Long time behavior of finite volume schemes for some dissipative problems

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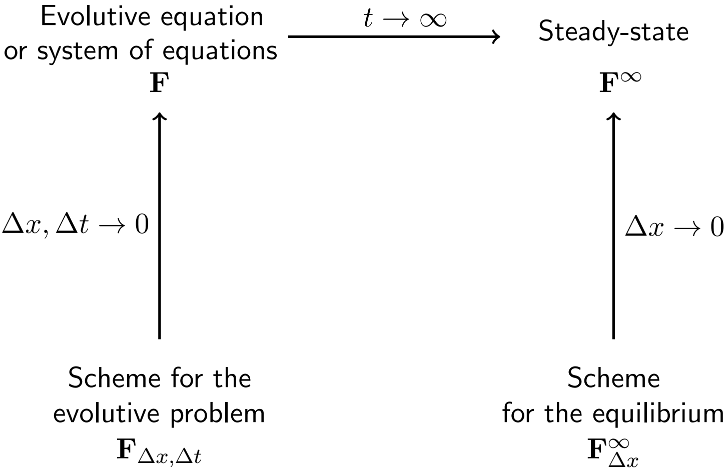
Séminaire Jacques-Louis Lions, 17/05/19

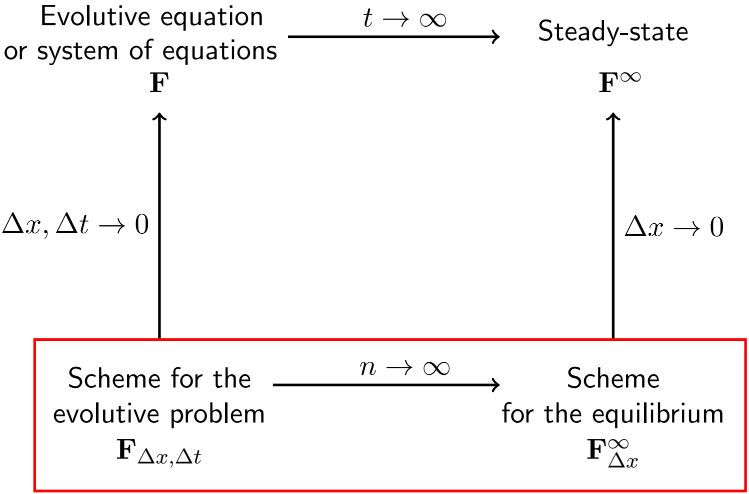
Joint work with M. Herda (Lille)

Outline of the talk

Overview


Evolutive equation
or system of equations
$\mathbf{F}$
$t \to \infty$
Steady-state
$\mathbf{F}^{\infty}$
$\Delta x, \Delta t \to 0$
$\Delta x \to 0$
Scheme for the
evolutive problem
$\mathbf{F}_{\Delta x, \Delta t}$
Scheme
for the equilibrium
$\mathbf{F}^{\infty}_{\Delta x}$

Overview



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Evolutive equation
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Steady-state
$\mathbf{F}^\infty$

$\Delta x, \Delta t \to 0$ ↑

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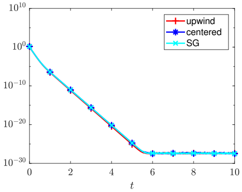


$+$ exponential convergence ?

Scheme for the
evolutive problem
$\mathbf{F}_{\Delta x, \Delta t}$

$n \to \infty$ →

Scheme
for the equilibrium
$\mathbf{F}^\infty_{\Delta x}$

Models under consideration

- Fokker-Planck equations

$$\partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f + \mathbf{U} f.$$

- Porous media equation

$$\partial_t f = \Delta f^m, \quad m \geq 1.$$

- Drift-diffusion-Poisson system of equations

$$\begin{cases} \partial_t N + \nabla \cdot \mathbf{J}_N = 0, & \mathbf{J}_N = -\nabla N + N \nabla \Psi, \\ \partial_t P + \nabla \cdot \mathbf{J}_P = 0, & \mathbf{J}_P = -\nabla P - P \nabla \Psi, \\ -\lambda^2 \Delta \Psi = P - N + C. \end{cases}$$

$+$ "general" Dirichlet-Neumann boundary conditions.

Focus on Fokker-Planck equations

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f + \mathbf{U} f, \text{ in } \Omega \times \mathbb{R}_+ \\ \mathbf{J} \cdot \mathbf{n} = 0 \text{ on } \Gamma^N \times \mathbb{R}_+ \\ f = f^D \text{ on } \Gamma^D \times \mathbb{R}_+ \\ f(\cdot, 0) = f_0 > 0. \end{cases}$$

Some references

- Carrillo, Toscani, '98
- Arnold, Markowich, Toscani, Unterreiter, '01
- Carrillo et al., '01
- Bodineau, Lebowitz, Mouhot, Villani, '14
- Gajewski, Gröger, '86, '89
- Jüngel, '95

Thermal equilibrium, when $\mathbf{U} = -\nabla\Psi$

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f - \nabla\Psi f, \text{ in } \Omega \times \mathbb{R}_+ \\ \mathbf{J} \cdot \mathbf{n} = 0 \text{ on } \Gamma^N \times \mathbb{R}_+ \\ f = f^D \text{ on } \Gamma^D \times \mathbb{R}_+ \\ f(\cdot, 0) = f_0 > 0. \end{cases}$$

$$f = \lambda e^{-\Psi} \Longrightarrow \mathbf{J} = 0$$

Existence of a thermal equilibrium $\quad f^\infty = \lambda e^{-\Psi}$

- if $\Gamma^D = \emptyset$, with $\lambda = \int_\Omega f_0 \,/\, \int_\Omega e^{-\Psi}$,
- if $\log f^D + \Psi^D = \alpha$, with $\lambda = e^\alpha$.

$$\Longrightarrow \quad \mathbf{J} = -f\nabla(\log f + \Psi) = -f\nabla \log \frac{f}{f^\infty}$$

Entropy-dissipation property

$$\partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -f \nabla \log \frac{f}{f^\infty}$$

Relative entropy

$$\Phi_1(x) = x \log x - x + 1$$
$$H_1(t) = \int_\Omega f^\infty \Phi_1(\frac{f}{f^\infty})$$

Dissipation of the entropy

$$\frac{d}{dt} H_1(t) = -D_1(t),$$

$$\text{with } D_1(t) = \int_\Omega f \left| \nabla \log \frac{f}{f^\infty} \right|^2 \geq 0$$

Exponential decay towards thermal equilibrium

No-flux boundary conditions

- conservation of mass : $\int_\Omega f = \int_\Omega f_0 = \int_\Omega f^\infty$
- $H_1(t) = \int_\Omega f \log(f/f^\infty)$
- $D_1(t) = \int_\Omega f |\nabla \log(f/f^\infty)|^2 = 4 \int_\Omega f^\infty \left|\nabla \sqrt{f/f^\infty}\right|^2$
- thanks to Logarithmic Sobolev inequality :

$$0 \leq H_1(t) \leq H_1(0) e^{-\kappa t}$$

- and with Csiszar-Kullback inequality :

$$\|f(t) - f^\infty\|_1^2 \leq 2 H_1(0) e^{-\kappa t}$$

Exponential decay towards thermal equilibrium

Dirichlet boundary conditions

- Upper and lower bounds on f and f^∞
- $H_1(t) = \int_\Omega \Phi_1(f) - \Phi_1(f^\infty) - (f - f^\infty)\Phi_1'(f^\infty)$

$$c\|f(t) - f^\infty\|_2^2 \le H_1(t) \le C\|f(t) - f^\infty\|_2^2$$

- $D_1(t) = \int_\Omega f\,|\nabla(\log f - \log f^\infty)|^2$
- with Poincaré inequality :

$$D_1(t) \ge \mathcal{C}\|f(t) - f^\infty\|_2^2$$

- Conclusion :

$$c\|f(t) - f^\infty\|_2^2 \le H_1(t) \le H_1(0)e^{-\kappa t}$$

General case

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f + \mathbf{U} f, \text{ in } \Omega \times \mathbb{R}_+ \\ f = f^D \text{ on } \Gamma^D \times \mathbb{R}_+ \text{ and } \mathbf{J} \cdot \mathbf{n} = 0 \text{ on } \Gamma^N \times \mathbb{R}_+ \end{cases}$$

Steady-state

$$\begin{cases} \nabla \cdot \mathbf{J}^\infty = 0, \quad \mathbf{J}^\infty = -\nabla f^\infty + \mathbf{U} f^\infty, \text{ in } \Omega \times \mathbb{R}_+ \\ f^\infty = f^D \text{ on } \Gamma^D \times \mathbb{R}_+ \text{ and } \mathbf{J}^\infty \cdot \mathbf{n} = 0 \text{ on } \Gamma^N \times \mathbb{R}_+. \end{cases}$$

$$f = f^\infty h \quad \Longrightarrow \quad \mathbf{J} = \mathbf{J}^\infty h - f^\infty \nabla h$$

Exponential decay towards the steady-state

- Entropy/dissipation, with $\Phi_2(x) = (x-1)^2$,

$$H_2(t) = \int_\Omega f^\infty \Phi_2(h) \text{ and } D_2(t) = \int_\Omega f^\infty \Phi_2''(h) |\nabla h|^2$$

- Poincaré inequality + bounds on f^∞

Adaptation to the discrete level ?

❑ Filbet, Herda, '17

Strategy

- Forward/backward Euler in time + finite volume in space
- Numerical scheme for the steady-state f^∞

  $\Longrightarrow$ approximation of the steady flux $\mathbf{J}^\infty$
- Approximation of the flux $\mathbf{J}$ as $\mathbf{J} = \mathbf{J}^\infty h - f^\infty \nabla h$

Main result

$$\|f_\delta(t^n) - f_\delta^\infty\|_1^2 \leq C e^{-\kappa t^n}$$

"Drawback"

Pre-computation of the steady-state needed for the definition of the scheme

Outline of the talk

Schemes for the evolutive drift-diffusion equation

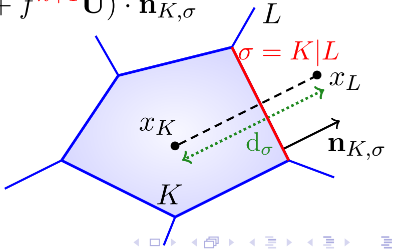
From the equation...

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f + \mathbf{U} f, \\ f(\cdot, 0) = f_0 \geq 0 \ \text{ + boundary conditions} \end{cases}$$

... to the scheme

$$\begin{cases} \mathsf{m}(K) \dfrac{f_K^{n+1} - f_K^n}{\Delta t} + \displaystyle\sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{K,\sigma}^{n+1} = 0 \\ \mathcal{F}_{K,\sigma}^{n+1} \approx \displaystyle\int_\sigma (-\nabla f^{n+1} + f^{n+1} \mathbf{U}) \cdot \mathbf{n}_{K,\sigma} \end{cases}$$

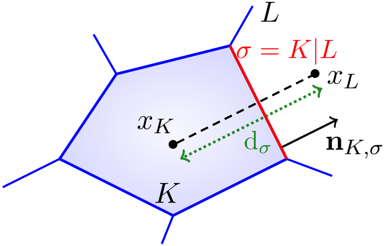
- $\mathcal{T}$: control volumes, $K \in \mathcal{T}$
- $\mathcal{E}$: edges, $\sigma \in \mathcal{E}$
- Δt : time step



Numerical fluxes

$$\mathcal{F}_{K,\sigma} \approx \int_\sigma (-\nabla f + f\mathbf{U}) \cdot \mathbf{n}_{K,\sigma}$$

$$U_{K,\sigma} \approx \frac{1}{\mathrm{m}(\sigma)} \int_\sigma \mathbf{U} \cdot \mathbf{n}_{K,\sigma}$$



Generic form

$$\mathcal{F}_{K,\sigma} = \tau_\sigma \Big(B(-U_{K,\sigma}\mathrm{d}_\sigma) f_K - B(U_{K,\sigma}\mathrm{d}_\sigma) f_L \Big), \ \tau_\sigma = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}$$

with $B(0) = 1, \ B(x) > 0$ and $B(x) - B(-x) = -x \ \forall x \in \mathbb{R}$

Classical examples

$$B_{up}(s) = 1 + s^-, \quad B_{ce}(s) = 1 - \frac{s}{2}$$

❑ C.-H., Droniou, ’05

Scharfetter-Gummel fluxes

Generic form

$$\mathcal{F}_{K,\sigma} = \tau_\sigma \Big(B(-U_{K,\sigma}\mathrm{d}_\sigma) f_K - B(U_{K,\sigma}\mathrm{d}_\sigma) f_L \Big), \ \tau_\sigma = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}$$

with $B(0) = 1, \ B(x) > 0$ and $B(x) - B(-x) = -x \ \forall x \in \mathbb{R}$

Preservation of a thermal equilibrium $\quad \mathbf{U} = -\nabla\Psi$

$$f = \lambda e^{-\Psi} \Longrightarrow -\nabla f - f\nabla\Psi = 0$$

At the discrete level $\quad U_{K,\sigma}\mathrm{d}_\sigma = (\Psi_K - \Psi_L)$

$$\left(f_K = \lambda e^{-\Psi_K} \Longrightarrow \mathcal{F}_{K,\sigma} = 0\right) \Longleftrightarrow B(x) = \frac{x}{e^x - 1}$$

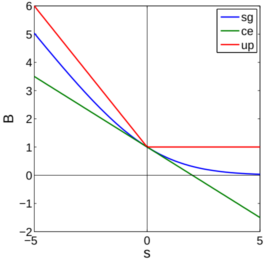
- Scharfetter, Gummel, 1969

Family of B-schemes for the Fokker-Planck equation

$$
\begin{cases}
\mathsf{m}(K)\dfrac{f_K^{n+1}-f_K^n}{\Delta t}+\displaystyle\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{K,\sigma}^{n+1}=0\\[2ex]
\mathcal{F}_{K,\sigma}^{n+1}=\begin{cases}
\tau_\sigma\Big(B(-U_{K,\sigma}\mathrm{d}_\sigma)f_K^{n+1}-B(U_{K,\sigma}\mathrm{d}_\sigma)f_L^{n+1}\Big), & \sigma=K|L,\\
\tau_\sigma\Big(B(-U_{K,\sigma}\mathrm{d}_\sigma)f_K^{n+1}-B(U_{K,\sigma}\mathrm{d}_\sigma)f_\sigma^{D}\Big), & \sigma\in\mathcal{E}_{ext}^D,\\
0, & \sigma\in\mathcal{E}_{ext}^N.
\end{cases}
\end{cases}
$$

Hypotheses on B

- $B(0)=1$,
- $B(x)>0 \quad \forall x\in\mathbb{R}$,
- $B(x)-B(-x)=-x$.



Additional hypotheses

- Admissibility and regularity of the mesh
- $\mathcal{E}_{ext}^D \neq \emptyset$
- $f_K^0 \geq 0 \quad \forall K \in \mathcal{T}$
- $\exists m^D$ and M^D such that

$$0 < m^D \leq f_\sigma^D \leq M^D \quad \forall \sigma \in \mathcal{E}_{ext}^D.$$

- $\exists V \geq 0$ such that

$$\max_{K \in \mathcal{T}} \max_{\sigma \in \mathcal{E}_K} |U_{K,\sigma}| \leq V.$$

Proposition

The scheme has a unique nonnegative solution $(f_K^n)_{K \in \mathcal{T}, n \geq 0}$.

Associated steady-state

$$\begin{cases} \displaystyle\sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{K,\sigma}^{\infty} = 0 \\ \mathcal{F}_{K,\sigma}^{\infty} = \begin{cases} \tau_\sigma \Big(B(-U_{K,\sigma} \mathrm{d}_\sigma) f_K^{\infty} - B(U_{K,\sigma} \mathrm{d}_\sigma) f_L^{\infty} \Big), & \sigma = K|L \\ \tau_\sigma \Big(B(-U_{K,\sigma} \mathrm{d}_\sigma) f_K^{\infty} - B(U_{K,\sigma} \mathrm{d}_\sigma) f_\sigma^{D} \Big), & \sigma \in \mathcal{E}_{ext}^{D} \\ 0, & \sigma \in \mathcal{E}_{ext}^{N} \end{cases} \end{cases}$$

Proposition

- Existence and uniqueness of a solution to the scheme $(f_K^{\infty})_{K \in \mathcal{T}}$.
- $\exists m^{\infty}, M^{\infty}$ such that

$$0 < m^{\infty} \leq f_K^{\infty} \leq M^{\infty} \quad \forall K \in \mathcal{T}.$$

Outline of the talk

How to rewrite the numerical fluxes ?

$$f = f^{\infty} h \Longrightarrow \mathbf{J} = \mathbf{J}^{\infty} h - f^{\infty} \nabla h$$

$$\begin{aligned}
\mathcal{F}_{K,\sigma} &= \tau_\sigma \Big(B(-U_{K,\sigma}\mathrm{d}_\sigma) f_K - B(U_{K,\sigma}\mathrm{d}_\sigma) f_L \Big), \\
&= \tau_\sigma \Big(B(-U_{K,\sigma}\mathrm{d}_\sigma) h_K f_K^{\infty} - B(U_{K,\sigma}\mathrm{d}_\sigma) h_L f_L^{\infty} \Big), \\
&= \mathcal{F}_{K,\sigma}^{\infty} h_K + \tau_\sigma B(U_{K,\sigma}\mathrm{d}_\sigma) f_L^{\infty} (h_K - h_L), \\
&= \mathcal{F}_{K,\sigma}^{\infty} h_L + \tau_\sigma B(-U_{K,\sigma}\mathrm{d}_\sigma) f_K^{\infty} (h_K - h_L)
\end{aligned}$$

Reformulation of the fluxes

$$\mathcal{F}_{K,\sigma} = \mathcal{F}_{K,\sigma}^{upw} + \tau_\sigma f_{B,\sigma}^{\infty} (h_K - h_L)$$

with $\mathcal{F}_{K,\sigma}^{upw} = (\mathcal{F}_{K,\sigma}^{\infty})^{+} h_K - (\mathcal{F}_{K,\sigma}^{\infty})^{-} h_L$

and $f_{B,\sigma}^{\infty} = \min\Big(B(-U_{K,\sigma}\mathrm{d}_\sigma) f_K^{\infty}, B(U_{K,\sigma}\mathrm{d}_\sigma) f_L^{\infty} \Big)$

Entropy-entropy dissipation property

$$\Phi'' > 0,\ \Phi(1) = 0,\ \Phi'(1) = 0$$

Discrete relative Φ-entropy

$$H_\Phi^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\Phi(h_K^n)f_K^\infty$$

Discrete dissipation

$$D_\Phi^n = \sum_{\sigma\in\mathcal{E}} \tau_\sigma f_{B,\sigma}^\infty (h_K^n - h_L^n)(\Phi'(h_K^n) - \Phi'(h_L^n)).$$

Discrete entropy-entropy dissipation property

$$\frac{H_\Phi^{n+1} - H_\Phi^n}{\Delta t} + D_\Phi^{n+1} \le 0 \quad \forall n \ge 0.$$

Main results

Uniform bounds

$$m^\infty \min(1, \min_{K\in\mathcal{T}} \frac{f_K^0}{f_K^\infty}) \le f_K^n \le M^\infty \max(1, \max_{K\in\mathcal{T}} \frac{f_K^0}{f_K^\infty})$$

Proof

- $\Phi_+(s) = (s-M)^+, \quad M = \max(1, \max h_K^0)$
- $\Phi_-(s) = (s-m)^-, \quad m = \min(1, \min h_K^0)$

Exponential decay

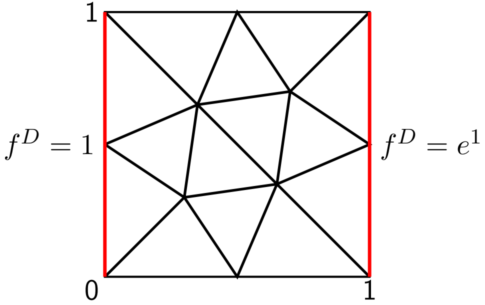
$$\Phi_2(s) = (s-1)^2,$$

$$H_{\Phi_2}^n \le H_{\Phi_2}^0 e^{-\kappa t^n},$$

$$\left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)|f_K^n - f_K^\infty|\right)^2 \le H_{\Phi_2}^0 \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) f_K^\infty\right) e^{-\kappa t^n}.$$

Test case

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f + \mathbf{U} f \\ \mathbf{U} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{cases}$$



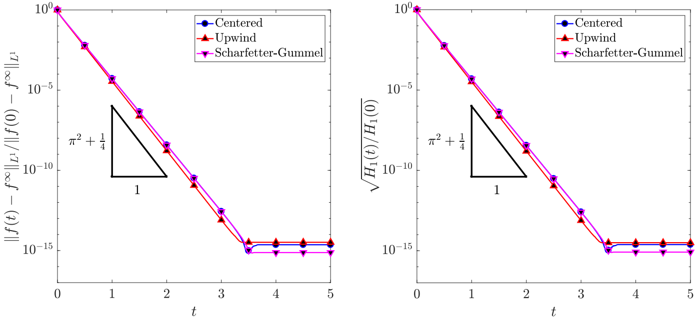
Solution and steady-state

$$f(x_1, x_2, t) = \exp(x_1) + \exp\left(\frac{x_1}{2} - \left(\pi^2 + \frac{1}{4}\right) t\right) \sin(\pi x_1)$$

$$f^\infty(x_1, x_2) = \exp(x_1)$$

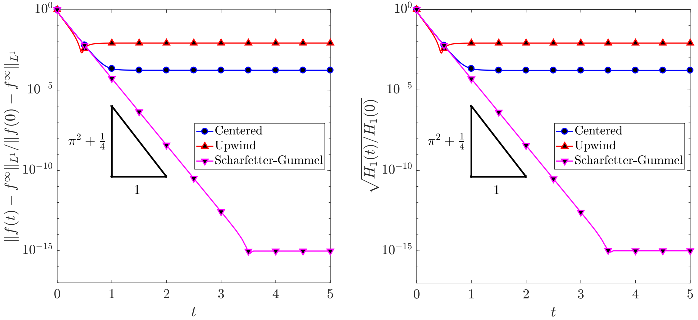
Long time behavior

Decay to the steady-state associated to the scheme



Long time behavior

Decay to the real steady-state



At this stage

Results

- Quantification of the exponential return to equilibrium
- For B-schemes for Fokker-Planck equations
- Results based on a relative entropy principle, adapted to the discrete level.

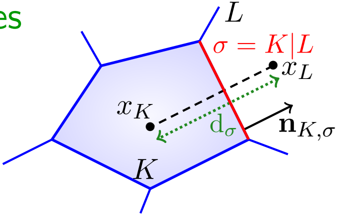
Limitations

- Use of TPFA schemes limited to admissible meshes
- Not extendable to anisotropic equations

Outline of the talk

1. Motivation
2. Finite volume schemes for the drift-diffusion equations
3. Long-time behavior of the B-schemes
4. About nonlinear schemes

Design of nonlinear TPFA schemes



Numerical fluxes

$$\mathbf{J} = -\nabla f - f\nabla\Psi = -f\nabla(\log f + \Psi)$$

$$\mathcal{F}_{K,\sigma} \approx \int_\sigma -f\nabla(\log f + \Psi)\cdot\mathbf{n}_{K,\sigma}$$

$$\mathcal{F}_{K,\sigma} = \tau_\sigma\ r(f_K, f_L)\Big(\log f_K + \Psi_K - \log f_L - \Psi_L\Big)$$

Examples of r functions

$$r(x,y) = \frac{x+y}{2}, \quad r(x,y) = \frac{x-y}{\log x - \log y}, \ldots$$

Design of nonlinear TPFA schemes

$$\begin{cases} \partial_t f + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = -\nabla f - \nabla \Psi f \text{ in } \Omega \times \mathbb{R}_+, \\ \mathbf{J} \cdot \mathbf{n} = 0 \text{ on } \Gamma \times \mathbb{R}_+, \\ f(.,0) = f_0 \geq 0. \end{cases}$$

The nonlinear schemes

$$\begin{cases} \mathrm{m}(K) \dfrac{f_K^{n+1} - f_K^n}{\Delta t} + \displaystyle\sum_{\sigma \in \mathcal{E}_K^{int}} \mathcal{F}_{K,\sigma}^{n+1} = 0, \\ \mathcal{F}_{K,\sigma} = \tau_\sigma \; r(f_K, f_L) \Big(\log f_K + \Psi_K - \log f_L - \Psi_L \Big). \end{cases}$$

Preservation of the thermal equilibrium

- $f_K^\infty = \lambda e^{-\Psi_K}$ is a steady-state,
- λ is fixed by the conservation of mass.

Dissipativity of the schemes

$$\begin{cases} \mathsf{m}(K)\dfrac{f_K^{n+1}-f_K^n}{\Delta t}+\displaystyle\sum_{\sigma\in\mathcal{E}_K^{int}}\mathcal{F}_{K,\sigma}^{n+1}=0, \\ \mathcal{F}_{K,\sigma}=\tau_\sigma r(f_K,f_L)\Big(\log\dfrac{f_K}{f_K^\infty}-\log\dfrac{f_L}{f_L^\infty}\Big). \end{cases}$$

Dissipation of the discrete entropies

Discrete relative entropy : $H_\Phi^n=\displaystyle\sum_{K\in\mathcal{T}}f_K^\infty\Phi(\frac{f_K^n}{f_K^\infty})$

$$\frac{H_\Phi^{n+1}-H_\Phi^n}{\Delta t}+D_\Phi^{n+1}\leq 0$$

with

$$D_\Phi=\sum_{\sigma\in\mathcal{E}_{int}}\tau_\sigma r(f_K,f_L)\big(\log\frac{f_K}{f_K^\infty}-\log\frac{f_L}{f_L^\infty}\big)\big(\Phi'(\frac{f_K}{f_K^\infty})-\Phi'(\frac{f_L}{f_L^\infty})\big)$$

Main results for the nonlinear TPFA schemes

A priori estimates

- Uniform bounds obtained with

$$\Phi(s) = (s-M)^+ \text{ and } \Phi(s) = (s-m)^-$$

for $M = \max(1, \max \frac{f_K^0}{f_K^\infty})$, $m = \min(1, \min \frac{f_K^0}{f_K^\infty})$

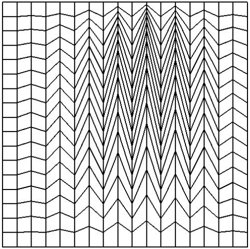
Existence of a solution to the scheme

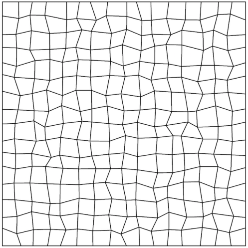
- via a topological degree argument

Exponential decay of H_1^n

- based on a discrete Log-Sobolev inequality

On general meshes ?





- The nonlinear strategy is applicable to other kinds of finite volume schemes.
- DDFV schemes, for instance.

❑ Cancès, Guichard, 2016

❑ Cancès, C.-H., Krell, 2018

Convergence with respect to the grid

On Kershaw meshes

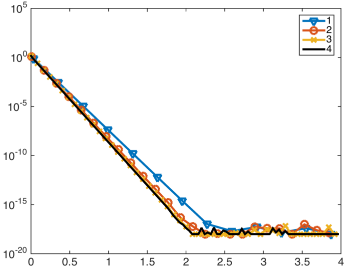
M	dt	errf	ordf	N_{max}	N_{mean}	Min f^n
1	2.0E-03	7.2E-03	—	9	2.15	1.010E-01
2	5.0E-04	1.7E-03	2.09	8	2.02	2.582E-02
3	1.2E-04	7.2E-04	2.20	7	1.49	6.488E-03
4	3.1E-05	4.0E-04	2.11	7	1.07	1.628E-03
5	3.1E-05	2.6E-04	1.98	7	1.04	1.628E-03

On quadrangle meshes

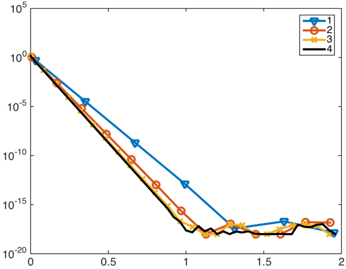
M	dt	errf	ordf	N_{max}	N_{mean}	Min f^n
1	4.0E-03	2.1E-02	—	9	2.26	1.803E-01
2	1.0E-03	5.1E-03	2.08	9	2.04	5.079E-02
3	2.5E-04	1.3E-03	2.06	8	1.96	1.352E-02
4	6.3E-05	3.3E-04	2.09	8	1.22	3.349E-03
5	1.2E-05	7.7E-05	1.70	7	1.01	8.695E-04

Long time behavior

Exponential decay of the discrete relative entropy



Kershaw



quadrangles