An entropy structure preserving space–time Galerkin method for cross–diffusion systems

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Cross-diffusion system

- Vector-valued unknown $\rho(t) = (\rho_1, \ldots, \rho_N)(\cdot, t) : \Omega \to \mathbb{R}^N$
- Diffusion matrix $A(\rho) \in \mathbb{R}^{N\times N}$

$$\begin{cases} \partial_t \rho - \nabla \cdot (A(\rho)\nabla\rho) = f(\rho) & \text{in } \Omega,\ t > 0, \\ (A(\rho)\nabla\rho)\cdot\nu = 0 & \text{on } \partial\Omega,\ t > 0, \\ \rho(0) = \rho_0 & \text{in } \Omega. \end{cases}$$

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Weak formulation:

$$\int_\Omega \phi(T) \cdot \rho(T) dx - \int_\Omega \phi(0) \cdot \rho_0 dx - \int_0^T \int_\Omega \partial_t \phi \cdot \rho dx dt$$
$$+ \sum_{i,j=1}^N \int_0^T \int_\Omega \nabla\phi_i \cdot A_{ij}(\rho) \nabla(\rho)_j dx dt$$
$$= \int_0^T \int_\Omega \phi \cdot f(\rho) dx dt \qquad \forall \phi \in H^1(Q_T)^N$$

Crucial Idea

Introduce entropy variable w and *bounded* transformation u s.t.

$$\rho = u(w)$$

- convex function $s \in C^2(\mathcal{D}, [0,\infty)) \cap C^0(\overline{\mathcal{D}})$, $\mathcal{D} \subset (0,\infty)^N$
- $s' : \mathcal{D} \to \mathbb{R}^N$ invertible and $u := (s')^{-1} \in C^1(\mathbb{R}^N, \mathcal{D})$,
  (a) There exists a constant $\gamma > 0$ such that
  $$z \cdot s''(\rho)A(\rho)z \geq \gamma |z|^2 \qquad \forall z \in \mathbb{R}^N,\ \rho \in \mathcal{D}.$$
  (b) There exists a constant $C_f \geq 0$ such that
  $$f(\rho) \cdot s'(\rho) \leq C_f \qquad \forall \rho \in \mathcal{D}.$$

Space-time Galerkin method

Find $w_h \in \boldsymbol{V}_h$ such that, by setting $\rho_h := u(w_h)$, it holds true that

$$\int_\Omega \phi(T) \cdot \rho_h(T) dx - \int_\Omega \phi(0) \cdot \rho_0 dx - \int_0^T \int_\Omega \partial_t \phi \cdot \rho_h dx dt \\ + \sum_{i,j=1}^N \int_0^T \int_\Omega \nabla \phi_i \cdot A_{ij}(\rho_h) \nabla (\rho_h)_j dx dt \\ = \int_0^T \int_\Omega \phi \cdot f(\rho_h) dx dt \qquad \forall \phi \in \boldsymbol{V}_h \tag{1}$$

Space-time Galerkin method

Find $w_h^\varepsilon \in \boldsymbol{V}_h$ such that, by setting $\rho_h^\varepsilon := u(w_h^\varepsilon)$, it holds true that

$$\begin{aligned}
&\varepsilon(\phi, w_h^\varepsilon)_{H^1(Q_T)^N} + \\
&\int_\Omega \phi(T)\cdot\rho_h^\varepsilon(T)dx - \int_\Omega \phi(0)\cdot\rho_0 dx - \int_0^T\int_\Omega \partial_t\phi\cdot\rho_h^\varepsilon dxdt \\
&+ \sum_{i,j=1}^N \int_0^T\int_\Omega \nabla\phi_i\cdot A_{ij}(\rho_h^\varepsilon)\nabla(\rho_h^\varepsilon)_j dxdt \\
&= \int_0^T\int_\Omega \phi\cdot f(\rho_h^\varepsilon)dxdt \qquad \forall\phi\in\boldsymbol{V}_h
\end{aligned} \tag{1}$$

$\Rightarrow$ gives nice bounds on $\|w_h^\varepsilon\|_{H^1(Q_T)}$

Proposition (Existence of discrete solutions)

Assume that $\rho_0 : \Omega \to \overline{\mathcal{D}}$ *is measurable. Then there exists a solution* $w_h^\varepsilon \in \boldsymbol{V}_h$ *of method* (1)*.*

Proof idea:

Consider $\Phi : \boldsymbol{V}_h \to \boldsymbol{V}_h$, $v \mapsto w$, where w denotes the unique solution of (1) for $\rho = u(v)$. Then by the Leray-Schauder fixed-point theorem, we obtain that Φ admits a fixed-point if

$$\{w \in \boldsymbol{V}_h : w = \sigma\Phi(w),\ \sigma \in [0,1]\}$$

is bounded.

Proposition (Convergence)

Assume that $\rho_0 : \Omega \to \overline{\mathcal{D}}$ *is measurable, and let* $w_h^\varepsilon \in \boldsymbol{V}_h$ *be a solution of* (1) *for* $\varepsilon, h > 0$*. Then there exist a weak solution*

$$\rho \in L^2(0,T;H^1(\Omega)^N) \cap H^1(0,T;(H^1(\Omega)')^N) \cap L^\infty((0,T)\times\Omega)^N$$

and sequences $h_i, \varepsilon_i \to 0$*, as* $i \to \infty$*, such that*

$$u(w_{h_i}^{\varepsilon_i}) \to \rho \qquad \text{in } L^r(Q_T)^N, \text{ as } i \to \infty$$

for all $r \in [1,\infty)$*.*

Proof idea:

1. Fix ε, take $h \to 0$
   Banach-Alaoglu + Rellich's theorem $\Rightarrow w_{h_\ell}^\varepsilon \xrightarrow{\ell\to\infty} w^\varepsilon$ in $L^2(Q_T)$ ✓
2. Take the limit $\varepsilon \to 0$
   compensated compactness

Lemma (div-curl lemma)

Let $\alpha, \alpha^\ell \in L^2(Q_T)^{1+d}$ *and* $\beta, \beta^\ell \in L^2(Q_T)^{1+d}$. *Then*

$$\alpha^\ell \rightharpoonup \alpha \quad \text{in } L^2(Q_T)^{1+d}, \text{ and } \quad (\operatorname{div}_{(t,x)}\alpha^\ell)_{\ell\in\mathbb{N}} \text{ bounded } L^2(Q_T),$$
$$\beta^\ell \rightharpoonup \beta \quad \text{in } L^2(Q_T)^{1+d}, \text{ and } \quad (\operatorname{curl}_{(t,x)}\beta^\ell)_{\ell\in\mathbb{N}} \text{ bounded } L^2(Q_T)^{(1+d)^2}$$

implies that

$$\int_{Q_T} \phi\alpha^\ell \cdot \beta^\ell \to \int_{Q_T} \phi\alpha \cdot \beta \qquad \forall \phi \in C_c^\infty(Q_T)$$

Proof idea (continued):

$$\alpha^\varepsilon = \begin{pmatrix} \rho_i^\varepsilon - \varepsilon\partial_t w_i^\varepsilon \\ J_i^\varepsilon - \varepsilon\nabla w_i^\varepsilon \end{pmatrix} \text{ and } \beta^\varepsilon := \begin{pmatrix} \rho_i^\varepsilon \\ 0 \end{pmatrix}, \text{ where } J_i^\varepsilon = -\sum_{j=1}^N A(\rho^\varepsilon)_{ij}\nabla\rho_j^\varepsilon.$$

Apply div-curl lemma

$$\int_{Q_T} \phi(\rho_i^{\varepsilon_\ell} - \varepsilon_\ell\partial_t w_i^{\varepsilon_\ell})\rho_i^{\varepsilon_\ell} \to \int_{Q_T} \phi\rho_i^2 \Rightarrow \rho_i^{\varepsilon_\ell} \to \rho_i \text{ in } L^2(Q_T)$$

Numerical Examples

- Heat equation
- Porous medium equation
- Fisher-KPP equation
- Maxwell-Stefan equation

Entropy density

In all cases, we consider the entropy density $s : \mathcal{D} \to [0, +\infty)$ defined by

$$s(\rho) = \sum_{j=1}^{N} \rho_j \log \rho_j + \left(1 - \sum_{j=1}^{N} \rho_j\right) \log \left(1 - \sum_{j=1}^{N} \rho_j\right) + \log(N+1),$$

where $\mathcal{D} := \left\{\rho \in (0,1)^N : \sum_{i=1}^{N} \rho_i < 1\right\}$. Moreover, $u : \mathbb{R}^N \to \mathcal{D}$ defined as

$$u_\ell(w) = \frac{e^{w_\ell}}{1 + \sum_{i=1}^{N} e^{w_i}} \quad \text{for } \ell = 1, \dots, N$$

is in $C^1(\mathbb{R}^N, \mathcal{D})$, and is the inverse of s'.

Heat equation

$$\partial_t \rho = \Delta\rho \qquad \text{in } \Omega,\ t > 0$$

Exact solution given by

$$\rho(t, \boldsymbol{x}) = 0.5\exp(-2\pi^2 t/\tau)\cos(\pi x_1)\cos(\pi x_2) + 0.5,$$

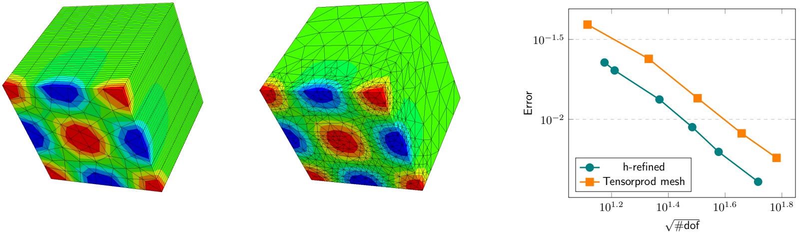


Figure: Comparison of a mesh made from time slabs (left) and an adapted space-time mesh (middle). The convergence of the two methods with respect to the number of degrees of freedom is shown on the right for $p = 1$.

Porous medium equation

$$\partial_t \rho = \Delta \rho^m \qquad \text{in } \Omega \; t > 0$$

Exact solution for $m = 2$:

$$\rho(x,t) = \frac{(x-5)^2}{12(5-t)}$$

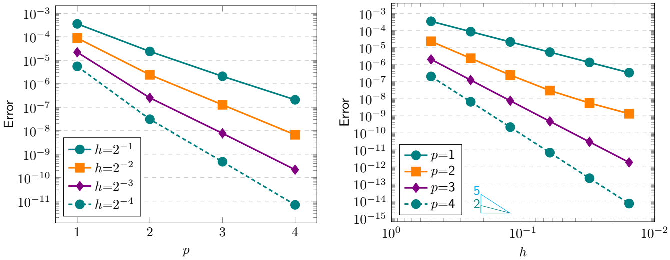


Figure: Convergence rates towards the exact solution of the porous medium equation, in polynomial degree p (left), and mesh size h (right).

Porous medium: finite propagaiton speed

$$\rho_0(x) = \begin{cases} \sin^{2/(m-1)}(x) & \text{if } 0 \leq x \leq \pi, \\ 0 & \text{otherwise,} \end{cases}$$

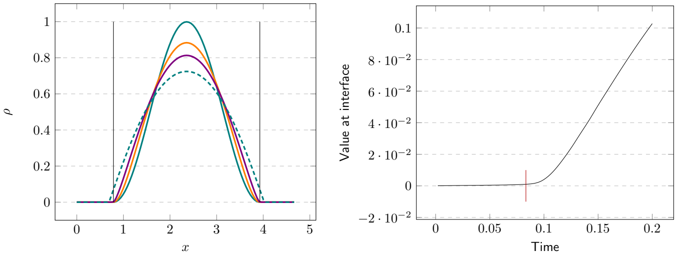


Figure: Snapshots of the solution of the porous medium equation emitting a waiting time, at different times (left) and the value at the left interface (right).

Fisher-KPP equation

$$\partial_t \rho = \Delta\rho + \rho(1-\rho) \qquad \text{in } \Omega,\ t>0$$

$$\rho(x,t) = \frac{1}{\left[1+\exp(-\frac{5}{6}t + \frac{1}{\sqrt{6}}x)\right]^2}$$

We set $\varepsilon = 10^{-16}$ and solve on unstructured simplicial space-time meshes.

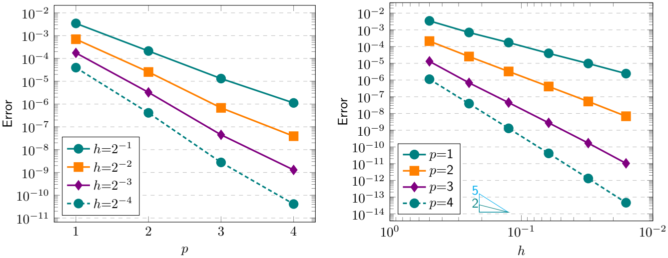


Figure: Convergence rates in polynomial degree p (left) and mesh size h for the exact solution of the Fisher-KPP equation.

Fisher-KPP equation: choice of entropy

Entropy 1: $\rho\log(\rho) - \rho + 1$

Entropy 2: $\rho\log\rho + (2-\rho)\log(2-\rho)$

Entropy 3: $\rho\log\rho + (2.1-\rho)\log(2.1-\rho)$

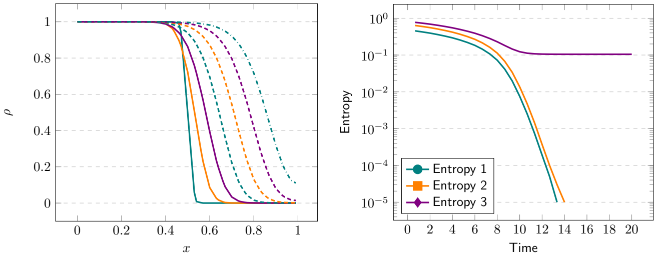


Figure: Snapshots of the numerical solution for the Fisher-KPP (left) and different choices of the entropy (right).

Francesca Bonizzoni, Marcel Braukhoff, Ansgar Jüngel, Ilaria Perugia
A structure-preserving discontinuous Galerkin scheme for the Fischer-KPP equation 2019, arxiv:1903.04212

Maxwell-Stefan system for $N = 2$

$$\partial_t \rho_i = \nabla \cdot \left(\sum_{j=1}^{2} A_{ij}(\rho_1, \rho_2) \nabla \rho_j \right) \text{ in } \Omega, \ t > 0$$

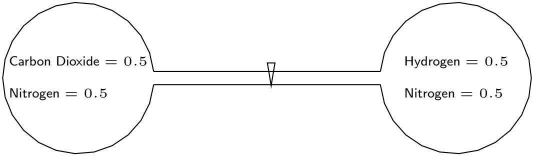
for $i = 1, 2$, with

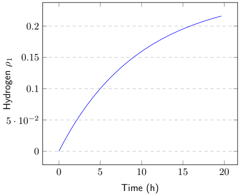
$$A(\rho_1, \rho_2) = \frac{1}{\delta(\rho_1, \rho_2)} \begin{pmatrix} d_1 + (d_3 - d_1)\rho_1 & (d_3 - d_2)\rho_1 \\ (d_3 - d_1)\rho_2 & d_2 + (d_3 - d_2)\rho_2 \end{pmatrix}$$

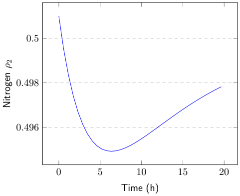
and

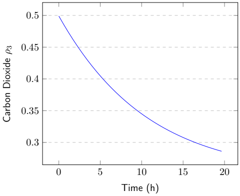
$$\delta(\rho_1, \rho_2) = d_1 d_2 (1 - \rho_1 - \rho_2) + d_2 d_3 \rho_1 + d_3 d_1 \rho_2.$$

Maxwell-Stefan: Duncan–Toor experiment









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