Entropy dissipative methods for parabolic problems

Clément Cancès

Equipe RAPSODI, Inria Lille - Nord Europe

Advanced numerical methods:
recent developments, analysis, and applications

Outline of the talk

1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

Outline of the talk

1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

A model problem

The Fokker-Planck equation

$$\begin{cases} \partial_t u - \boldsymbol{\nabla} \cdot (\boldsymbol{\Lambda}(\boldsymbol{\nabla} u + u \boldsymbol{\nabla} \Psi)) = 0 & \text{in } \Omega \times (0, \infty), \\ \boldsymbol{\Lambda} \left(u \boldsymbol{\nabla} \Psi + \boldsymbol{\nabla} u \right) \cdot \mathbf{n} = 0 & \text{on } \partial\Omega \times (0, \infty), \\ u_{|_{t=0}} = u_0 \geq 0 & \text{in } \Omega. \end{cases} \tag{FP}$$

with $\Psi \in C^2(\overline{\Omega})$ and $\boldsymbol{\Lambda}$ uniformly elliptic

$$0 \leq \lambda_\star \boldsymbol{I} \leq \boldsymbol{\Lambda} = \boldsymbol{\Lambda}^T \leq \lambda^\star \boldsymbol{I}.$$

A model problem

The Fokker-Planck equation

$$\begin{cases} \partial_t u - \nabla \cdot (\mathbf{\Lambda}(\nabla u + u \nabla \Psi)) = 0 & \text{in } \Omega \times (0, \infty), \\ \mathbf{\Lambda} (u \nabla \Psi + \nabla u) \cdot \mathbf{n} = 0 & \text{on } \partial\Omega \times (0, \infty), \\ u_{|_{t=0}} = u_0 \geq 0 & \text{in } \Omega. \end{cases} \tag{FP}$$

with $\Psi \in C^2(\overline{\Omega})$ and $\mathbf{\Lambda}$ uniformly elliptic

$$0 \leq \lambda_\star \boldsymbol{I} \leq \mathbf{\Lambda} = \mathbf{\Lambda}^T \leq \lambda^\star \boldsymbol{I}.$$

Very classical results

- The problem is well-posed
- $u \geq 0$ everywhere in $\overline{\Omega} \times \mathbb{R}_+$

Free energy and dissipation

Since $\nabla u = u \nabla \log(u)$, the problem rewrites as a nonlinear parabolic equation

$$\partial_t u - \nabla \cdot (u \Lambda \nabla (\log(u) + \Psi)) = 0. \tag{1}$$

Free energy: $\mathfrak{E}(u) = \underbrace{\int_\Omega (u \log u - u) \mathrm{d}\mathbf{x}}_{\text{entropy}} + \underbrace{\int_\Omega u \Psi \mathrm{d}\mathbf{x}}_{\text{pot. energy}} = \mathfrak{E}_{\text{ent}}(u) + \mathfrak{E}_{\text{pot}}(u),$

Dissipation: $\mathfrak{D}(u) = \int_\Omega u \Lambda \nabla (\log(u) + \Psi) \cdot \nabla (\log(u) + \Psi) \mathrm{d}\mathbf{x} \geq 0.$

Multiply (1) by $\log(u) + \Psi$ provides

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t} \mathfrak{E}(u) = -\mathfrak{D}(u) \leq 0.}$$

Three important remarks

[Arnold *et al.* '01], [Carrillo *et al.* '01], [Bolley, Gentil, and Guillin '12], ...

The crucial estimate is nonlinear

- Test with a nonlinear function of the unknown and use

$$\nabla\phi(u) = \phi'(u)\nabla u \qquad \big(\text{hence } \nabla u \nabla \log(u) = 4|\nabla\sqrt{u}|^2 \geq 0\big)$$

Three important remarks

[Arnold *et al.* '01], [Carrillo *et al.* '01], [Bolley, Gentil, and Guillin '12], ...

The crucial estimate is nonlinear

- Test with a nonlinear function of the unknown and use

$$\nabla \phi(u) = \phi'(u) \nabla u \qquad \left(\text{hence } \nabla u \nabla \log(u) = 4|\nabla \sqrt{u}|^2 \geq 0\right)$$

Convergence to equilibrium

- Define $u_\infty = e^{-\Psi}$, then

$$u(\cdot, t) \longrightarrow u_\infty \quad \text{in } L^2(\Omega) \text{ as } t \to \infty.$$

$+$ exponentially fast convergence if Ψ and Ω are convex.

Three important remarks

[Arnold *et al.* '01], [Carrillo *et al.* '01], [Bolley, Gentil, and Guillin '12], ...

The crucial estimate is nonlinear

- Test with a nonlinear function of the unknown and use

$$\nabla \phi(u) = \phi'(u)\nabla u \qquad \left(\text{hence } \nabla u \nabla \log(u) = 4|\nabla \sqrt{u}|^2 \geq 0\right)$$

Convergence to equilibrium

- Define $u_\infty = e^{-\Psi}$, then

$$u(\cdot, t) \longrightarrow u_\infty \quad \text{in } L^2(\Omega) \text{ as } t \to \infty.$$

  + exponentially fast convergence if Ψ and Ω are convex.

Extensions many other problems:

- Porous media flows, semiconductors, chemotaxis, ...

Outline of the talk

1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

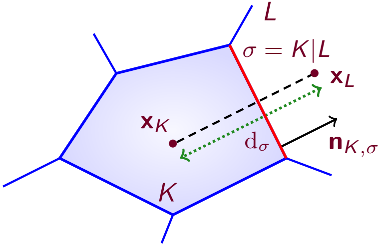
The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Isotropic diffusion tensor $\boldsymbol{\Lambda} = \boldsymbol{I}_d$

Super-admissible mesh

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



Implicit Finite Volume scheme

$$\left| \begin{array}{l} \dfrac{u_K^{n+1} - u_K^n}{\Delta t} m_K + \displaystyle\sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{K,\sigma}^{n+1} = 0 \\ \mathcal{F}_{K,\sigma}^{n+1} \simeq -\displaystyle\int_\sigma \left(\boldsymbol{\nabla} u^{n+1} + u^{n+1} \boldsymbol{\nabla} \Psi \right) \cdot \mathbf{n}_{K,\sigma} \mathrm{d}\mathbf{x} \end{array} \right.$$

Approximate solution

$$u_h^{n+1}(\mathbf{x}) = u_K^{n+1} \text{ if } \mathbf{x} \in K, \qquad u_h(\cdot, t) = u_h^{n+1} \text{ if } t \in (n\Delta t, (n+1)\Delta t].$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma} \left(B(\Psi_L - \Psi_K) u_K^{n+1} - B(\Psi_K - \Psi_L) u_L^{n+1} \right), \qquad \sigma = K|L$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma} \left(B(\Psi_L - \Psi_K) u_K^{n+1} - B(\Psi_K - \Psi_L) u_L^{n+1} \right), \qquad \sigma = K|L$$

Key properties of the SG scheme

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma} \left(B(\Psi_L - \Psi_K) u_K^{n+1} - B(\Psi_K - \Psi_L) u_L^{n+1} \right), \qquad \sigma = K|L$$

Key properties of the SG scheme

(a) Linearity: the scheme amounts to a linear system

$$(\mathbb{M} + \mathbb{A}_\Psi) \boldsymbol{U}^{n+1} = \mathbb{M} \boldsymbol{U}^n, \qquad \boldsymbol{U}^{n+1} = \left(u_K^{n+1} \right)_K$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma}\left(B(\Psi_L - \Psi_K)u_K^{n+1} - B(\Psi_K - \Psi_L)u_L^{n+1}\right), \qquad \sigma = K|L$$

Key properties of the SG scheme

(a) Linearity: the scheme amounts to a linear system

$$(\mathbb{M} + \mathbb{A}_\Psi)\,\boldsymbol{U}^{n+1} = \mathbb{M}\boldsymbol{U}^n, \qquad \boldsymbol{U}^{n+1} = \left(u_K^{n+1}\right)_K$$

(b) Monotonicity: the scheme rewrites

$$\mathcal{H}_K\Big(\underset{\nearrow}{u_K^{n+1}}, \underset{\searrow}{u_K^n}, \underset{\searrow}{\left(u_L^{n+1}\right)_{L\neq K}}\Big) = 0$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma}\left(B(\Psi_L - \Psi_K)u_K^{n+1} - B(\Psi_K - \Psi_L)u_L^{n+1}\right), \qquad \sigma = K|L$$

Key properties of the SG scheme

(c) Exact preservation of the equilibrium

$$u_K^\infty = e^{-\Psi_K} \text{ and } u_L^\infty = e^{-\Psi_L} \implies \mathcal{F}_{K,\sigma}^\infty = 0$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

Set $\Psi_K = \Psi(\mathbf{x}_K)$ and $B(s) = \frac{s}{e^s - 1} \geq 0$

$$\mathcal{F}_{K,\sigma}^{n+1} = \frac{m_\sigma}{\mathrm{d}_\sigma}\left(B(\Psi_L - \Psi_K)u_K^{n+1} - B(\Psi_K - \Psi_L)u_L^{n+1}\right), \qquad \sigma = K|L$$

Key properties of the SG scheme

(c) Exact preservation of the equilibrium

$$u_K^\infty = e^{-\Psi_K} \text{ and } u_L^\infty = e^{-\Psi_L} \implies \mathcal{F}_{K,\sigma}^\infty = 0$$

(d) Free energy dissipation:

$$\mathfrak{E}(u_h^{n+1}) \leq \mathfrak{E}(u_h^{n+1}) + \Delta t \sum_{K \in \mathcal{T}} \mathcal{F}_{K,\sigma}^{n+1}(\log(u_K^{n+1}) + \Psi_K) \leq \mathfrak{E}(u_h^n)$$

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

- The scheme is convergent

$$u_h \longrightarrow u \quad \text{in } L^1_{\text{loc}}(\overline{\Omega} \times \mathbb{R}_+) \text{ as } h, \Delta t \to 0$$

- Cheap computations (linear system)
- Positivity preserving
- 2nd order accuracy in space
- Convergence towards the equilibrium

$$u_h(\cdot, t) \longrightarrow u_h^\infty = e^{-\Psi_h} \quad \text{as } t \to \infty$$

- possible extensions to nonlinear problems [Bessemoulin-Chatard, *PhD thesis* '12]

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69], [Chatard '11], ...

- The scheme is convergent

$$u_h \longrightarrow u \quad \text{in } L^1_{\text{loc}}(\overline{\Omega} \times \mathbb{R}_+) \text{ as } h, \Delta t \to 0$$

- Cheap computations (linear system)
- Positivity preserving
- 2nd order accuracy in space
- Convergence towards the equilibrium

$$u_h(\cdot, t) \longrightarrow u_h^\infty = e^{-\Psi_h} \quad \text{as } t \to \infty$$

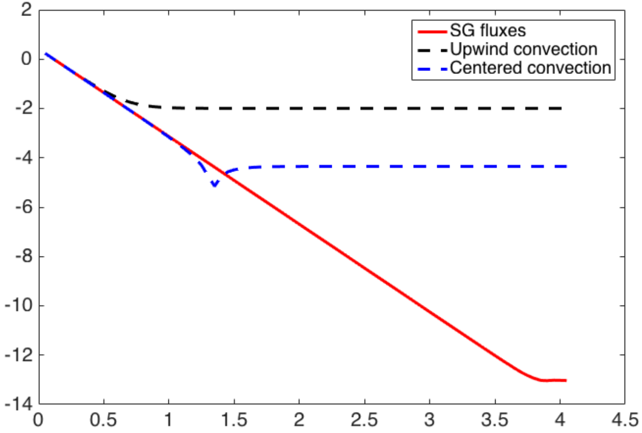
- possible extensions to nonlinear problems [Bessemoulin-Chatard, *PhD thesis* '12]

But...

- Extension when $\mathbf{\Lambda} \neq \lambda \mathbf{I}_d$?
- More general grids ?

The Scharfetter-Gummel scheme

[Scharfetter and Gummel '69, Chatard '11]



$\mathrm{Log}_{10}\left(\|u_h(\cdot,t) - u_h^\infty\|_{L^1(\Omega)}\right)$ as a function of t

Outline of the talk

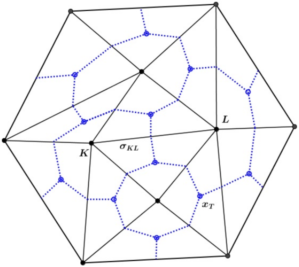
1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

A nonlinear upstream mobility CVFE scheme

[C. and Guichard, *MCOM* '16], [Ait Hammou, C., and Chainais-Hillairet, *submitted*]

Simplicial mesh

- $\mathcal{T}$: triangles or tetrahedra, $T \in \mathcal{T}$
- $\mathcal{V}$: vertices, $K \in \mathcal{V}$
- $\mathcal{E}$: edges connected vertices, $\sigma \in \mathcal{E}$
- $\mathcal{D}$: dual barycentric mesh, $\omega_K \in \mathcal{D}$
- Δt: time step



mass-lumped $\mathbb{P}_1$-finite elements

- Diagonal mass matrix

$$m_K := \int_{\omega_K} \mathrm{d}\mathbf{x} = \int_\Omega \phi_K \mathrm{d}\mathbf{x}, \quad K \in \mathcal{V}$$

- Transmittivity coefficients (possibly <0)

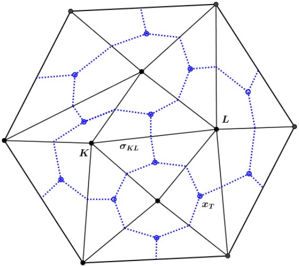
$$a_{KL} = -\int_\Omega \boldsymbol{\Lambda} \boldsymbol{\nabla} \phi_K \cdot \boldsymbol{\nabla} \phi_L \mathrm{d}\mathbf{x}, \quad K \neq L \in \mathcal{V}$$

A nonlinear upstream mobility CVFE scheme

[C. and Guichard, *MCOM* '16], [Ait Hammou, C., and Chainais-Hillairet, *submitted*]

Simplicial mesh

- $\mathcal{T}$: triangles or tetrahedra, $T \in \mathcal{T}$
- $\mathcal{V}$: vertices, $K \in \mathcal{V}$
- $\mathcal{E}$: edges connected vertices, $\sigma \in \mathcal{E}$
- $\mathcal{D}$: dual barycentric mesh, $\omega_K \in \mathcal{D}$
- Δt: time step



discrete reconstructions

- Piecewise linear reconstruction

$$v_h(\mathbf{x}, t) = \sum_{K \in \mathcal{V}} v_K^{n+1} \phi_K(\mathbf{x}) \qquad \text{if } t \in (t_n, t_{n+1}].$$

- Piecewise constant reconstruction

$$\overline{v}_h(\mathbf{x}, t) = \sum_{K \in \mathcal{V}} v_K^{n+1} \mathbf{1}_{\omega_K}(\mathbf{x}) \qquad \text{if } t \in (t_n, t_{n+1}].$$

A nonlinear upstream mobility CVFE scheme

[C. and Guichard, *MCOM* '16], [Ait Hammou, C., and Chainais-Hillairet, *submitted*]

Discretization of the nonlinear version of the equation:

$$\partial_t u - \nabla \cdot (u \boldsymbol{\Lambda} \nabla (\log(u) + \Psi)) = 0$$

into a nonlinear system $\mathcal{F}_n(\boldsymbol{u}^{n+1}) = \mathbf{0}$.

Conservation on the dual cell ω_K: Define $p_K^{n+1} = \log(u_K^{n+1}) + \Psi_K$

$$\frac{u_K^{n+1} - u_K^n}{\Delta t} m_K + \sum_{\sigma_{KL} \in \mathcal{E}_K} u_{KL}^{n+1} a_{KL} \left(p_K^{n+1} - p_L^{n+1}\right) = 0$$

Upwind mobility on σ_{KL}:

$$u_{KL}^{n+1} = \begin{cases} \left(u_K^{n+1}\right)^+ & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) \geq 0 \\ \left(u_L^{n+1}\right)^+ & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) < 0 \end{cases}$$

A priori estimates

- Loss of monotonicity when $a_{KL} < 0$...

A priori estimates

- Loss of monotonicity when $a_{KL} < 0$...

Positivity preservation

$$u_K^n \ \geq 0, \qquad \forall K \in \mathcal{V},\ \forall n \geq 0$$

Proof by induction:

- Base case: $u_K^0 = \dfrac{1}{m_K} \displaystyle\int_{\omega_K} u_0 \mathrm{d}\mathbf{x} \geq 0.$
- Inductive step: assume $u_K^{n+1} = \min_K \ u_K^{n+1} < 0.$

$$u_K^{n+1} = \underbrace{u_K^n}_{\geq 0} - \frac{\Delta t}{m_K} \sum_{\sigma_{KL} \in \mathcal{E}_K} \Big[\underbrace{\left(u_L^{n+1}\right)^+}_{\geq 0} \times [\leq 0] + \underbrace{\left(u_K^{n+1}\right)^+}_{=0} \times [\geq 0] \Big] \geq 0$$

A priori estimates

- Loss of monotonicity when $a_{KL} < 0$...

Positivity preservation

$$u_K^n \ \geq 0, \qquad \forall K \in \mathcal{V},\ \forall n \geq 0$$

Remark

$$u_{KL}^{n+1} \ = \begin{cases} \left(u_K^{n+1}\right)^+ & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) \geq 0 \\ \left(u_L^{n+1}\right)^+ & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) < 0 \end{cases}$$

A priori estimates

- Loss of monotonicity when $a_{KL} < 0$...

Positivity preservation

$$u_K^n \geq 0, \qquad \forall K \in \mathcal{V}, \ \forall n \geq 0$$

Remark

$$u_{KL}^{n+1} = \begin{cases} u_K^{n+1} & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) \geq 0 \\ u_L^{n+1} & \text{if } a_{KL}\left(p_K^{n+1} - p_L^{n+1}\right) < 0 \end{cases}$$

Entropy stability and dissipation control

Proposition

There exists C *depending on* $\boldsymbol{\Lambda}$, $reg(\mathcal{T})$, *and* t_f *such that*

- **Entropy stability**

$$\mathfrak{E}_{ent}(\overline{u}_h^n) \leq C, \qquad \forall n \geq 0$$

- **Dissipation control**

$$\sum_{n=0}^{N} \Delta t \sum_{\sigma_{KL}} |a_{KL}| u_{KL}^{n+1} \left(\log(u_K^{n+1}) - \log(u_L^{n+1})\right)^2 \leq C.$$

Entropy stability and dissipation control

Proposition

There exists C depending on $\boldsymbol{\Lambda}$, $reg(\mathcal{T})$, and t_{f} such that

- **Entropy stability**

$$\mathfrak{E}_{ent}(\overline{u}_h^n) \leq C, \qquad \forall n \geq 0$$

- **Dissipation control**

$$\sum_{n=0}^{N} \Delta t \sum_{\sigma_{KL}} |a_{KL}| u_{KL}^{n+1} \left(\log(u_K^{n+1}) - \log(u_L^{n+1})\right)^2 \leq C.$$

We proved that

$$\mathfrak{E}_{\mathrm{ent}}(\overline{u}_h^n) \leq C \quad \text{hence} \quad \mathfrak{E}(\overline{u}_h^n) \leq C$$

We **did not prove**

$$\mathfrak{E}(\overline{u}_h^{n+1}) \leq \mathfrak{E}(\overline{u}_h^n) \qquad \text{if } \boldsymbol{\nabla}\Psi \neq 0.$$

Existence of a solution to the scheme

Proposition

There exists (at least) one solution $\boldsymbol{u}^{n+1} = \left(u_K^{n+1}\right)_K$ to the nonlinear scheme

Sketch of the proof

Step 1: there exists $\epsilon > 0$ and $R > 0$ depending on $\mathcal{T}$ and Δt such that

$$0 < \epsilon \le u_K^n \le R, \qquad \forall K, \ \forall n$$

Step 2: the system $\mathcal{F}_n(\boldsymbol{u}^{n+1}) = \mathbf{0}$ admits one solution $\boldsymbol{u}^{n+1}$ in $[\epsilon, R]^{\#\mathcal{V}}$

- $\mathcal{F}_n$ is continuous on $[\epsilon, R]^{\#\mathcal{V}}$ (singularity of the log near 0 avoided)
- A topological degree argument to conclude
  [Leray and Schauder '34], [Deimling '85], [Eymard *et al.* '98]

Convergence of the scheme

[C. and Guichard, *MCOM* '16], [Ait Hammou, C., and Chainais-Hillairet, *submitted*]

- h_T: diameter of the simplex T
- ρ_T: diameter of the largest inner sphere of T

$$\text{size}(\mathcal{T}) = \max_{T\in\mathcal{T}} h_T, \qquad \text{reg}(\mathcal{T}) = \max_{T\in\mathcal{T}} \frac{h_T}{\rho_T}$$

Theorem

Assume that $size(\mathcal{T})$ and Δt tend to 0 and $reg(\mathcal{T}) \le C$, then

$$\overline{u}_h \to u \quad in\ L^1_{loc}(\overline{\Omega} \times \mathbb{R}_+)$$

where u is the unique solution to the Fokker-Planck equation

Proof based on compactness arguments

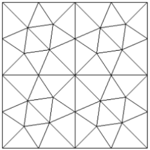
A test case with an analytic solution

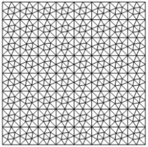
[Ait Hammou, C., and Chainais-Hillairet, *submitted*]

- **The domain:** $\Omega = [0,1]^2$
- **The equation:** $\Psi(x,y) = -x$

$$\partial_t u + \nabla \cdot (\boldsymbol{\Lambda} (u \mathbf{e}_x - \nabla u)) = 0$$

- **The diffusion tensor:** $\boldsymbol{\Lambda} = \boldsymbol{I}_d$ and $\boldsymbol{\Lambda} = \mathrm{diag}(1, 20)$
- **The mesh:** successive refinements of a Delaunay mesh

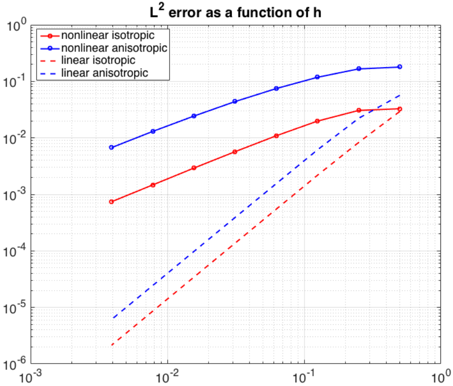




- **The analytic solution**:

$$u_{\mathrm{ex}}(x,y,t) = \exp\left(-(\pi^2 + \frac{1}{4})t + \frac{x}{2}\right)\left(\pi \cos(\pi x) + \frac{1}{2}\sin(\pi x)\right) + \pi \exp(x - \frac{1}{2})$$

Numerical results



- Preservation of the positivity by the nonlinear scheme
- Nonlinear scheme merely of order 1: $\|u - u_h\|_{L^2(Q)} \leq Ch$
- The constant C strongly depends on the anisotropy ratio

Outline of the talk

1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

Motivation

Specification

Tune your preferred numerical method to make it

- Free Energy diminishing

$$\mathfrak{E}(\overline{u}_h^{n+1}) \leq \mathfrak{E}(\overline{u}_h^n), \qquad n \geq 0$$

- Second order accurate (w.r.t. space)

$$\|\overline{u}_h - u_{\mathrm{ex}}\| \leq Ch^2$$

- Robust w.r.t. the anisotropy ratio (or the grid)
- Reasonably cheap (coding and computations)

- Vertex Approximate Gradient (VAG) scheme: [C. and Guichard, *JFoCM* '16]
- P_1 Finite Elements: [C., Nabet, and Vohralík, *in preparation*]
- Discrete Duality Finite Volumes: [C., Chainais-Hillairet, and Krell, *in preparation*]
- ...

Motivation

Specification

Tune your preferred numerical method to make it

- Free Energy diminishing

$$\mathfrak{E}(\overline{u}_h^{n+1}) \leq \mathfrak{E}(\overline{u}_h^n), \qquad n \geq 0$$

- Second order accurate (w.r.t. space)

$$\|\overline{u}_h - u_{\text{ex}}\| \leq Ch^2$$

- Robust w.r.t. the anisotropy ratio (or the grid)
- Reasonably cheap (coding and computations)

- Vertex Approximate Gradient (VAG) scheme: [C. and Guichard, *JFoCM* '16]
- P_1 Finite Elements: [C., Nabet, and Vohralík, *in preparation*]
- Discrete Duality Finite Volumes: [C., Chainais-Hillairet, and Krell, *in preparation*]
- ...

The scheme and first elementary properties

Define $p_K^{n+1} = \log(u_K^{n+1}) + \Psi_K$ and $\boldsymbol{u}^{n+1}$ by

$$\int_\Omega \frac{\overline{u}_h^{n+1} - \overline{u}_h^n}{\Delta t} \overline{v}_h \mathrm{d}\mathbf{x} + \int_\Omega \check{u}_h^{n+1} \boldsymbol{\Lambda} \boldsymbol{\nabla} p_h^{n+1} \cdot \boldsymbol{\nabla} v_h \mathrm{d}\mathbf{x} = 0, \qquad \forall \boldsymbol{v} \in \mathbb{R}^{\#\mathcal{V}}$$

The scheme and first elementary properties

Define $p_K^{n+1} = \log(u_K^{n+1}) + \Psi_K$ and $\boldsymbol{u}^{n+1}$ by

$$\int_\Omega \frac{\overline{u}_h^{n+1} - \overline{u}_h^n}{\Delta t} \overline{v}_h \mathrm{d}\mathbf{x} + \int_\Omega \check{u}_h^{n+1} \boldsymbol{\Lambda} \boldsymbol{\nabla} p_h^{n+1} \cdot \boldsymbol{\nabla} v_h \mathrm{d}\mathbf{x} = 0, \qquad \forall \boldsymbol{v} \in \mathbb{R}^{\#\mathcal{V}}$$

Proposition

- *If $\check{u}_h^{n+1} \geq 0$, then the scheme is free energy diminishing*

$$\mathfrak{E}(\overline{u}_h^{n+1}) + \Delta t \int_\Omega \check{u}_h^{n+1} \boldsymbol{\Lambda} \boldsymbol{\nabla} p_h^{n+1} \cdot \boldsymbol{\nabla} p_h^{n+1} \mathrm{d}\mathbf{x} \leq \mathfrak{E}(\overline{u}_h^n), \qquad n \geq 0$$

The scheme and first elementary properties

Define $p_K^{n+1} = \log(u_K^{n+1}) + \Psi_K$ and $\boldsymbol{u}^{n+1}$ by

$$\int_\Omega \frac{\overline{u}_h^{n+1} - \overline{u}_h^n}{\Delta t} \overline{v}_h \mathrm{d}\mathbf{x} + \int_\Omega \check{u}_h^{n+1} \boldsymbol{\Lambda} \boldsymbol{\nabla} p_h^{n+1} \cdot \boldsymbol{\nabla} v_h \mathrm{d}\mathbf{x} = 0, \qquad \forall \boldsymbol{v} \in \mathbb{R}^{\#\mathcal{V}}$$

Proposition

- *If $\check{u}_h^{n+1} \geq 0$, then the scheme is free energy diminishing*

$$\mathfrak{E}(\overline{u}_h^{n+1}) + \Delta t \int_\Omega \check{u}_h^{n+1} \boldsymbol{\Lambda} \boldsymbol{\nabla} p_h^{n+1} \cdot \boldsymbol{\nabla} p_h^{n+1} \mathrm{d}\mathbf{x} \leq \mathfrak{E}(\overline{u}_h^n), \qquad n \geq 0$$

- *The scheme is well-balanced*

$$u_K^\infty = e^{-\Psi_K} \implies p_h^\infty \equiv 0 \implies u_h^\infty \text{ is a steady solution to the scheme}$$

(the reciprocal also holds if $\check{u}_h^\infty > 0$)

Existence of a discrete solution

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

(H): There exists $\alpha > 0$ such that $\oint_T \check{v}_h \mathrm{d}\mathbf{x} \geq \alpha \max_{K \in \mathcal{V}_T} v_K$ for all $v_h \geq 0$

Positivity of the solutions

There exists $\epsilon > 0$ depending on $\mathcal{T}$, Δt such that

$$u_K^{n+1} \geq \epsilon > 0, \qquad \forall K,\ \forall n \geq 0.$$

Existence of a discrete solution

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

(H): There exists $\alpha > 0$ such that $\oint_T \check{v}_h \mathrm{d}\mathbf{x} \geq \alpha \max_{K \in \mathcal{V}_T} v_K$ for all $v_h \geq 0$

Positivity of the solutions

There exists $\epsilon > 0$ depending on $\mathcal{T}$, Δt such that

$$u_K^{n+1} \geq \epsilon > 0, \qquad \forall K, \ \forall n \geq 0.$$

This property comes from the singularity of the log near 0.
It may be lost for general nonlinear problems [C. and Guichard, *JFoCM* '16]

Existence of a discrete solution

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

(H): There exists $\alpha > 0$ such that $\oint_T \check{v}_h \mathrm{d}\mathbf{x} \geq \alpha \max_{K \in \mathcal{V}_T} v_K$ for all $v_h \geq 0$

Positivity of the solutions

There exists $\epsilon > 0$ depending on $\mathcal{T}$, Δt such that

$$u_K^{n+1} \geq \epsilon > 0, \qquad \forall K,\ \forall n \geq 0.$$

This property comes from the singularity of the log near 0.
It may be lost for general nonlinear problems [C. and Guichard, *JFoCM* '16]

How to choose $\check{u}_h^{n+1}$

A good choice is

$$\check{u}_h^{n+1} = u_h^{n+1} \quad \text{or} \quad \check{u}_h^{n+1} = \overline{u}_h^{n+1}$$

Existence of a discrete solution

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

(H): There exists $\alpha > 0$ such that $\oint_T \check{v}_h \mathrm{d}\mathbf{x} \geq \alpha \max_{K \in \mathcal{V}_T} v_K$ for all $v_h \geq 0$

Positivity of the solutions

There exists $\epsilon > 0$ depending on $\mathcal{T}$, Δt such that

$$u_K^{n+1} \geq \epsilon > 0, \qquad \forall K, \ \forall n \geq 0.$$

Existence of a discrete solution

Given $\boldsymbol{u}^n \in (\mathbb{R}_+)^{\#\mathcal{V}}$, there exists (at least) one solution $\boldsymbol{u}^{n+1} \in [\epsilon, R]^{\#\mathcal{V}}$ to the nonlinear system $\mathcal{F}_n(\boldsymbol{u}^{n+1}) = \mathbf{0}$ corresponding to the scheme.

Topological degree argument [Leray and Schauder '34], [Deimling '85], [Eymard *et al.* '98]

A convergence theorem

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

Theorem

Assume that $size(\mathcal{T})$ *and* Δt *tend to* 0 *and* $reg(\mathcal{T}) \leq C$*, then*

$$\overline{u}_h \to u \quad in\ L^1_{loc}(\overline{\Omega} \times \mathbb{R}_+)$$

where u *is the unique solution to the Fokker-Planck equation*

A convergence theorem

[C. and Guichard, *JFoCM* '16], [C., Nabet, and Vohralík, *in preparation*]

Theorem

Assume that $size(\mathcal{T})$ *and* Δt *tend to* 0 *and* $reg(\mathcal{T}) \leq C$*, then*

$$\overline{u}_h \to u \quad \text{in } L^1_{loc}(\overline{\Omega} \times \mathbb{R}_+)$$

where u *is the unique solution to the Fokker-Planck equation*

Sketch of the proof

- Up to a subsequence, $\overline{u}_h$ converges in $L^1(\Omega \times (0, t_{\mathrm{f}}))$ towards a function u [Andreianov, C., and Moussa, *submitted*], [Droniou and Eymard '16]
- u is the unique weak solution, then the whole sequence converges.

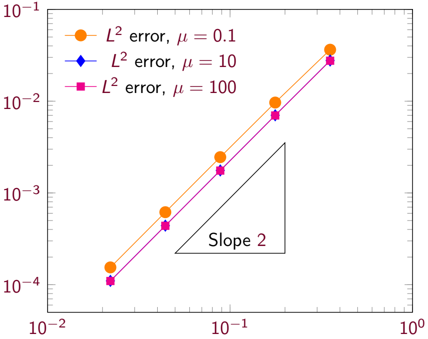
Numerical results

Equation:

$$\partial_t u - \nabla \cdot (u \boldsymbol{\Lambda} \nabla(\log u - \mathbf{e}_x)) = 0 \quad \text{with } \boldsymbol{\Lambda} = \begin{pmatrix} 1 & 0 \\ 0 & \mu \end{pmatrix}.$$

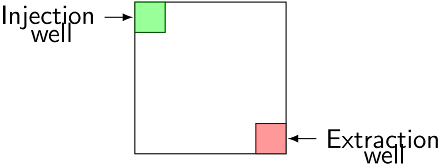
Exact solution:

$$u((x,y),t) = \exp\left(-(\pi^2 + \frac{1}{4})t + \frac{x}{2}\right)\left(\pi\cos(\pi x) + \frac{1}{2}\sin(\pi x)\right) + \pi\exp\left(x - \frac{1}{2}\right).$$



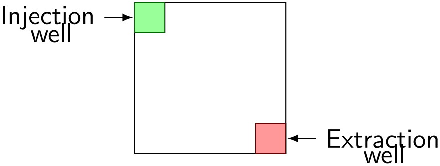
Going further

Two phase flows in porous media [C. and Nabet, *in preparation*]



Going further

Two phase flows in porous media [C. and Nabet, *in preparation*]



Equilibrated flux reconstruction [C., Nabet, and Vohralík, *in preparation*]

There exists $\boldsymbol{\sigma}_h^{n+1} \in RT_1$ such that

$$\frac{u_h^{n+1} - u_h^n}{\Delta t} + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}^{n+1} = 0.$$

- locally conservative method
- *a posteriori* error analysis and adaptive stopping criteria [Ern-Vohralík, '13]

Outline of the talk

1. Entropy and dissipation for a model parabolic problem
2. Scharfetter-Gummel: a monotone, linear, and well-balanced scheme
3. Upstream mobility schemes
4. Schemes with positive local dissipation tensors
5. Conclusion and prospects

To sum up...

Scharfetter-Gummel

- ✔ "Optimal" for linear isotropic problems
- ✘ No longer valid with anisotropy (or on general grids)

To sum up. . .

Scharfetter-Gummel

- ✓ "Optimal" for linear isotropic problems
- ✗ No longer valid with anisotropy (or on general grids)

Upstream mobility

- ✓ Positivity preserving
- ✓ Convergence theorem
- ✓ Exact on the equilibrium
- ✗ 1^{st} order accurate w.r.t. space
- ✗ Robustness w.r.t. the anisotropy
- ✓ Extension to nonlinear problems
- ? 2^{nd} order extensions (limiters) ?

To sum up...

Scharfetter-Gummel

- ✓ "Optimal" for linear isotropic problems
- ✗ No longer valid with anisotropy (or on general grids)

Upstream mobility

- ✓ Positivity preserving
- ✓ Convergence theorem
- ✓ Exact on the equilibrium
- ✗ 1st order accurate w.r.t. space
- ✗ Robustness w.r.t. the anisotropy
- ✓ Extension to nonlinear problems
- ? 2nd order extensions (limiters) ?

Positive local dissipation tensor

- ✓ Convergence theorem
- ✓ Exact on the equilibrium
- ✓ 2nd order accurate w.r.t. space
- ✓ Robustness w.r.t. the anisotropy
- ✓ Extension to nonlinear problems
- ⚠ Positivity under conditions
- ? higher order extensions ?

Finite Volumes for Complex Applications

FVCA 8

Lille - France
June 12-16, 2017

Topics

- Numerical methods
- Numerical analysis
- Scientific computing
- Industrial applications

Invited speakers

- A. R. Brodkorb
- A. Chertock
- I. Faille
- E. Fernandez-Nieto
- T. Gallouët
- B. Haasdonk
- S. Mishra
- C. W. Shu

- Peer-reviewed proceedings (submission deadline: January 6, 2017)
- Special benchmark session on incompressible flows

https://indico.math.cnrs.fr/event/1299/overview