error compared to $[D1Q2]^n$.
- Using the flux-vector splitting FV method we obtain new [D1Q3]ⁿ.
- The $[D1Q3]^n$ Osher scheme is generic for hyperbolic systems.
- We propose a new $[D1Q3]^n$ scheme for low-Mach. Problem: stability for $\omega \approx 1$. Modification ?

Kinetic scheme and LBM for diffusion

- These methods allows to treat also the diffusion equations using the splitting error.
- Poor/correct accuracy for anisotropic diffusion/heat equation. Need to be increased.

Future works

 2D/3D diffusion and low-Mach, MHD, BC, Dispersive waves, Limiting methods, Machine Learning.

