

# A free energy diminishing DDFV scheme for convection-diffusion equations

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# Outline of the talk

1 Motivation

2 About DDFV schemes for diffusion equations

3 The nonlinear DDFV scheme

4 Some numerical results

# About convection-diffusion equations

Model problem : Fokker-Planck equation

$$\begin{cases} \partial_t u + \operatorname{div} \mathbf{J} = 0, & \mathbf{J} = \boldsymbol{\Lambda}(-\nabla u - u \nabla V), \text{ in } \Omega \times (0, T) \\ & + \text{Neumann boundary conditions} \\ u(\cdot, 0) = u_0 \geq 0 \end{cases}$$

## Examples

- Semiconductor models, corrosion models
  - ⇒  $\boldsymbol{\Lambda} = \mathbf{I}$
  - ⇒ coupling with a Poisson equation for  $V$
- Porous media flow
  - ⇒  $\boldsymbol{\Lambda}$  bounded, symmetric and uniformly elliptic
  - ⇒  $V = gz$

Assumptions :  $V \in C^1(\Omega, \mathbb{R}^+)$ ,  $\int_{\Omega} u_0 > 0$ .

## Structural properties

$$\begin{cases} \partial_t u + \operatorname{div} \mathbf{J} = 0, & \mathbf{J} = \mathbf{\Lambda}(-\nabla u - u \nabla V), \\ u(\cdot, 0) = u_0 \geq 0 & \text{+ Neumann boundary conditions} \end{cases}$$

- Existence and uniqueness of the solution
- Nonnegativity of  $u$  and mass conservation
- An energy/energy dissipation relation :  $\frac{d\mathbb{E}}{dt} + \mathbb{I} = 0$

$$\mathbb{E}(t) = \int_{\Omega} (H(u) + Vu) dx, \quad (H(s) = s \log s - s + 1)$$

$$\mathbb{I}(t) = \int_{\Omega} u \mathbf{\Lambda} \nabla (\log u + V) \cdot \nabla (\log u + V) dx$$

- Convergence towards the thermal equilibrium :

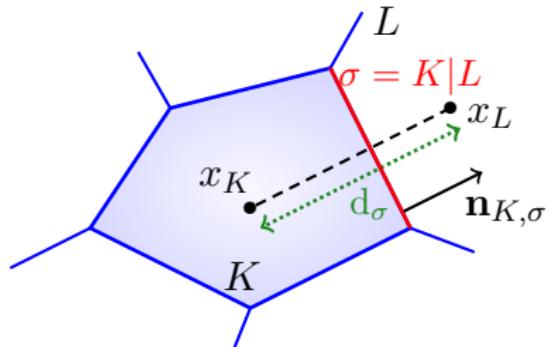
$$u_{\infty} = \lambda e^{-V} \quad (\implies \mathbf{J} = 0)$$

# $\Lambda = \mathbf{I}$ , TPFA scheme on admissible meshes

$$\begin{cases} \partial_t u + \operatorname{div} \mathbf{J} = 0, & \mathbf{J} = -\nabla u - u \nabla V, \text{ in } \Omega \\ u(\cdot, 0) = u_0 \geq 0 & + \text{Neumann boundary conditions} \end{cases}$$

Classical TPFA scheme

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



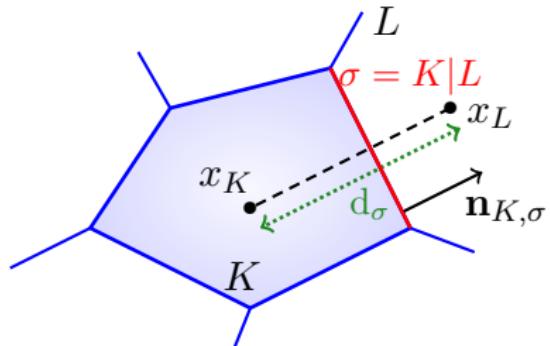
$$\left\{ \begin{array}{l} \mathbf{m}(K) \frac{u_K^{n+1} - u_K^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K^{int}} \mathcal{F}_{K,\sigma}^{\textcolor{red}{n+1}} = 0 \\ \mathcal{F}_{K,\sigma} \approx \int_{\sigma} (-\nabla u - u \nabla V) \cdot \mathbf{n}_{K,\sigma} \end{array} \right.$$

# $\Lambda = \mathbf{I}$ , TPFA scheme on admissible meshes

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$$\left\{ \begin{array}{l} \mathbf{m}(K) \frac{u_K^{n+1} - u_K^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K^{int}} \mathcal{F}_{K,\sigma}^{\textcolor{red}{n+1}} = 0 \\ \mathcal{F}_{K,\sigma} = \frac{\mathbf{m}(\sigma)}{d_\sigma} \left( B(V_L - V_K) u_K - B(-V_L + V_K) u_L \right) \end{array} \right.$$

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

# TPFA + Scharfetter-Gummel fluxes

Definition

□ SCHARFETTER, GUMMEL, 1969

$$\mathcal{F}_{K,\sigma} = \frac{m(\sigma)}{d_\sigma} \left( B_{sg}(V_L - V_K) u_K - B_{sg}(-V_L + V_K) u_L \right)$$

$$B_{sg}(x) = \frac{x}{e^x - 1} \quad (B_{sg}(0) = 1).$$

Properties

- Existence, uniqueness of the solution to the scheme
- Preservation of positivity, conservation of mass
- Preservation of the thermal equilibrium :

$$u_K = \lambda \exp(-V_K) \implies \mathcal{F}_{K,\sigma} = 0.$$

- Discrete counterpart of the energy/dissipation relation
- CHATARD, 2011

# Motivation

Main drawbacks of the TPFA scheme

- Admissibility of the mesh
- $\Lambda = \mathbf{I}$

Requirements wanted for a new scheme

- To be applicable on almost-general meshes
- To be applicable for anisotropic equations
- To preserve thermal equilibrium
- To be energy-diminishing
- To ensure the positivity

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# Introduction to DDFV schemes

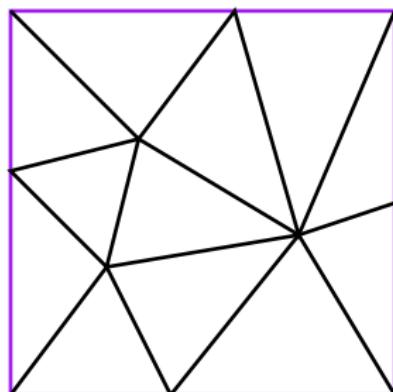
## Some (partial) references

- DOMELEVO, OMNES, 2005
- COUDIÈRE, VILA, VILLEDIEU, 1999
- ANDREIANOV, BOYER, HUBERT, 2007
- ANDREIANOV, BENDAHMANE, KARLSEN, 2010
- ...

## Principles (for diffusion equations)

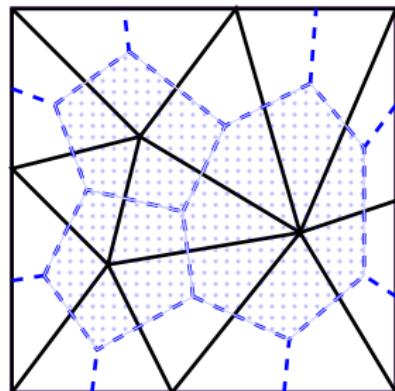
- Unknowns located at the centers and the vertices of the mesh
- Discrete gradient defined on a diamond mesh
- Discrete divergence defined on primal and dual meshes
- Integration of the equation on primal cells and dual cells
- Discrete-duality formula

## Meshes : primal and dual meshes



$\mathfrak{M}$  : primal mesh  
 $\partial\mathfrak{M}$  : exterior primal mesh

→ approximate values :  
 $(u_K)_{K \in \mathfrak{M} \cup \partial\mathfrak{M}}$

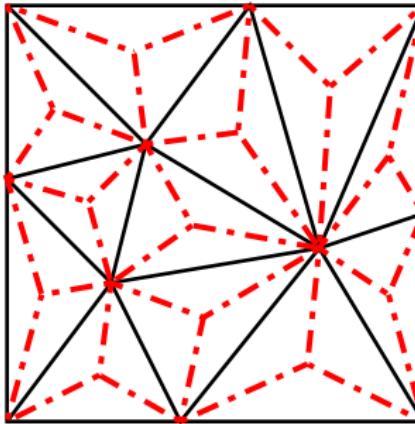


$\mathfrak{M}^*$  : interior dual mesh  
 $\partial\mathfrak{M}^*$  : exterior dual mesh

→ approximate values :  
 $(u_{K^*})_{K^* \in \mathfrak{M}^* \cup \partial\mathfrak{M}^*}$

$$u_T = ((u_K)_{K \in \mathfrak{M} \cup \partial\mathfrak{M}}, (u_{K^*})_{K^* \in \mathfrak{M}^* \cup \partial\mathfrak{M}^*})$$

## Meshes : diamond mesh



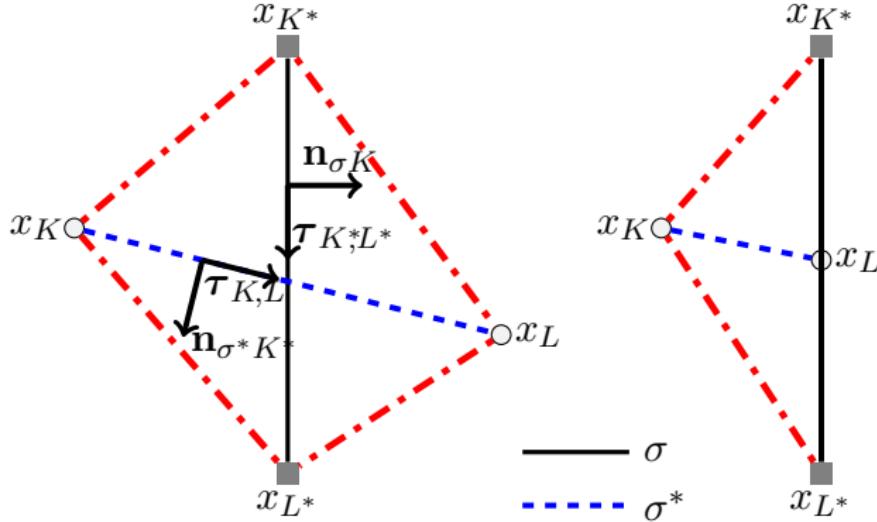
$\mathfrak{D}$  : diamond mesh

→ for the definition of the discrete gradient

$$\nabla^{\mathfrak{D}} : \mathbb{R}^T \rightarrow (\mathbb{R}^2)^{\mathfrak{D}}$$

$$u_T \mapsto (\nabla^{\mathfrak{D}} u_T)_{\mathcal{D} \in \mathfrak{D}}$$

# Discrete gradient operator



$$\nabla^{\mathfrak{D}} u_{\mathcal{T}} = (\nabla^{\mathcal{D}} u_{\mathcal{T}})_{\mathcal{D} \in \mathfrak{D}} \text{ with } \left\{ \begin{array}{lcl} \nabla^{\mathcal{D}} u_{\mathcal{T}} \cdot \tau_{K^* L^*} & = & \frac{u_{L^*} - u_{K^*}}{m_{\sigma}}, \\ \nabla^{\mathcal{D}} u_{\mathcal{T}} \cdot \tau_{K, L} & = & \frac{u_L - u_K}{m_{\sigma^*}}. \end{array} \right.$$

$$\nabla^{\mathcal{D}} u_{\mathcal{T}} = \frac{1}{2m_{\mathcal{D}}} \left( m_{\sigma} (u_L - u_K) \mathbf{n}_{\sigma K} + m_{\sigma^*} (u_{L^*} - u_{K^*}) \mathbf{n}_{\sigma^* K^*} \right).$$

# Discrete divergence operator

On the continuous level

$$\int_K \operatorname{div}(\boldsymbol{\xi}(x)) dx = \sum_{\sigma \in \partial K} \int_{\sigma} \boldsymbol{\xi}(s) \cdot \mathbf{n}_{\sigma K} ds, \quad \forall K \in \mathfrak{M}.$$

On the discrete level

$$\forall K \in \mathfrak{M}, \quad \operatorname{div}_K \boldsymbol{\xi}_{\mathfrak{D}} = \frac{1}{m_K} \sum_{\substack{\mathcal{D} \in \mathfrak{D}_K \\ \mathcal{D} = \mathcal{D}_{\sigma, \sigma^*}}} m_{\sigma} \boldsymbol{\xi}_{\mathcal{D}} \cdot \mathbf{n}_{\sigma K},$$

$$\forall K^* \in \mathfrak{M}^*, \quad \operatorname{div}_{K^*} \boldsymbol{\xi}_{\mathfrak{D}} = \frac{1}{m_{K^*}} \sum_{\substack{\mathcal{D} \in \mathfrak{D}_{K^*} \\ \mathcal{D} = \mathcal{D}_{\sigma, \sigma^*}}} m_{\sigma^*} \boldsymbol{\xi}_{\mathcal{D}} \cdot \mathbf{n}_{\sigma^* K^*},$$

$$\operatorname{div}^{\mathcal{T}} : (\mathbb{R}^2)^{\mathfrak{D}} \rightarrow \mathbb{R}^{\mathcal{T}}$$

$$\boldsymbol{\xi}_{\mathfrak{D}} \mapsto \left( (\operatorname{div}_K \boldsymbol{\xi}_{\mathfrak{D}})_{K \in \mathfrak{M}}, 0, (\operatorname{div}_{K^*} \boldsymbol{\xi}_{\mathfrak{D}})_{K^* \in \mathfrak{M}^* \cup \partial \mathfrak{M}^*} \right)$$

# Discrete duality property

Scalar products and norms

$$\begin{aligned}\llbracket v_{\mathcal{T}}, u_{\mathcal{T}} \rrbracket_{\mathcal{T}} &= \frac{1}{2} \left( \sum_{K \in \mathfrak{M}} m_K u_K v_K + \sum_{K^* \in \overline{\mathfrak{M}^*}} m_{K^*} u_{K^*} v_{K^*} \right), \\ (\boldsymbol{\xi}_{\mathfrak{D}}, \boldsymbol{\varphi}_{\mathfrak{D}})_{\mathfrak{D}} &= \sum_{\mathcal{D} \in \mathfrak{D}} m_{\mathcal{D}} \boldsymbol{\xi}_{\mathcal{D}} \cdot \boldsymbol{\varphi}_{\mathcal{D}},\end{aligned}$$

On the continuous level : the Green formula

$$\int_{\Omega} \operatorname{div} \boldsymbol{\xi} v = - \int_{\Omega} \boldsymbol{\xi} \cdot \nabla v + \int_{\partial \Omega} \boldsymbol{\xi} \cdot \mathbf{n} v$$

On the discrete level : the discrete duality formula

$$\llbracket \operatorname{div}^{\mathcal{T}} \boldsymbol{\xi}_{\mathfrak{D}}, v_{\mathcal{T}} \rrbracket_{\mathcal{T}} = -(\boldsymbol{\xi}_{\mathfrak{D}}, \nabla^{\mathfrak{D}} v_{\mathcal{T}})_{\mathfrak{D}} + \langle \gamma^{\mathfrak{D}}(\boldsymbol{\xi}_{\mathfrak{D}}) \cdot \mathbf{n}, \gamma^{\mathcal{T}}(v_{\mathcal{T}}) \rangle_{\partial \Omega},$$

## DDFV scheme for an anisotropic diffusion equation

$$\begin{cases} -\operatorname{div}\boldsymbol{\Lambda}\nabla u = f \\ + \text{boundary conditions} \end{cases}$$

The DDFV scheme

$$\begin{cases} -\operatorname{div}^{\mathcal{T}}(\boldsymbol{\Lambda}_{\mathfrak{D}}\nabla^{\mathfrak{D}} u_{\mathcal{T}}) = f_{\mathcal{T}} \\ + \text{boundary conditions} \end{cases}$$

“Variational” formulation

$$(\boldsymbol{\Lambda}_{\mathfrak{D}}\nabla^{\mathfrak{D}} u_{\mathcal{T}}, \nabla^{\mathfrak{D}} v_{\mathcal{T}})_{\mathfrak{D}} = [f_{\mathcal{T}}, v_{\mathcal{T}}]_{\mathcal{T}} \quad \forall v_{\mathcal{T}} \in \mathbb{R}^{\mathcal{T}}$$

# DDFV scheme for an anisotropic diffusion equation

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“Variational” formulation

$$\underbrace{(\Lambda_{\mathfrak{D}}\nabla^{\mathfrak{D}} u_{\mathcal{T}}, \nabla^{\mathfrak{D}} v_{\mathcal{T}})_{\mathfrak{D}}}_{(\nabla^{\mathfrak{D}} u_{\mathcal{T}}, \nabla^{\mathfrak{D}} v_{\mathcal{T}})_{\Lambda, \mathfrak{D}}} = [\![f_{\mathcal{T}}, v_{\mathcal{T}}]\!]_{\mathcal{T}} \quad \forall v_{\mathcal{T}} \in \mathbb{R}^{\mathcal{T}}$$

# DDFV scheme for an anisotropic diffusion equation

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$$\text{with } (\boldsymbol{\xi}_{\mathfrak{D}}, \varphi_{\mathfrak{D}})_{\boldsymbol{\Lambda}, \mathfrak{D}} = \sum_{\mathcal{D} \in \mathfrak{D}} m_{\mathcal{D}} \boldsymbol{\xi}_{\mathcal{D}} \cdot \boldsymbol{\Lambda}_{\mathcal{D}} \varphi_{\mathcal{D}}, \quad \boldsymbol{\Lambda}_{\mathcal{D}} = \frac{1}{m_{\mathcal{D}}} \int_{\mathcal{D}} \boldsymbol{\Lambda}.$$

# Structure of the scalar product of two discrete gradients

Discrete gradient

$$\nabla^{\mathcal{D}} u_{\mathcal{T}} = \frac{1}{2m_{\mathcal{D}}} \left( m_{\sigma} (u_L - u_K) \mathbf{n}_{\sigma K} + m_{\sigma^*} (u_{L^*} - u_{K^*}) \mathbf{n}_{\sigma^* K^*} \right).$$

$$\delta^{\mathcal{D}} u_{\mathcal{T}} = \begin{pmatrix} u_K - u_L \\ u_{K^*} - u_{L^*} \end{pmatrix}$$

Scalar product

$$\begin{aligned} (\nabla^{\mathcal{D}} u_{\mathcal{T}}, \nabla^{\mathcal{D}} v_{\mathcal{T}})_{\Lambda, \mathfrak{D}} &= \sum_{\mathcal{D} \in \mathfrak{D}} m_{\mathcal{D}} \nabla^{\mathcal{D}} u_{\mathcal{T}} \cdot \Lambda_{\mathcal{D}} \nabla^{\mathcal{D}} v_{\mathcal{T}}, \\ &= \sum_{\mathcal{D} \in \mathfrak{D}} m_{\mathcal{D}} \delta^{\mathcal{D}} u_{\mathcal{T}} \cdot \mathbb{A}_{\mathcal{D}} \delta^{\mathcal{D}} v_{\mathcal{T}}. \end{aligned}$$

Local matrices  $\mathbb{A}_{\mathcal{D}}$

⇒ Uniform bound on  $\text{Cond}_2(\mathbb{A}_{\mathcal{D}})$

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## Nonlinear formulation of the problem

$$\begin{cases} \partial_t u + \operatorname{div} \mathbf{J} = 0, & \mathbf{J} = -u \boldsymbol{\Lambda} \nabla(\log u + V), \text{ in } \Omega \times (0, T) \\ u(\cdot, 0) = u_0 \geq 0 + \text{Neumann boundary conditions} \end{cases}$$

How to approximate the current ?

- $V_T$  given. For  $u_T \in \mathbb{R}^T$ , we define  $g_T = \log u_T + V_T$ .
- $\nabla^{\mathfrak{D}} g_T$  has a sense.
- Reconstruction of  $u$  on the diamond mesh,  $r^{\mathfrak{D}}(u_T)$

$$r^{\mathfrak{D}}(u_T) = \frac{1}{4}(u_K + u_L + u_{K^*} + u_{L^*}) \quad \forall \mathfrak{D} \in \mathfrak{D}$$

- We can define a discrete current on the diamond mesh :

$$\mathbf{J}_{\mathfrak{D}} = -r^{\mathfrak{D}}(u_T) \boldsymbol{\Lambda}_{\mathfrak{D}} \nabla^{\mathfrak{D}} g_T.$$

# The scheme

$$\begin{cases} \partial_t u + \operatorname{div} \mathbf{J} = 0, & \mathbf{J} = -u \boldsymbol{\Lambda} \nabla (\log u + V), \text{ in } \Omega \times (0, T) \\ u(\cdot, 0) = u_0 \geq 0 + \text{Neumann boundary conditions} \end{cases}$$

“Classical” formulation

$$\frac{u_{\mathcal{T}}^{n+1} - u_{\mathcal{T}}^n}{\Delta t} + \operatorname{div}_{\mathcal{T}}(J_{\mathfrak{D}}^{n+1}) = 0, \quad J_{\mathfrak{D}}^{n+1} = -r^{\mathfrak{D}}[u_{\mathcal{T}}^{n+1}] \boldsymbol{\Lambda}^{\mathfrak{D}} \nabla^{\mathfrak{D}} g_{\mathcal{T}}^{n+1},$$

$$m_{\sigma} J_{\mathcal{D}}^{n+1} \cdot \mathbf{n} = 0, \quad \forall \mathcal{D} = \mathcal{D}_{\sigma, \sigma^*} \in \mathfrak{D}_{ext}.$$

Compact form

$$\left[ \left[ \frac{u_{\mathcal{T}}^{n+1} - u_{\mathcal{T}}^n}{\Delta t}, \psi_{\mathcal{T}} \right] \right]_{\mathcal{T}} + T_{\mathfrak{D}}(u_{\mathcal{T}}^{n+1}; g_{\mathcal{T}}^{n+1}, \psi_{\mathcal{T}}) = 0, \quad \forall \psi_{\mathcal{T}} \in \mathbb{R}^{\mathcal{T}},$$

$$T_{\mathfrak{D}}(u_{\mathcal{T}}^{n+1}; g_{\mathcal{T}}^{n+1}, \psi_{\mathcal{T}}) = \sum_{\mathcal{D} \in \mathfrak{D}} r^{\mathcal{D}}(u_{\mathcal{T}}^{n+1}) \delta^{\mathcal{D}} g_{\mathcal{T}}^{n+1} \cdot \mathbb{A}^{\mathcal{D}} \delta^{\mathcal{D}} \psi_{\mathcal{T}},$$

$$g_{\mathcal{T}}^{n+1} = \log(u_{\mathcal{T}}^{n+1}) + V_{\mathcal{T}}.$$

# Key discrete properties

$$\left[ \left[ \frac{u_{\mathcal{T}}^{n+1} - u_{\mathcal{T}}^n}{\Delta t}, \psi_{\mathcal{T}} \right] \right]_{\mathcal{T}} + T_{\mathfrak{D}}(u_{\mathcal{T}}^{n+1}; g_{\mathcal{T}}^{n+1}, \psi_{\mathcal{T}}) = 0, \quad \forall \psi_{\mathcal{T}} \in \mathbb{R}^{\mathcal{T}},$$

$$T_{\mathfrak{D}}(u_{\mathcal{T}}^{n+1}; g_{\mathcal{T}}^{n+1}, \psi_{\mathcal{T}}) = \sum_{\mathcal{D} \in \mathfrak{D}} r^{\mathcal{D}}(u_{\mathcal{T}}^{n+1}) \delta^{\mathcal{D}} g_{\mathcal{T}}^{n+1} \cdot \mathbb{A}^{\mathcal{D}} \delta^{\mathcal{D}} \psi_{\mathcal{T}},$$

$$g_{\mathcal{T}}^{n+1} = \log(u_{\mathcal{T}}^{n+1}) + V_{\mathcal{T}}.$$

## A priori estimates

- Mass conservation :  $\llbracket u_{\mathcal{T}}^n, 1_{\mathcal{T}} \rrbracket_{\mathcal{T}} = \int_{\Omega} u_0 \quad \forall n \geq 0$
- Energy/dissipation property
  - Discrete free energy :  $\mathbb{E}_{\mathcal{T}}^n = \llbracket H(u_{\mathcal{T}}^n), 1_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket V_{\mathcal{T}}, u_{\mathcal{T}}^n \rrbracket_{\mathcal{T}}$
  - Discrete dissipation :  $\mathbb{I}_{\mathcal{T}}^n = T_{\mathfrak{D}}(u_{\mathcal{T}}^n; g_{\mathcal{T}}^n, g_{\mathcal{T}}^n), \quad \forall n \geq 1$

$$\frac{\mathbb{E}_{\mathcal{T}}^{n+1} - \mathbb{E}_{\mathcal{T}}^n}{\Delta t} + \mathbb{I}_{\mathcal{T}}^{n+1} \leq 0, \quad \forall n \geq 0.$$

# Consequences

- Decay of the free energy + bounds
- Further a priori estimates related to Fisher information
- Positivity + lower bound of the approximate solution
- Existence of a solution to the scheme
- Compactness of a sequence of approximate solutions
- Convergence (if penalization term)

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# Test case

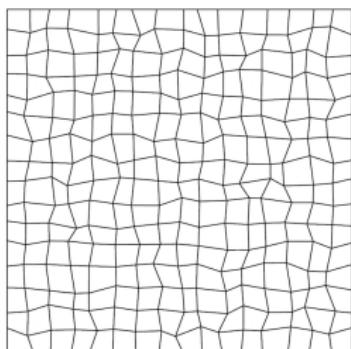
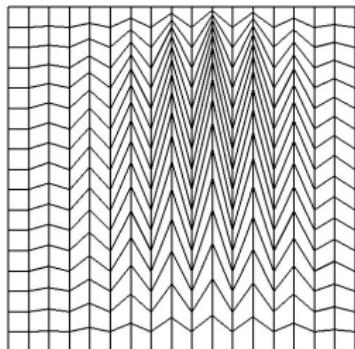
## Data and solution

- $\Omega = (0, 1)^2$ , and  $V(x_1, x_2) = -x_2$ .
- Exact solution, with  $\alpha = \pi^2 + \frac{1}{4}$ ,

$$u_{\text{ex}}((x_1, x_2), t) = e^{-\alpha t + \frac{x_2}{2}} \left( \pi \cos(\pi x_2) + \frac{1}{2} \sin(\pi x_2) \right) + \pi e^{(x_2 - \frac{1}{2})}$$

- Initial condition :  $u_0(x) = u_{\text{ex}}(x, 0)$ .

## Meshes



## Convergence with respect to the grid

On Kershaw meshes

M	dt	erru	ordu	$N_{\max}$	$N_{\text{mean}}$	Min $u^n$
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	erru	ordu	$N_{\max}$	$N_{\text{mean}}$	Min $u^n$
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

## Discrete stationary solution

$$u_K^\infty = \rho e^{-V(x_K)}, \quad u_{K^*}^\infty = \rho^* e^{-V(x_{K^*})}$$

$\rho, \rho^*$  such that  $\sum_{K \in \mathfrak{M}} u_K^\infty m_K = \sum_{K \in \overline{\mathfrak{M}}^*} u_{K^*}^\infty m_{K^*} = \int_{\Omega} u_0(x) dx.$

## Relative energy

$$\mathbb{E}_{\mathcal{T}}^n - \mathbb{E}_{\mathcal{T}}^\infty = \left[ \left[ u_{\mathcal{T}}^n \log \left( \frac{u_{\mathcal{T}}^n}{u_{\mathcal{T}}^\infty} \right) - u_{\mathcal{T}}^n + u_{\mathcal{T}}^\infty, 1_{\mathcal{T}} \right] \right]_{\mathcal{T}}, \quad n \geq 0$$

