Linear/nonlinear approaches for the approximation of convection-diffusion equations

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FVOT, Orsay, 2024/11/19

Outline of the talk

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1. Basics on convection-diffusion equations
2. Two-Point Flux Approximation of linear convection-diffusion
3. Hybrid finite volume schemes

Fokker-Planck equation (with anisotropy)

$$\begin{cases} \partial_t u + \text{div}\, \mathbf{J} = 0, \quad \mathbf{J} = \mathbf{\Lambda}(-\nabla u - u\nabla\Phi), \text{ in } \Omega \times (0,T) \\ + \text{ Dirichlet on } \Gamma^D \text{ and no-flux on } \Gamma^N,\ \partial\Omega = \Gamma^D \bigcup \Gamma^N \\ u(\cdot, 0) = u_0 \geq 0 \end{cases}$$

Examples

- Semiconductor models, corrosion models
  - ➠ $\mathbf{\Lambda} = \mathbf{I}$ or $\mathbf{\Lambda} = \frac{1}{1+b^2}\begin{pmatrix} 1 & \pm b \\ \mp b & 1 \end{pmatrix}$ (with magnetic field)
  - ➠ coupling with a Poisson equation for Φ
- Porous media flow
  - ➠ $\mathbf{\Lambda}$ bounded, symmetric and uniformly elliptic
  - ➠ $\Phi = gz$

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

Structural properties

$$\begin{cases} \partial_t u + \text{div } \mathbf{J} = 0, \quad \mathbf{J} = \mathbf{\Lambda}(-\nabla u - u \nabla \Phi), \\ u(\cdot, 0) = u_0 \geq 0 \;\; + \text{ boundary conditions} \end{cases}$$

- Existence and uniqueness of the solution
- Nonnegativity of u, mass conservation if $\Gamma^D = \emptyset$
- Existence of a thermal equilibrium :

$$u_\infty = \rho e^{-\Phi} (\Longrightarrow \mathbf{J} = 0)$$

➟ if $\Gamma^D = \emptyset$,

$$\rho = \frac{\displaystyle\int_\Omega u_0}{\displaystyle\int_\Omega e^{-\Phi}}, \quad \text{so that} \quad \int_\Omega u_\infty = \int_\Omega u_0$$

➟ if $\Gamma^D \neq \emptyset$ and $u^D = \rho e^{-\Phi^D}$ on Γ^D.

Reformulation of the convection-diffusion fluxes

$$\begin{cases} \partial_t u + \text{div } \mathbf{J} = 0, \quad \mathbf{J} = -\nabla u - u\nabla\Phi, \\ \mathbf{J}\cdot\mathbf{n} = 0 \text{ on } \Gamma^N \text{ and } \; u = u^D \text{ on } \Gamma^D. \end{cases} \qquad u^\infty = \rho e^{-\Phi}$$

Equivalence

$$\begin{aligned} \mathbf{J} &= -\nabla u - u\nabla\Phi \\ &= -u^\infty \nabla \frac{u}{u^\infty} \\ &= -u\nabla \log \frac{u}{u^\infty} \\ &= -u\nabla(\log u + \Phi) \end{aligned}$$

Towards nonlinear convection diffusion fluxes (*à la* Onsager)

$$\mathbf{J} = -\eta(u)\nabla(\mu(u) + z_u\Phi)$$

η : mobility, μ : chemical potential, z_u : charge

Long time behaviour of the Fokker-Planck equation

$$\begin{cases} \partial_t u + \text{div } \mathbf{J} = 0, \quad \mathbf{J} = -\nabla u - u\nabla\Phi, \\ \mathbf{J}\cdot\mathbf{n} = 0 \text{ on } \Gamma^N \text{ and } \ u = u^D \text{ on } \Gamma^D. \end{cases} \qquad u^\infty = \rho e^{-\Phi}$$

Dissipation of some relative Ψ-entropies

Ψ C^2-convex function, $\Psi(1) = \Psi'(1) = 0$

$$\left.\begin{aligned} \mathbb{E}(t) &= \int_\Omega u^\infty \Psi(\frac{u}{u^\infty}) \\ \mathbb{I}(t) &= \int_\Omega u^\infty \nabla\Psi'(\frac{u}{u^\infty}) \cdot \nabla\frac{u}{u^\infty} \\ &= \int_\Omega u\nabla\Psi'(\frac{u}{u^\infty}) \cdot \nabla \log\frac{u}{u^\infty} \end{aligned}\right\} \qquad \frac{d\mathbb{E}}{dt} + \mathbb{I} = 0, \text{ with } \mathbb{I} \geq 0.$$

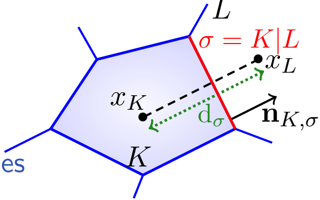
Exponential decay of the relative Ψ-entropies

For some specific choice of Ψ and thanks to functional inequalities,

$$\exists \nu \in \mathbb{R}, \quad \mathbb{E}(t) \leq \mathbb{E}(0)e^{-\nu t}.$$

Outline of the talk

TPFA finite volume schemes



$$\partial_t u + \mathsf{div}\ \mathbf{J} = 0$$

Generic form of the finite volume schemes

- (forward Euler) scheme in time

$$\frac{u^{n+1} - u^n}{\Delta t} + \mathsf{div}\ \mathbf{J}^{n+1} = 0$$

- integration of the balance law over control volumes

$$\begin{cases} \mathsf{m}(K)\dfrac{u_K^{n+1} - u_K^n}{\Delta t} + \displaystyle\sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{K,\sigma}^{n+1} = 0, \forall K \in \mathcal{T} \\ \mathcal{F}_{K,\sigma} \approx \displaystyle\int_\sigma \mathbf{J} \cdot \mathbf{n}_{K,\sigma} \quad \forall \sigma \in \mathcal{E}_K. \end{cases}$$

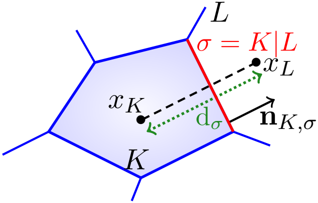
First examples of numerical fluxes (TPFA)

- $\mathbf{J} = -\nabla u \quad \mathcal{F}_{K,\sigma} = \mathrm{m}(\sigma)\dfrac{u_K - u_L}{\mathrm{d}_\sigma} = \tau_\sigma(u_K - u_L)$
- $\mathbf{J} = \mathbf{v}u \quad \mathcal{F}_{K,\sigma} = \mathrm{m}(\sigma)v_{K,\sigma}\dfrac{u_K + u_L}{2},\ v_{K,\sigma} \approx \displaystyle\oint_\sigma \mathbf{v} \cdot \mathbf{n}_{K,\sigma}$

B-numerical fluxes / B-schemes

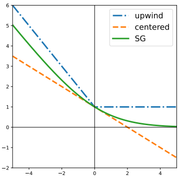
$$\mathcal{F}_{K,\sigma} \approx \int_\sigma \mathbf{J} \cdot \mathbf{n}_{K,\sigma}$$

with $\mathbf{J} = -\nabla u - u \nabla \Phi.$



$$\mathcal{F}_{K,\sigma} = \tau_\sigma \Big(B\big(\Phi_L - \Phi_K\big) u_K - B\big(\Phi_K - \Phi_L\big) u_L \Big),$$

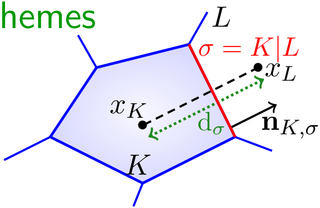
$$B(x) \geq 0, \quad B(0) = 1, \quad B(x) - B(-x) = -x.$$



- upwind flux : $B_{up}(x) = 1 + \max(-x, 0)$
- centered flux : $B_{ce}(x) = 1 - \dfrac{x}{2}$
- SG flux : $B_{SG}(x) = \dfrac{x}{\exp x - 1}$

❑ C.-H., Droniou, 2011

S-numerical fluxes / exp. fitting schemes



$$\mathcal{F}_{K,\sigma} \approx \int_\sigma \mathbf{J} \cdot \mathbf{n}_{K,\sigma}$$

with $\mathbf{J} = -u^\infty \nabla \frac{u}{u^\infty}, \quad u^\infty = e^{-\Phi}.$

$$\mathcal{F}_{K,\sigma} = \tau_\sigma S(u_K^\infty, u_L^\infty)\left(\frac{u_K}{u_K^\infty} - \frac{u_L}{u_L^\infty}\right),$$

with S Stolarsky mean : $S_{\alpha,\beta}(x,y) = \left(\frac{\beta}{\alpha}\frac{x^\alpha - y^\alpha}{x^\beta - y^\beta}\right)^{\frac{1}{\alpha-\beta}}$

- $S_{1,-1}(x,y) = \sqrt{xy}$
- $S_{0,-1} = xy(\log x - \log y)/(x-y)$
- $S_{2,1} = (x+y)/2$
- $S_{-2,-1} = 2xy/(x+y)$

❑ Heida, Kantner, Stefan, 2021

❑ Brezzi, Marini, Pietra, 1989

S-numerical fluxes / exp. fitting schemes

$$\mathcal{F}_{K,\sigma} \approx \int_\sigma \mathbf{J}\cdot\mathbf{n}_{K,\sigma}$$

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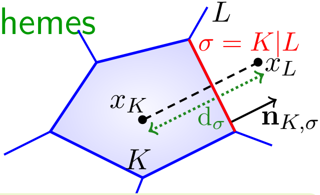

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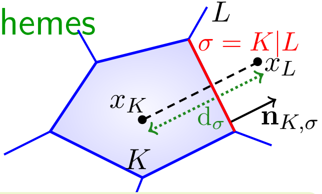
Properties of the S-functions

$$\left.\begin{array}{l} S(x,y) = xS(1,\frac{y}{x}) \\[2ex] S(x,y) = yS(1,\frac{x}{y}) \end{array}\right\} \Longrightarrow \left\{\begin{array}{l} \dfrac{S(u_K^\infty,u_L^\infty)}{u_K^\infty} = S(1, e^{-(\Phi_L-\Phi_K)}) \\[2ex] \dfrac{S(u_K^\infty,u_L^\infty)}{u_L^\infty} = S(1, e^{-(\Phi_K-\Phi_L)}) \end{array}\right.$$

S-numerical fluxes / exp. fitting schemes



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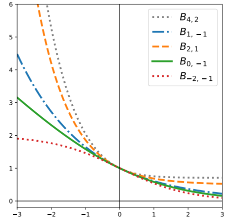
S-flux vs B-flux

The S-flux rewrites as a B-flux with

$$B(x) = S(1, e^{-x})$$



B-scheme vs S-scheme ?

- S-flux $\Longrightarrow$ B-flux, with $B(x) = S(1, e^{-x})$,

  but $B(x) - B(-x) = -x$ iff $S = S_{0,-1}$ and $B = B_{SG}$.

- B-flux $\Longrightarrow$ S-flux ?

  if $S(u_K^\infty, u_L^\infty) = u_K^\infty B(\Phi_L - \Phi_K) = u_L^\infty B(\Phi_K - \Phi_L)$

  iff $B = B_{SG}$, and therefore $S = S_{0,-1}$.

- Preservation of the thermal equilibrium ?

  always true for the S-flux.

- Preservation of the positivity ?

  yes, for both schemes (monotonicity of the fluxes).

- Exponential decay towards thermal equilibrium ?

  discrete counterpart of the entropy-dissipation estimate ?

Reformulation of the SG B-fluxes

$$\mathbf{J} = -u\nabla \log \frac{u}{u^\infty} = -u\nabla(\log u + \Phi)$$

With the Bernoulli function $B(x) = x/(e^x - 1)$

$$\mathcal{F}_{K,\sigma} = \tau_\sigma \Big(B\big(\Phi_L - \Phi_K\big) u_K - B\big(-\Phi_L + \Phi_K\big) u_L \Big)$$

$$0 = \tau_\sigma \Big(B(\log u_K - \log u_L) u_K - B(\log u_L - \log u_K) u_L \Big)$$

This implies

$$\mathcal{F}_{K,\sigma} = \tau_\sigma \left(\frac{B(y) - B(x)}{x - y} u_K + \frac{B(-x) - B(-y)}{x - y} u_L \right) (x - y)$$

with $x = \log u_K - \log u_L,\ y = \Phi_L - \Phi_K,$

so that $x - y = \log u_K + \Phi_K - (\log u_L + \Phi_L)$

❑ Cancès, C.-H., Fuhrmann, Gaudeul, 2021

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$$0 = \tau_\sigma \Big(B(\log u_K - \log u_L) u_K - B(\log u_L - \log u_K) u_L \Big)$$

This implies

$$\mathcal{F}_{K,\sigma} = \tau_\sigma r_{KL} \Big(\log u_K + \Phi_K - (\log u_L + \Phi_L) \Big)$$

with r_{KL} convex combination of u_K and u_L

(depending also on Φ_K and Φ_L)

❑ Cancès, C.-H., Fuhrmann, Gaudeul, 2021

More generally : nonlinear numerical fluxes

$$\mathbf{J} = -\nabla u - u\nabla\Phi = -u\nabla(\log u + \Phi)$$

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

$$\mathcal{F}_{K,\sigma} = \tau_\sigma r(u_K, u_L)\Big(\log u_K + \Phi_K - \log u_L - \Phi_L\Big)$$

with $r(u_K, u_L)$ a given mean value between u_K and u_L

❑ Cancès, C.-H., Herda, Krell, 2020

Beyond the TPFA schemes

Drawbacks of the TPFA schemes

- Admissibility of the mesh (orthogonality property)
- $\mathbf{\Lambda} = \mathbf{I}$

Main objectives from now on

- Design of schemes that are applicable
  - on almost-general meshes,
  - for anisotropic equations,
- while preserving :
  - positivity, conservation of mass,
  - thermal equilibrium and long-time behaviour,
- and with the possibility of extension to high order schemes.

➔ Hybrid finite volume schemes.

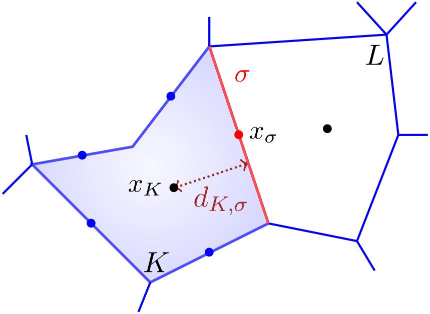
❑ Eymard, Gallouët, Herbin, 2010

Outline of the talk

Mesh and unknowns

Mesh $\mathcal{D} = (\mathcal{M}, \mathcal{E}, \mathcal{P})$

- $\mathcal{M}$: set of the control volumes (K)
- $\mathcal{E}$: set of the faces (σ)
- $\mathcal{P}$: set of the cell centers $(x_K)_{K\in\mathcal{M}}$



Set of discrete unknowns $\underline{V}_{\mathcal{D}}$

$$\underline{u}_{\mathcal{D}} = \{(u_K)_{K\in\mathcal{M}}, (u_\sigma)_{\sigma\in\mathcal{E}}\} \text{ and } u_{\mathcal{M}} : \Omega \to \mathbb{R}$$

Mesh and unknowns

Mesh $\mathcal{D} = (\mathcal{M}, \mathcal{E}, \mathcal{P})$

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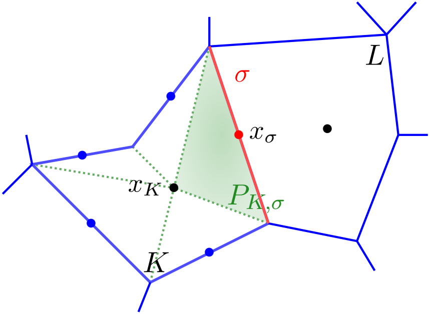


Set of discrete unknowns $\underline{V}_{\mathcal{D}}$

$$\underline{u}_{\mathcal{D}} = \{(u_K)_{K \in \mathcal{M}}, (u_\sigma)_{\sigma \in \mathcal{E}}\} \text{ and } u_{\mathcal{M}} : \Omega \to \mathbb{R}$$

HFV scheme for a diffusion equation

$$-\text{div}\,(\mathbf{\Lambda}\nabla u) = f \qquad + \text{ boundary conditions}$$

Foundations of the HFV scheme

- A discrete gradient operator $\nabla_{\mathcal{D}}$ on $\underline{V}_{\mathcal{D}}$:
  - ✻ $\nabla_{\mathcal{D}}\underline{v}_{\mathcal{D}}$ is piecewise constant on the pyramidal submesh,
  - ✻ on $P_{K,\sigma}$, $\nabla_{\mathcal{D}}\underline{v}_{\mathcal{D}}$ depends only on $\underline{v}_K = (v_K, (v_\sigma)_{\sigma\in\mathcal{E}_K})$ and is made of a consistent part and a stabilisation part.

- Some discrete bilinear forms $a_{\mathcal{D}}^{\Lambda}$ and $(a_K^{\Lambda})_{K\in\mathcal{M}}$:

$$a_{\mathcal{D}}^{\Lambda}(\underline{u}_{\mathcal{D}}, \underline{v}_{\mathcal{D}}) = (\Lambda\nabla_{\mathcal{D}}\underline{u}_{\mathcal{D}}, \nabla_{\mathcal{D}}\underline{v}_{\mathcal{D}})_{\Omega} = \sum_{K\in\mathcal{M}} a_K^{\Lambda}(\underline{u}_K, \underline{v}_K).$$

➔ definition of the scheme *via* a variational formulation.

HFV scheme for a diffusion equation

Local discrete bilinear forms and numerical fluxes

$$a_K^\Lambda(\underline{u}_K, \underline{v}_K) = (v_K - v_\sigma)_{\sigma\in\mathcal{E}_K} \cdot \mathbb{A}_K (u_K - u_\sigma)_{\sigma\in\mathcal{E}_K}$$

$$\text{with } \mathbb{A}_K = (A_K^{\sigma,\sigma'})_{\sigma,\sigma'\in\mathcal{E}_K} \in \mathcal{S}^{++}_{|\mathcal{E}_K|}$$

$$F_{K,\sigma}^\Lambda(\underline{u}_\mathcal{D}) = \sum_{\sigma'\in\mathcal{E}_K} A_K^{\sigma,\sigma'}(u_K - u_{\sigma'})$$

The HFV scheme

$$\begin{cases} \displaystyle\sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^\Lambda(\underline{u}_\mathcal{D}) = \int_K f, \\ F_{K,\sigma}^\Lambda(\underline{u}_\mathcal{D}) + F_{L,\sigma}^\Lambda(\underline{u}_\mathcal{D}) = 0 \quad \forall \sigma = K|L, \\ u_\sigma = 0 \quad \forall \sigma \in \mathcal{E}_{ext}^D \quad (u^D = 0), \quad F_{K,\sigma}^\Lambda(\underline{u}_\mathcal{D}) = 0 \quad \forall \sigma \in \mathcal{E}_{ext}^N. \end{cases}$$

➔ a linear system of equations on $(u_\sigma)_{\sigma\in\mathcal{E}}$
(after elimination of the cell unknowns)

Linear HFV schemes for an advection-diffusion equation

The Hybrid Mixed Method $\mathbf{J} = -\boldsymbol{\Lambda}\nabla u + \mathbf{w}u$

❑ Beirão da Vega, Droniou, Manzini, 2011

- Keep the same diffusive fluxes $F^{\Lambda}_{K,\sigma}(\underline{u}_{\mathcal{D}})$,
- Define some convective fluxes $F^{c}_{K,\sigma}(\underline{u}_{\mathcal{D}}) \approx \int_\sigma u\mathbf{w}\cdot\mathbf{n}_{K,\sigma}$,
- Write the balance law and the conservativity of the fluxes.

The exponential fitting scheme $\mathbf{J} = -\boldsymbol{\Lambda}(\nabla u + u\nabla\Phi)$

- Rewrite $\mathbf{J} = \omega\boldsymbol{\Lambda}\nabla\rho$ with $\rho = \dfrac{u}{\omega}$, $\omega = e^{-\Phi}$
- Write the HFV scheme for this anisotropic diffusion equation, with a specific averaging of $\omega\Lambda$ on the pyramids $P_{K,\sigma}$.
- Solve the linear system either in the ρ or in the u variable.

Properties of the linear schemes

	HMM	Exponential fitting
Well-posedness	needs coercivity or smallness of the mesh ✔	✔
Preservation of the thermal equilibrium	✘	✔
Positivity	✘	✘
Mass conservation	✔	✔
Asymptotic stability $\|u_{\mathcal{M}}^n - u_{\mathcal{M}}^\infty\|_{L^2(\Omega)}$	✔	✔

Introduction of a nonlinear HFV scheme

$$\text{div }(\mathbf{J}) = f, \quad \mathbf{J} = -u\boldsymbol{\Lambda}\nabla(\log u + \Phi)$$

Principles of the nonlinear HFV scheme

- Define the nonlinear numerical fluxes :

$$\mathcal{G}^{\Lambda}_{K,\sigma}(\underline{u}_{\mathcal{D}}, \underline{\Phi}_{\mathcal{D}}) = r_K(\underline{u}_{\mathcal{D}}) F^{\Lambda}_{K,\sigma}(\log \underline{u}_{\mathcal{D}} + \underline{\Phi}_{\mathcal{D}})$$

$$\text{with } r_K(\underline{u}_{\mathcal{D}}) = \frac{1}{2}\left(u_K + \frac{1}{|\mathcal{E}_K|}\sum_{\sigma\in\mathcal{E}_K} u_\sigma\right).$$

- Write balance law and conservativity of the fluxes.

❑ C.-H., Herda, Lemaire, Moatti, 2023

❑ Moatti 2023 (PhD thesis)

About the nonlinear scheme

$$\begin{cases} \partial_t u + \mathsf{div}\, \mathbf{J} = 0, \quad \mathbf{J} = -u\boldsymbol{\Lambda}\nabla(\log u + \Phi) = -u\boldsymbol{\Lambda}\nabla \log \dfrac{u}{\omega}, \\ u(\cdot, 0) = u_0 \geq 0 \ + \text{homogeneous Neumann boundary conditions}, \\ M = \displaystyle\int_\Omega u_0 > 0 \end{cases}$$

The scheme under its compact form

$$\frac{1}{\Delta t}(u_{\mathcal{M}}^n - u_{\mathcal{M}}^{n-1}, v_{\mathcal{M}})_\Omega + T_{\mathcal{D}}(\underline{u}_{\mathcal{D}}^n, \underline{w}_{\mathcal{D}}^n, \underline{v}_{\mathcal{D}}) = 0 \quad \forall \underline{v}_{\mathcal{D}} \in \underline{V}_{\mathcal{D}},$$

$$\underline{w}_{\mathcal{D}} = \log \frac{\underline{u}_{\mathcal{D}}}{\underline{\omega}_D}$$

$$T_{\mathcal{D}}(\underline{u}_{\mathcal{D}}^n, \underline{w}_{\mathcal{D}}, \underline{v}_{\mathcal{D}}) = \sum_{K \in \mathcal{M}} r_K(\underline{u}_K) a_K^\Lambda(\underline{w}_K, \underline{v}_K).$$

First a priori estimate : conservation of mass

Choose $\underline{v}_{\mathcal{D}} = \underline{1}_D$ in order to obtain

$$\int_\Omega u_{\mathcal{M}}^n = \int_\Omega u_{\mathcal{M}}^{n-1} \text{ for all } n \geq 1.$$

About the nonlinear scheme

Second a priori estimate : entropy-dissipation estimate

- Discrete relative entropy :

$$\mathbb{E}^n = \int_\Omega u_{\mathcal{M}}^\infty \Psi(\frac{u_{\mathcal{M}}^n}{u_{\mathcal{M}}^\infty}) \text{ with } \Psi(s) = s \log s - s + 1.$$

- Discrete dissipation :

$$\mathbb{D}^n = T_{\mathcal{D}}(\underline{u}_{\mathcal{D}}^n, \underline{w}_{\mathcal{D}}^n, \underline{w}_{\mathcal{D}}^n).$$

- With the test function $\underline{v}_{\mathcal{D}} = \underline{w}_{\mathcal{D}}^n$ in the scheme, we get

$$\frac{\mathbb{E}^{n+1} - \mathbb{E}^n}{\Delta t} + \mathbb{D}^{n+1} \leq 0$$

if the scheme has a positive solution.

Main results

Theorem 1

Existence of a positive discrete solution to the nonlinear scheme.

Theorem 2

Exponential decay of the discrete entropy in time :

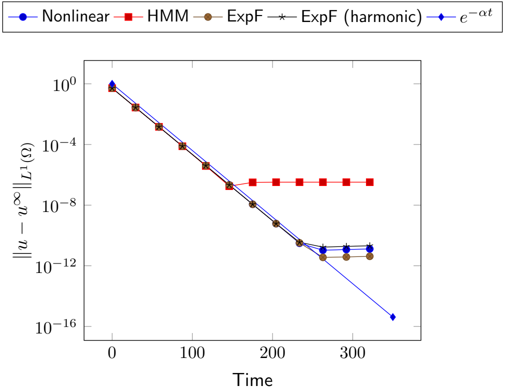
$$\mathbb{E}^{n+1} \leq (1 + \tilde{\nu}\Delta t)^{-1}\mathbb{E}^n, \forall n \geq 0$$

Exponential decay of the L^1-distance to the equilibrium

$$\|u_{\mathcal{M}}^n - u_{\mathcal{M}}^\infty\|_{L^1(\Omega)} \leq C(1 + \tilde{\nu}\Delta t)^{-\frac{n}{2}}.$$

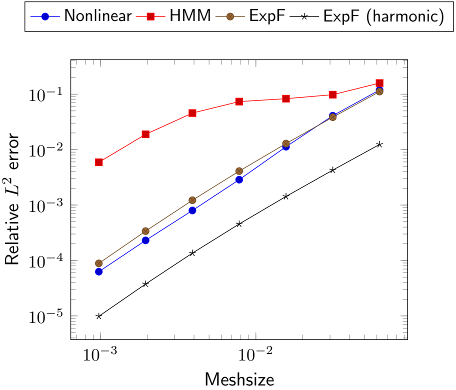
Numerical results

Long-time behaviour (on a fine Kershaw mesh)



Numerical results

Accuracy of stationary solutions (advection-dominated test case)



Concluding remarks

About the non linear hybrid scheme

- Well posedness, positivity and preservation of the equilibrium
- Exponential decay towards the equilibrium
- A first step towards Hybrid High Order schemes

❑ Lemaire, Moatti, 2024

- Possible extension to nonlinear convection-diffusion equations

TPFA schemes and nonlinear convection-diffusion fluxes

$$\mathbf{J} = -\eta(u)\nabla(\mu(u) + z_u\Phi)$$

❑ Cancès, C.H., Fuhrmann, Gaudeul, 2021

❑ Cancès, Venel, 2023

❑ Cancès, Herda, Massimini, 2023