

Several finite volume cookpots for the heat equation

Joseph Fourier, clever peoples thus mostly not B. Gaudreul

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August 17, 2022

- 1 The Finite Difference method for the Heat equation
- 2 The Finite Element method for the Heat equation
- 3 The Finite Volume method for the Heat equation
- 4 Application to a Research-level example

The Heat equation

$$\partial_t u - \Delta u = 0$$

The Heat equation

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$$u(x, t = 0) = u^0(x)$$

key properties

$$u(t, x) = u^0(\bullet) * e^{-\bullet^2/t}$$

- information travels at infinite speed
- monotonicity
- conservation of $\int u$
- decay of $\int u^2$
- decay of $\int u \log u$

Outline

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Simplest approximations

$$\partial_t u(x, t) \simeq \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t}$$

$$\partial_{xx} u(x, t) \simeq \frac{u(x + \Delta x, t) + u(x - \Delta x, t) - 2u(x, t)}{\Delta x^2}$$

Explicit scheme

$$u_i^{n+1} = u_i^n + \Delta t \frac{u_{i+1}^n + u_{i-1}^n - 2u_i^n}{\Delta x^2}$$

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Solving a linear system

$$Au^{n+1} = u^n$$

$$A = \begin{pmatrix} \ddots & & & \\ & \ddots & & \\ & & 1 + 2\frac{\Delta t}{\Delta x^2} & -\frac{\Delta t}{\Delta x^2} \\ & & -\frac{\Delta t}{\Delta x^2} & 1 + 2\frac{\Delta t}{\Delta x^2} \\ & & & \ddots \\ & & & & \ddots \end{pmatrix}$$

Natural questions

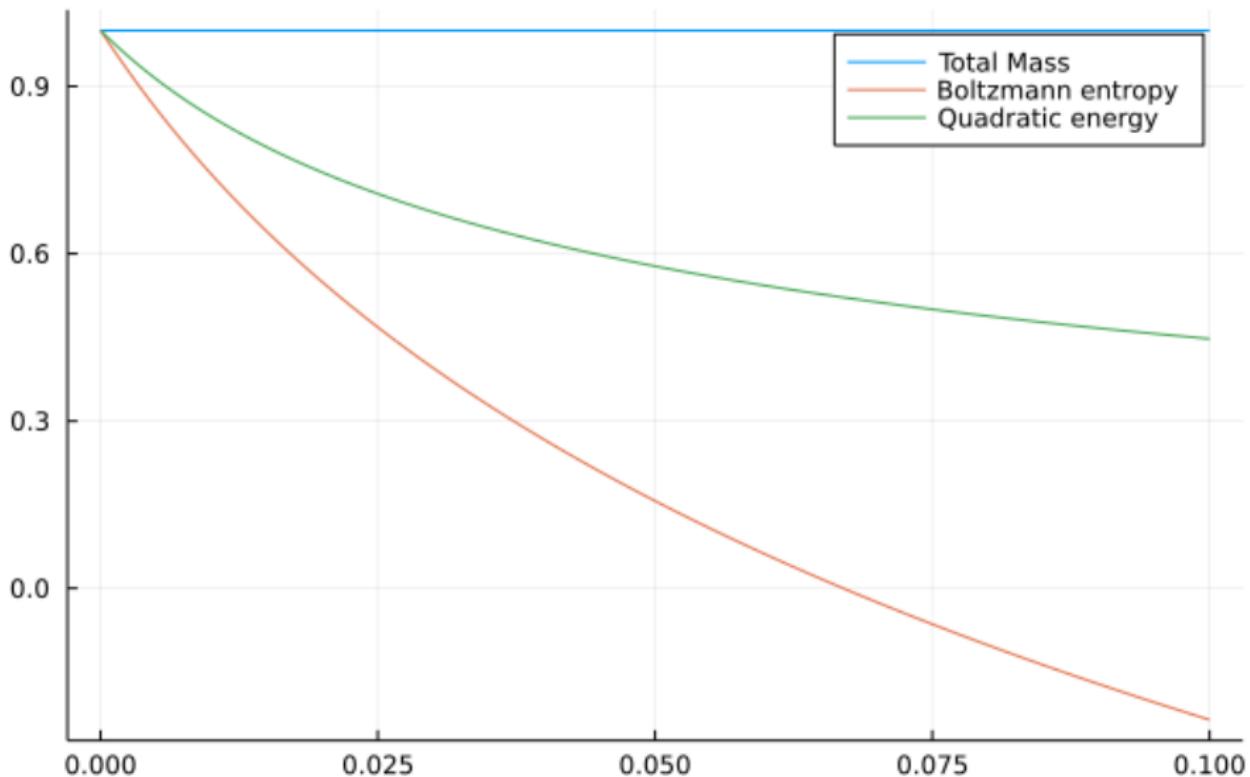
- is my scheme defined ?
- do I preserve some properties of the continuous equation ?
- does my approximate solution converge ? in what sense ? is the limit a (weak ?) solution of the heat equation ?
- how good is my approximation ?

Properties

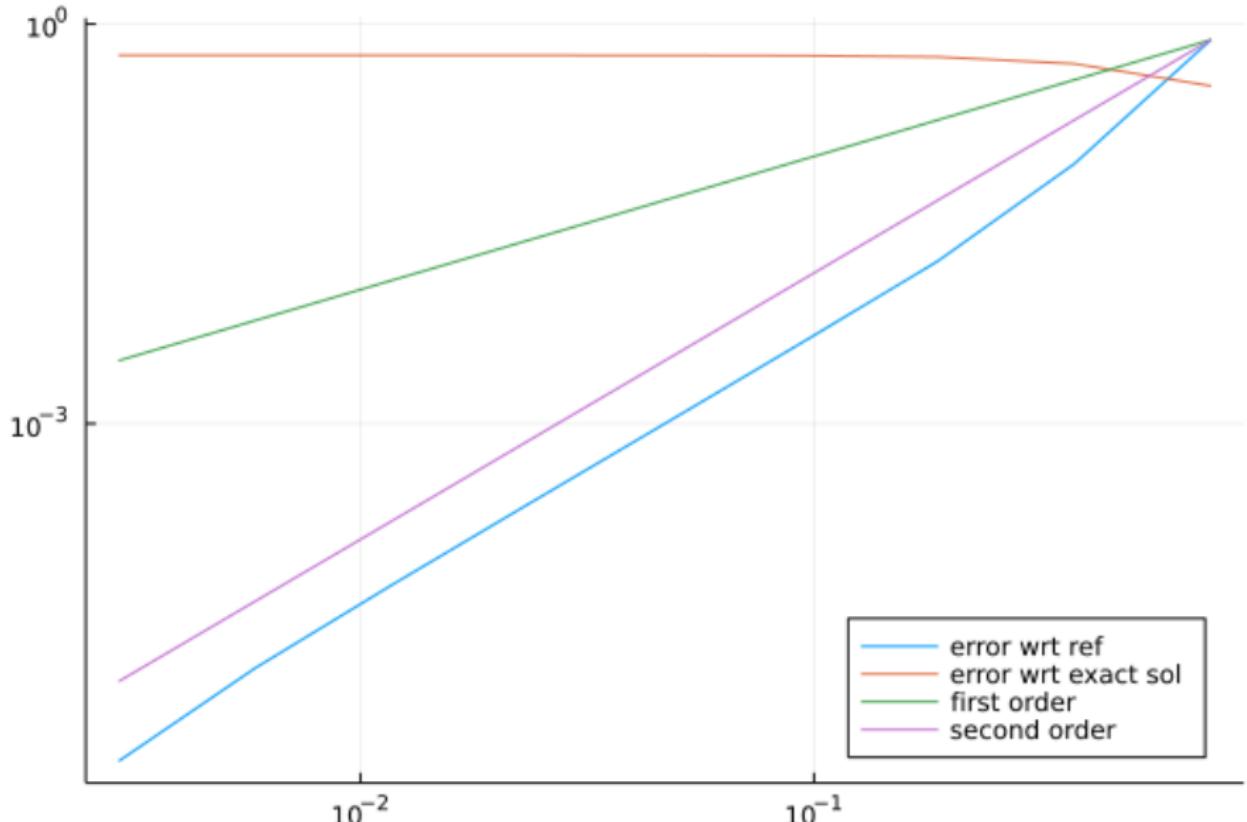
- ✓ information travels at infinite speed
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Properties

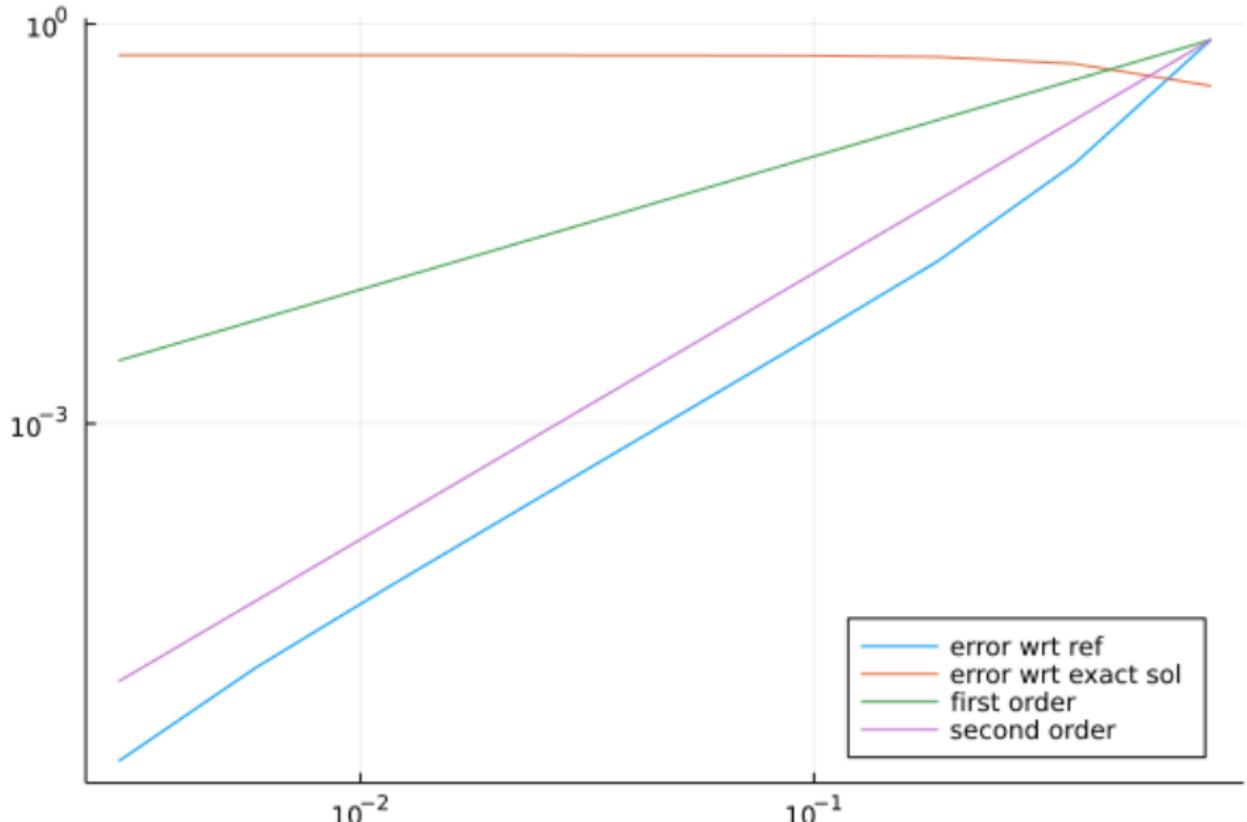
Finite difference reconstruction



Convergence curve



Convergence curve



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Key idea

$$\partial_t u = \Delta u \implies \forall v, \int (\partial_t u)v = \int (\Delta u)v = - \int \nabla u \cdot \nabla v$$

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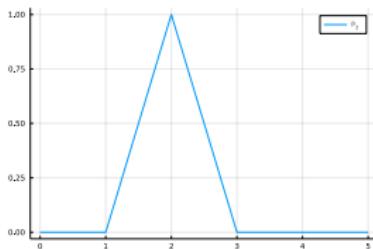
$$\partial_t u = \Delta u \implies \forall v, \int (\partial_t u)v = \int (\Delta u)v = - \int \nabla u \cdot \nabla v$$

discretized using

$$\int u^{n+1}(x)v(x) + \Delta t \nabla u^{n+1}(x) \cdot \nabla v(x) dx = \int u^n(x)v(x) dx$$

\mathbb{P}_1 discretization

$$u(x) = \sum u_i \phi_i(x)$$



$$\int \phi_i(x) \phi_i(x) = \frac{2\Delta x}{3} \quad \int \phi_i(x) \phi_{i+1}(x) = \frac{\Delta x}{6}$$

$$\int \partial_x \phi_i(x) \partial_x \phi_i(x) = \frac{2}{\Delta x} \quad \int \partial_x \phi_i(x) \partial_x \phi_{i+1}(x) = -\frac{1}{\Delta x}$$

$$(M + A)u^{n+1} = (M + I)u^n$$
$$M = \begin{pmatrix} \ddots & & & \\ & \ddots & & \\ & & -\frac{1}{3} & \frac{1}{6} \\ & & \frac{1}{6} & -\frac{1}{3} \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

Properties

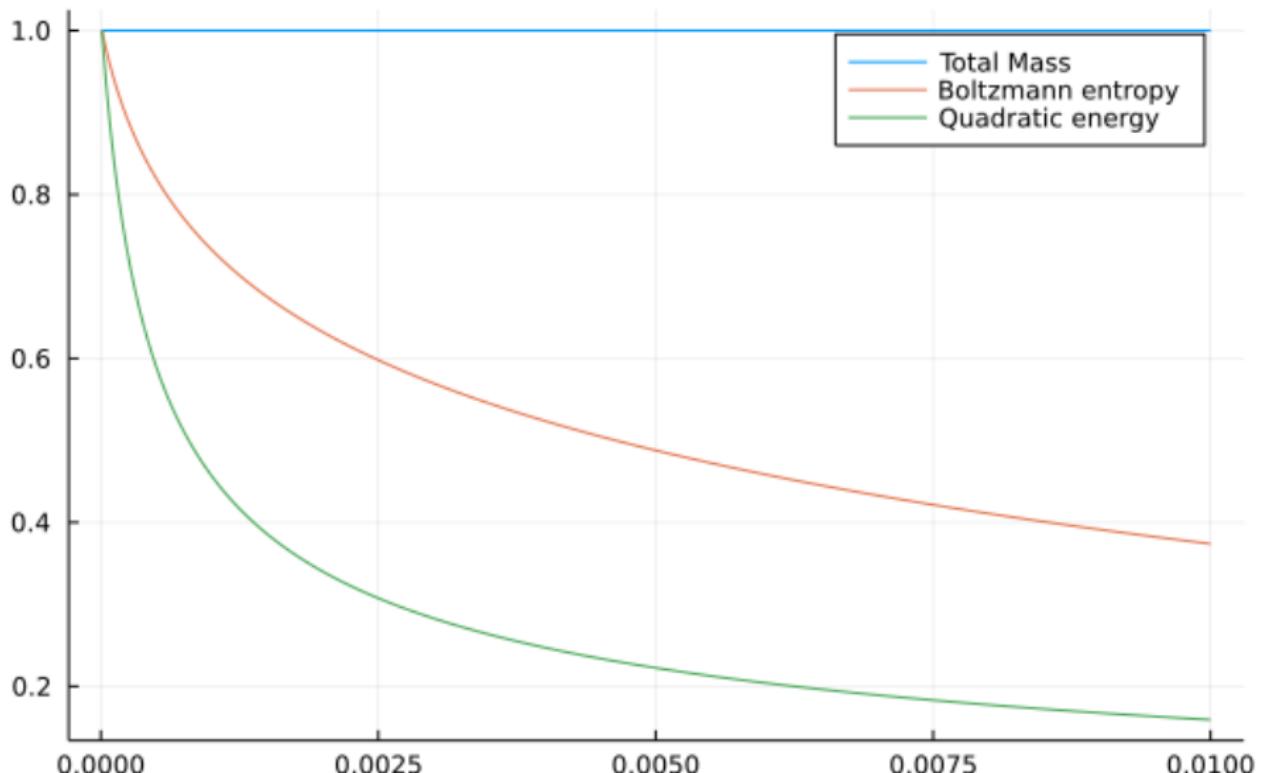
- ✓ information travels at infinite speed
- ✓ monotonicity
- ✓ conservation of $\int u$
- ✓ decay of $\int u^2$
- ? decay of $\int u \log u$

Properties

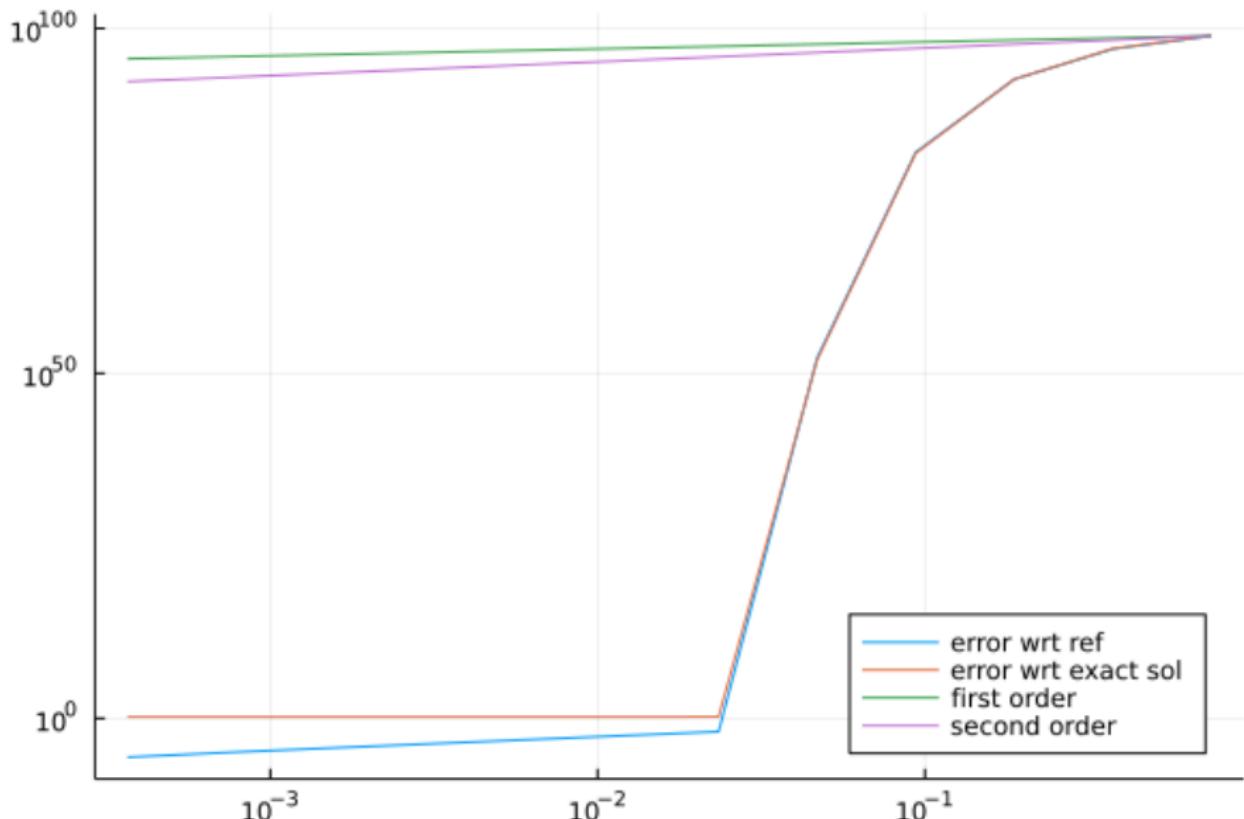
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Properties

Finite element reconstruction



Convergence curve

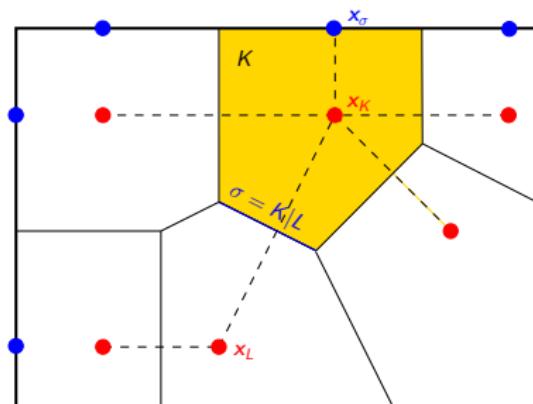


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$$\begin{aligned}\Delta u = \partial_t u &\quad \Rightarrow \quad \forall K, \int_K \Delta u = \int_K \partial_t u \\ &\Rightarrow \quad \forall K, \int_{\partial K} -\nabla u \cdot n = \int_K \partial_t u\end{aligned}$$

The mesh



A first scheme

$$\forall K, \sum_{\sigma} \int_{\sigma} -\nabla u \cdot n = \int_K \partial_t u$$

$$-\sum_{\sigma=K|L} \tau_{\sigma} (u_K^{n+1} - u_L^{n+1}) = |K| \frac{u_K^{n+1} - u_K^n}{\Delta t}, \quad \tau_{\sigma} = \frac{m_{\sigma}}{d_{\sigma}}$$

Towards other schemes

$$\nabla c = c \nabla \log(c)$$

Other schemes

$$-\sum_{\sigma=K|L} \tau_\sigma u_\sigma^{n+1} (\log(u_K^{n+1}) - \log(u_L^{n+1})) = |K| \frac{u_K^{n+1} - u_K^n}{\Delta t}, \quad \tau_\sigma = \frac{m_\sigma}{d_\sigma}$$

where

$$u_{K|L} = \frac{u_K + u_L}{2} \tag{C}$$

$$u_{K|L} = \frac{u_K - u_L}{\log u_K - \log u_L} \tag{\ln}$$

$$u_{K|L} = \max(u_K, u_L) \tag{upw}$$

1D Formulation

For (C) and (upw):

$$u_i^{n+1} + \frac{\Delta t}{\Delta x^2} (u_{i-1,i}^{n+1} (\log u_i^{n+1} - \log u_{i-1}^{n+1}) + u_{i+1,i}^{n+1} (\log u_i^{n+1} - \log u_{i+1}^{n+1})) = u_i^n$$

For (ln):

$$u_i^{n+1} + \frac{\Delta t}{\Delta x^2} (2u_i^{n+1} - u_{i-1}^{n+1} - u_{i+1}^{n+1}) = u_i^n$$

Properties

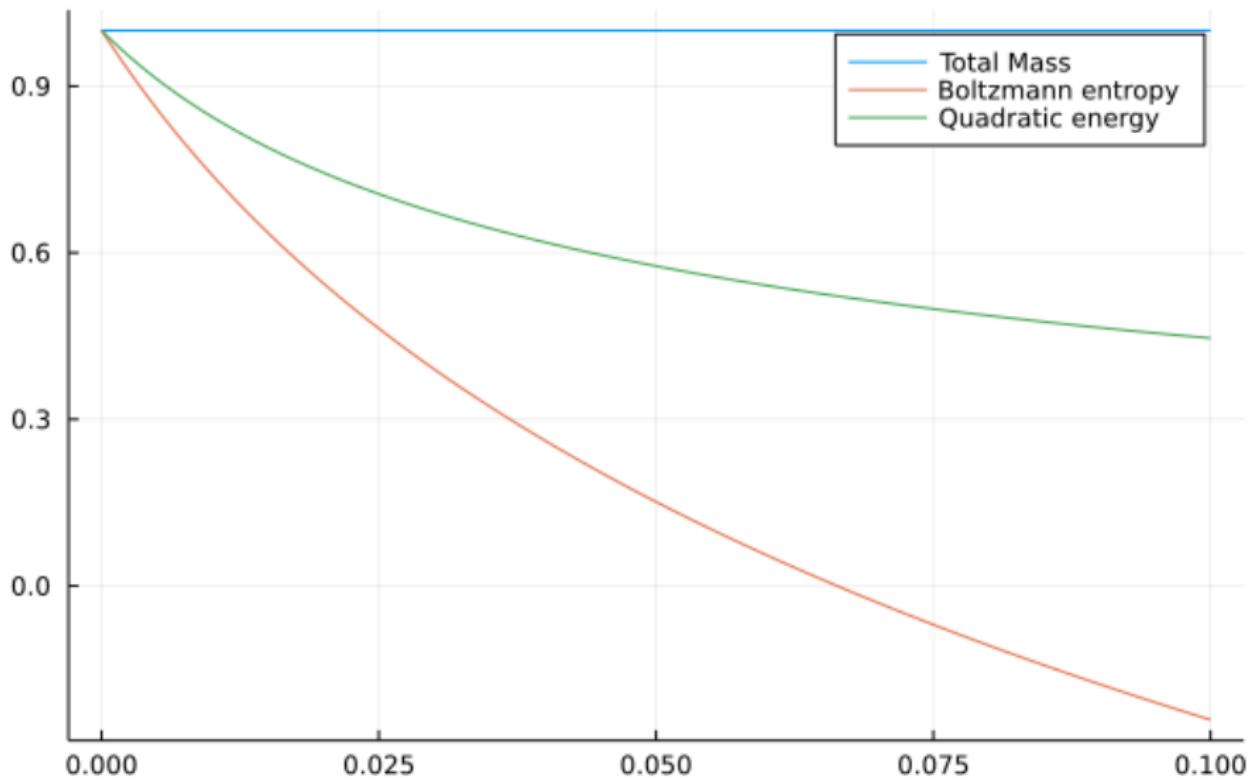
	(ln)	(c)	(upw)
information travels at infinite speed	✓	✓	✓
monotonicity	?	?	?
conservation of $\int u$	✓	✓	✓
decay of $\int u^2$	✓	?	?
decay of $\int u \log u$	✓	✓	✓

Properties

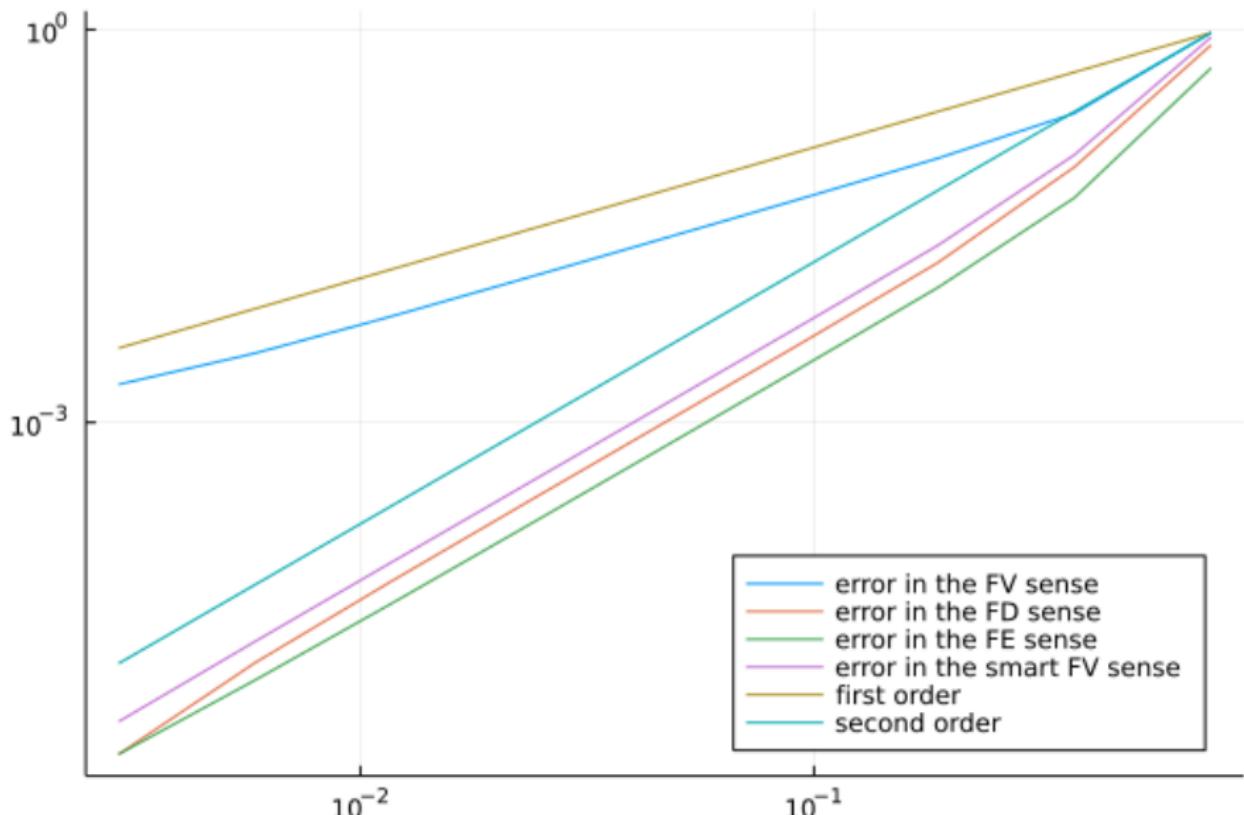
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Properties

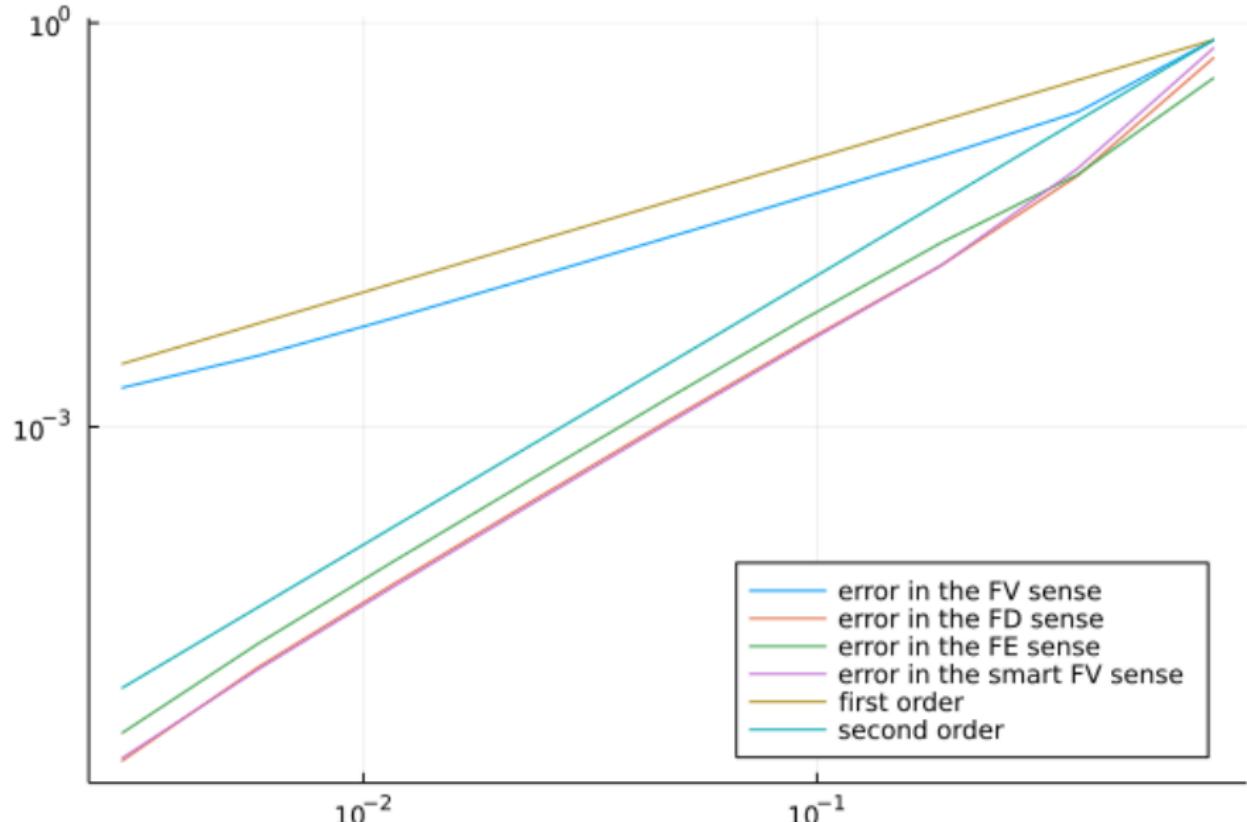
Centered Finite volume reconstruction



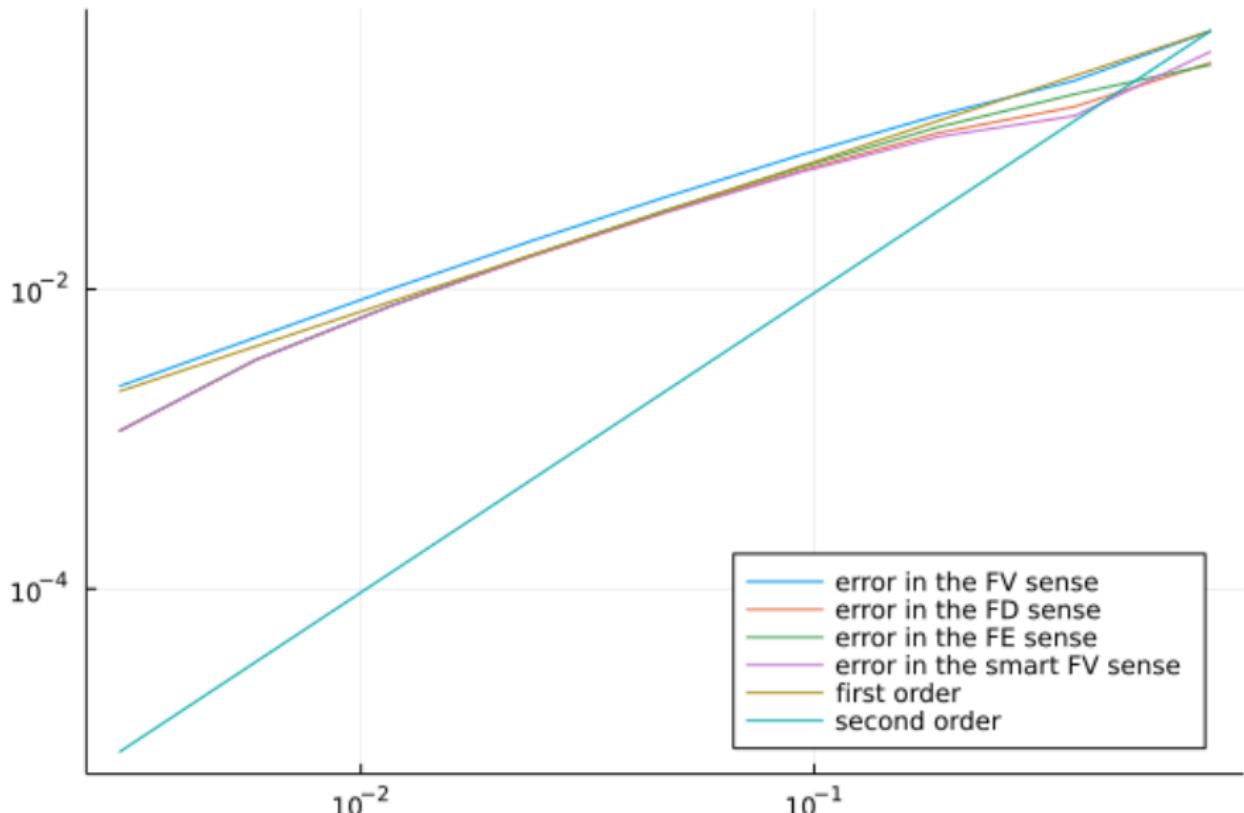
Convergence curve with log average



Convergence curve with centered scheme



Convergence curve with upwind scheme



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Thank you for your attention

La conclusion de cet exposé est laissée en exercice à l'auditoire

A numerical-analysis-focused comparison of several finite volume schemes for a unipolar degenerate drift-diffusion model

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Univ. Lille, Inria, Laboratoire Paul Painlevé

August 17, 2022

Nonlinear Drift-diffusion model

Equations:

$$\begin{aligned}\partial_t c + \operatorname{div} \left(-c \nabla \left(\log \frac{c}{1-c} + \Phi \right) \right) &= 0 \\ -\lambda^2 \Delta \Phi &= \left(c - \frac{1}{2} \right)\end{aligned}$$

Boundary and initial conditions :

- Reasonable initial condition
- Homogeneous Neumann boundary condition for the concentration
- Mixed Dirichlet-Neumann for the potential

The classical NPP system

$$\partial_t c + \operatorname{div}(-c \nabla (\log c + \Phi)) = 0$$

$$-\lambda^2 \Delta \Phi = \left(c - \frac{1}{2} \right)$$

Equivalent definitions of the fluxes

Chemical potential based:

$$\mathcal{N} = -c \nabla (h(c) + \Phi)$$

$$h : c \mapsto \log \frac{c}{1-c}$$

Diffusion enhanced based:

$$\mathcal{N} = -r'(c) \nabla c - c \nabla \Phi$$

$$r'(c) = ch'(c)$$

Excess potential based:

$$\mathcal{N} = -\nabla c - c \nabla (\Phi + \nu(c))$$

$$\nu : c \mapsto -\log(1-c)$$

Activity based:

$$\mathcal{N} = -\beta(\nabla a + a \nabla \Phi)$$

$$a = \frac{c}{1-c}; \quad \beta = 1 - c$$

The centered scheme

Continuous expression

$$\mathcal{N} = -c \nabla (h(c) + \Phi) \quad h : c \mapsto \log \frac{c}{1-c}$$

Discrete counterpart

$$F_{KL} = \tau_\sigma \frac{c_K + c_L}{2} D_{KL}(h(c) + \Phi)$$

The Bessemoulin-Chatard scheme

Continuous reformulation

$$\begin{aligned}\mathcal{N} &= -r'(c)\nabla c + c\nabla\Phi & r \text{ s.t } r'(c) = ch'(c) = \frac{h'(c)}{\log'(c)} \\ &= -r'(c) \left(\nabla c + c \frac{\nabla\Phi}{r'(c)} \right)\end{aligned}$$

Discrete counterpart

$$F_{KL} = \tau_\sigma dr_{KL} \left(B \left(\frac{\Phi_L - \Phi_K}{dr_{KL}} \right) c_K - B \left(\frac{\Phi_K - \Phi_L}{dr_{KL}} \right) c_L \right)$$

with

$$dr_{KL} = \frac{h(c_K) - h(c_L)}{\log c_K - \log c_L}$$

- BESSEMOUTIN-CHATARD (2012)

The SEDAN III scheme

Continuous reformulation

$$\mathcal{N} = -\nabla c - c \nabla(\Phi + \nu(c)) \quad \nu : c \mapsto -\log(1 - c)$$

Discrete counterpart

$$F_{KL} = \tau_\sigma \left(B (\Phi_L + \nu_L - \Phi_K - \nu_K) c_K - B (\Phi_K + \nu_K - \Phi_L - \nu_L) c_L \right)$$

- DUTTON, YU (1998)

The activity scheme

Continuous reformulation

$$\mathcal{N} = -\beta(\nabla a + a \nabla \Phi) \quad a = \frac{c}{1-c}; \quad \beta = 1 - c$$

Discrete counterpart

$$F_{KL} = \tau_\sigma \frac{\beta_K + \beta_L}{2} (B(\Phi_L - \Phi_K)a_K - B(\Phi_K - \Phi_L)a_L)$$

□ FUHRMANN (2015)

Average property

$$c_{KL} = \frac{F_{KL}}{h(c_K) + \Phi_K - h(c_L) - \Phi_L}$$

Average property

For the centered, SEDAN, and Bessemoulin-Chatard schemes, we have:

$$\min(c_K, c_L) \leq c_{KL} \leq \max(c_K, c_L)$$

Some continuous property

Chemical free energy density:

$$H(c) = c \log(c) + (1 - c) \log(1 - c)$$

Free energy of the solution:

$$E = \int_{\Omega} \left(H + \lambda^2 \frac{|\nabla \Phi|^2}{2} \right) - \int_{\Gamma_D} \Phi^D \lambda^2 \nabla \Phi \cdot \vec{n}$$

Proposition : Energy, energy dissipation relation

The functional E is convex and :

$$\partial_t E + \int_{\Omega} c |\nabla h(c) + \Phi|^2 = 0$$

Discrete counterpart

let $\mathcal{P}_{K|L} = c_{KL} (h(c_K) + \Phi_K - h(c_L) - \Phi_L)^2$ and

$$E^n = \sum_{K \in \mathcal{T}} m_K H(c_K^n) + \frac{1}{2} \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma \Phi^n)^2 - \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}^D \cap \mathcal{E}_K} \tau_\sigma \Phi_\sigma^D D_{K\sigma} \Phi^n.$$

Proposition: Entropy dissipation relation

The discrete free energy is decreasing and we have:

$$E^n + \Delta t \sum_{\sigma=K|L} \tau_\sigma \mathcal{P}_{K|L}^n \leq E^{n-1}$$

A priori estimates

Assuming $0 < c < 1$:

- $|\Phi|_\infty \leq M$
- $E_{\min} \leq E^n \leq E^0 < \infty$
- $\Delta t \sum_{\sigma=K|L} \tau_\sigma \mathcal{P}_{K|L}^n \leq E^0 - E^{\min}$
- $0 < \epsilon \leq c \leq 1 - \epsilon$

A minimal coercivity result

$$\mathcal{P}_{KL} = \mathcal{P}(c_K, c_L, \Phi_K, \Phi_L)$$

$$\Psi_{\delta,M}(c_L) = \inf\{\mathcal{P}(c_K, c_L, \Phi_K, \Phi_L); c_K \in [\delta, 1), (\Phi_K, \Phi_L) \in [-M, M]^2\}$$

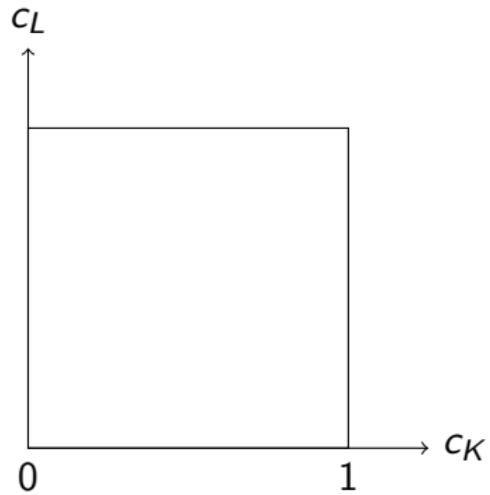
$$\Upsilon_{\delta,M}(c_L) = \inf\{\mathcal{P}(c_K, c_L, \Phi_K, \Phi_L); c_K \in (0, 1 - \delta], (\Phi_K, \Phi_L) \in [-M, M]^2\}$$

$$\lim_{c \rightarrow 0} \Psi_{\delta,M}(c) = +\infty$$

$$\lim_{c \rightarrow 1} \Upsilon_{\delta,M}(c) = +\infty$$

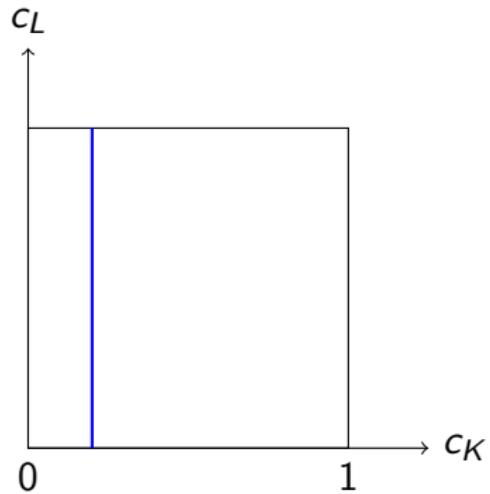
Second step: closed bounds on c_K^n

$$\mathcal{P}_{KL} = \mathcal{P}(c_K, c_L, \Phi_K, \Phi_L) \leq M$$



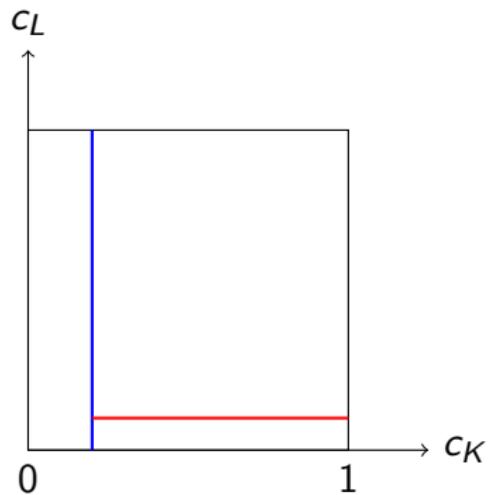
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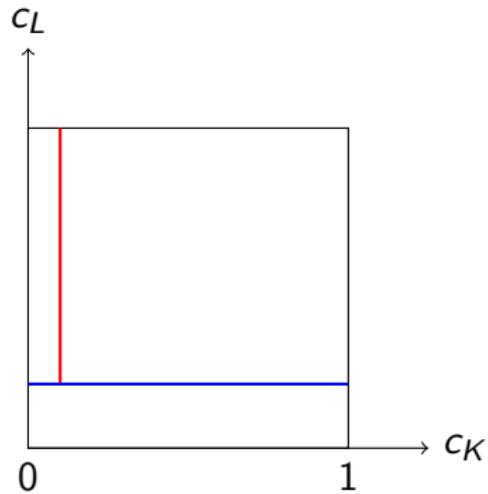
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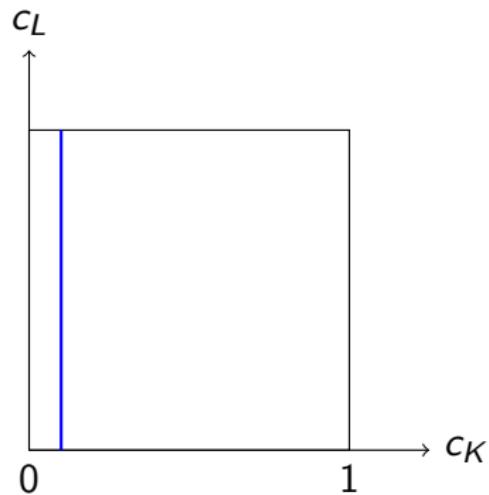
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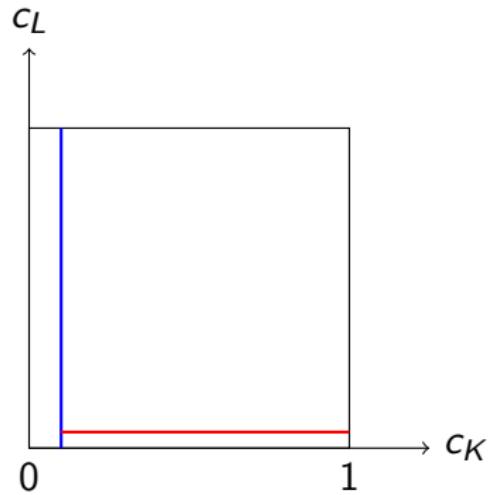
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Second step: closed bounds on c_K^n

$$\mathcal{P}_{KL} = \mathcal{P}(c_K, c_L, \Phi_K, \Phi_L) \leq M$$



Existence theorem

Theorem

For all 4 numerical fluxes, there exists (c_K^n, Φ_K^n) solution to the scheme.
Moreover, we have

$$0 < c_K^n < 1.$$

Sketch of the proof

Assume $0 < c_K^n < 1$

- ① Estimates on Φ
- ② $\Delta t \sum \tau_{K|L} \mathcal{P}_{KL} \leq C \implies \epsilon \leq c_K^n \leq 1 - \epsilon$
- ③ Topological degree argument

Convergence theorem

Theorem

Let c_m and Φ_m be solutions of the centered or SEDAN scheme.

If $h_m \rightarrow 0$, up to a subsequence:

$$c_m \xrightarrow[m \rightarrow \infty]{} c \quad \text{a.e. in } Q_T, \quad \nabla_m r(c_m) \xrightarrow[m \rightarrow \infty]{} \nabla r(c) \quad \text{in } L^2(Q_T),$$

$$\Phi_m \xrightarrow[m \rightarrow \infty]{} \Phi \quad \text{in } L^2(Q_T), \quad \nabla_m \Phi_m \xrightarrow[m \rightarrow \infty]{\star} \nabla \Phi \quad \text{in } L^\infty((0, T); L^2(\Omega)).$$

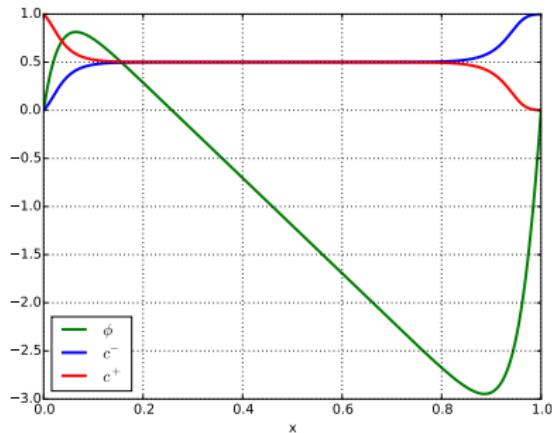
where (c, Φ) is a weak solution.

- A priori estimates;
- Compactness properties;
- Identification of the limit.

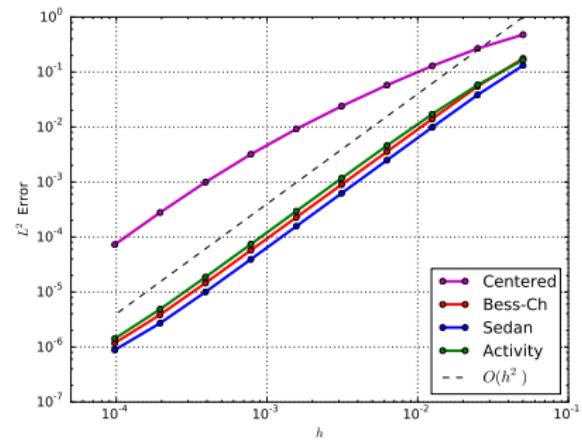
EYMARD, GALLOUËT, HERBIN (2000)

ANDREIANOV, CANCE, MOUSSA (2017)

1D test case



Stationnary problem solution



Error with respect to the reference solution

Thank you for your attention