Structure-preserving discretization of nonlinear cross-diffusion systems

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Joint work with

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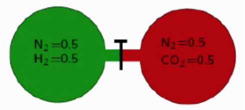
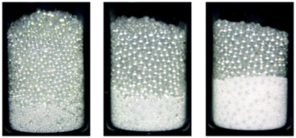
Cross-diffusion systems

- multi-component systems arise in physics, ecology, biology, and chemistry
  e.g. gas mixtures, competing population species, pattern formation, chemical reactions
- cross diffusion: the flux of one component is driven by the gradient of another
  (*uphill diffusion*, segregation)

interactions between species $\rightarrow$ spatial distribution





- space–time cylinder $Q_T = \Omega \times (0,T]$, $\Omega \subset \mathbb{R}^d$ Lipschitz polytope, $d \in \{1,2,3\}$
- densities/concentrations $\boldsymbol{\rho} := (\rho_1, \ldots, \rho_N) : Q_T \to \mathbb{R}^N$, $N \geq 1$ number of species
- diffusion matrix $A : \mathbb{R}^N \to \mathbb{R}^{N \times N}$
- reaction $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^N$

reaction-diffusion system

$$\begin{aligned} \partial_t \boldsymbol{\rho} - \nabla \circ (A(\boldsymbol{\rho}) \nabla \boldsymbol{\rho}) &= \boldsymbol{f}(\boldsymbol{\rho}) && \text{in } Q_T \\ (A(\boldsymbol{\rho}) \nabla \boldsymbol{\rho})\, \underline{n}_\Omega &= \mathbf{0} && \text{on } \partial\Omega \times (0,T) \\ \boldsymbol{\rho} &= \boldsymbol{\rho}_0 && \text{on } \Omega \times \{0\} \end{aligned}$$

- $A \in \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^{N \times N}\right)$ and $\boldsymbol{f} \in \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^N\right)$, for a bounded domain $\mathcal{D} \subset (0,\infty)^N$
- $\boldsymbol{\rho}_0 \in \mathcal{D}$ a.e. in Ω

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[Shigesada-Kawasaki-Teramoto, 1979]

- modeling spatial segregation and pattern formation of (two) competing species including cross-diffusion effects
- applications: ecology, environmental sciences, conservation biology

SKT system ($N = 2$)

$$\begin{cases} \dfrac{\partial \rho_1}{\partial t} - a_{10}\Delta\rho_1 - \nabla \cdot \Big(\rho_1(2a_{11}\nabla\rho_1 + a_{12}\nabla\rho_2) + a_{12}\rho_2\nabla\rho_1\Big) = \rho_1(b_{10} - b_{11}\rho_1 - b_{12}\rho_2) \\ \dfrac{\partial \rho_2}{\partial t} - a_{20}\Delta\rho_2 - \nabla \cdot \Big(\rho_2(a_{21}\nabla\rho_1 + 2a_{22}\nabla\rho_2) + a_{21}\rho_1\nabla\rho_2\Big) = \rho_2(b_{20} - b_{21}\rho_1 - b_{22}\rho_2) \end{cases}$$

Example: the Shigesada-Kawasaki-Teramoto system

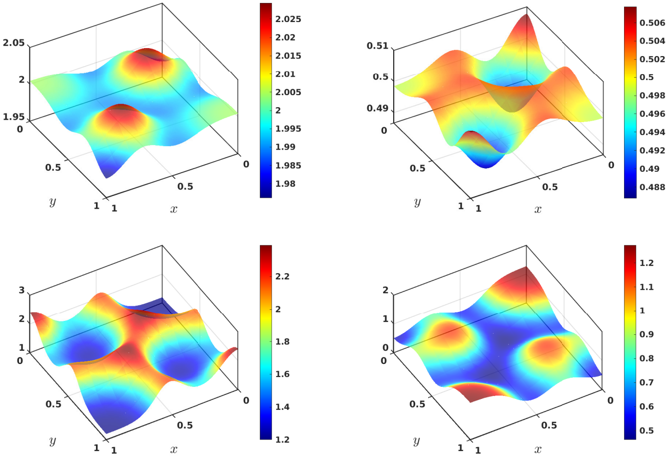
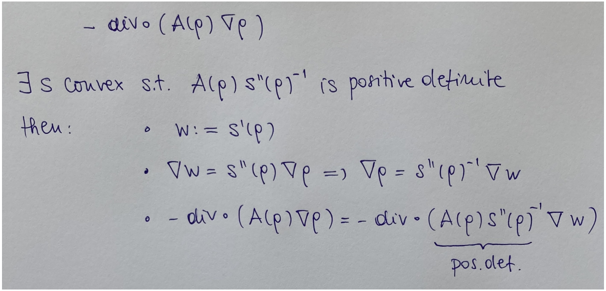


Figure: SKT system with data as in [Jüngel & Zurek, 2021] ($\rho_1|_{t=0}$ two bumps, $\rho_2|_{t=0} = 0.5$): ρ_1 (left) and ρ_2 (right) at $t = 0.5$ (top) and $t = 10$ (bottom).

- nonlinearity and coupled nature of equations
- the diffusion matrix $A(\cdot)$ may not be symmetric or positive definite
- a maximum principle may not be available
- positivity/boundedness of solutions

cross-diffusion systems with entropy structure

$\longrightarrow$ boundedness-by-entropy framework [Jüngel, 2015]



[Jüngel, 2015]

$$A \in \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^{N\times N}\right) \text{ and } \boldsymbol{f} \in \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^N\right), \text{ for a bounded domain } \mathcal{D} \subset (0,\infty)^N$$

assumptions

there exists a convex function $s \in \mathcal{C}^2(\mathcal{D}; (0,\infty)) \cap \mathcal{C}^0\left(\overline{\mathcal{D}}; (0,\infty)\right)$ satisfying

- $s' : \mathcal{D} \to \mathbb{R}^N$ invertible with inverse $\boldsymbol{u} := (s')^{-1} \in \mathcal{C}^1\left(\mathbb{R}^N; \mathcal{D}\right)$
- there exists a constant $\gamma > 0$ such that

$$\mathbf{z} \cdot \left(s''(\boldsymbol{\rho})A(\boldsymbol{\rho})\mathbf{z}\right) \geq \gamma\,|\mathbf{z}|^2 \qquad \forall \mathbf{z} \in \mathbb{R}^N,\ \boldsymbol{\rho} \in \mathcal{D} \qquad (\text{“coer}\,A\text{”})$$

- there exists a constant $C_f \geq 0$ such that

$$\boldsymbol{f}(\boldsymbol{\rho}) \cdot s'(\boldsymbol{\rho}) \leq C_f \quad \forall \boldsymbol{\rho} \in \mathcal{D} \qquad (\text{“cont}\,\boldsymbol{f}\text{”})$$

- the initial datum satisfies $\boldsymbol{\rho}_0 \in \mathcal{D}$ a.e. in Ω so that

$$\int_\Omega s(\boldsymbol{\rho}_0)\mathrm{d}\boldsymbol{x} < \infty$$

$s(\cdot)$ entropy density function

entropy
$$\mathcal{H}(\boldsymbol{\rho}) := \int_\Omega s(\boldsymbol{\rho})\,dx$$

- introduce the entropy variable $\boldsymbol{w} := s'(\boldsymbol{\rho})$
- s' invertible $\Rightarrow$ $\boldsymbol{\rho} = (s')^{-1}(\boldsymbol{w}) = \boldsymbol{u}(\boldsymbol{w})$
- $\mathcal{D}$ bounded, $\boldsymbol{u} \in \mathcal{C}^1\left(\mathbb{R}^N; \mathcal{D}\right)$ $\Rightarrow$ pointwise boundedness of $\boldsymbol{u}(\boldsymbol{w}) = \boldsymbol{\rho}$ (no max. princ. used)
- regularity of s $\Rightarrow$ $\nabla \boldsymbol{w} = \nabla\left(s'(\boldsymbol{\rho})\right) = s''(\boldsymbol{\rho})\nabla\boldsymbol{\rho}$ (chain rule)

entropy-stability estimate

test with $\boldsymbol{w} = s'(\boldsymbol{\rho})$, use the chain rule and "coer A", "cont $\boldsymbol{f}$":

$$\int_\Omega s(\boldsymbol{\rho}(\boldsymbol{x},\tau))\mathrm{d}\boldsymbol{x} + \gamma \int_0^\tau \|\nabla \boldsymbol{\rho}\|^2_{[L^2(\Omega)^d]^N} \mathrm{d}t \le \int_\Omega s(\boldsymbol{\rho}_0)\mathrm{d}\boldsymbol{x} + \tau C_f |\Omega| \qquad \text{for all } 0 < \tau \le T$$

SKT system ($N = 2$)

$$\begin{cases} \dfrac{\partial \rho_1}{\partial t} - a_{10}\Delta\rho_1 - \nabla\cdot\Big(\rho_1(2a_{11}\nabla\rho_1 + a_{12}\nabla\rho_2) + a_{12}\rho_2\nabla\rho_1\Big) = \rho_1(b_{10} - b_{11}\rho_1 - b_{12}\rho_2) \\ \dfrac{\partial \rho_2}{\partial t} - a_{20}\Delta\rho_2 - \nabla\cdot\Big(\rho_2(a_{21}\nabla\rho_1 + 2a_{22}\nabla\rho_2) + a_{21}\rho_1\nabla\rho_2\Big) = \rho_2(b_{20} - b_{21}\rho_1 - b_{22}\rho_2) \end{cases}$$

modified Boltzmann-Shannon entropy

$$s(\boldsymbol{\rho}) = \pi_1\left(\rho_1(\log\rho_1 - 1) + 1\right) + \pi_2\left(\rho_2(\log\rho_2 - 1) + 1\right)$$

with $\pi_1, \pi_2 > 0$, $\pi_i a_{ij} = \pi_j a_{ji}$ for $i \neq j$ (detailed balance condition)

[Chen, Daus, Jüngel, 2018]

Numerical approximation: desired properties

- arbitrary degrees of approximation (in space)
- positivity/boundedness of numerical solutions with no postprocessing or slope limiters
- discrete version of the entropy-stability estimate of the continuous problem
- nonlinearities not appearing within spatial differential operators or interface terms
  $\rightarrow$ natural parallelizable structure and high efficiency

positivity preservation in high-order methods (with no postprocessing/slope limiters)

- [Barrenechea, John, Knobloch, 2024]: recent survey
- [Barrenechea, Georgoulis, Pryer, Veeser, 2023] nodally bound-preserving FEM
- entropy variable
  [Bonizzoni, Braukhoff, Jüngel, Perugia, 2020], [Corti, Bonizzoni, Antonietti, 2023]: IPDG
  [Braukhoff, Perugia, Stocker, 2022]: space-time FEM
  [Lemaire & Moatti, 2024]: HHO

A conforming space-time discretization

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[Braukhoff, Perugia, Stocker, 2022]

1. space-time variational formulation
2. transformation to entropy variables
3. regularization
4. monolithic space-time Galerkin discretization

structure preservation

- space-time approach to the proof of existence of bounded, nonnegative weak solutions (space-time version of the boundedness-by-entropy method, [Jüngel, 2015])
- space-time continuous Galerkin discretization preserving the entropy structure of the continuous problem

✓ arbitrary degrees of approximation (in space and time)

✓ positivity/boundedness of numerical solutions with no postprocessing or slope limiters

✓ discrete version of the entropy-stability estimate of the continuous problem

✗ nonlinearities not appearing within spatial differential operators or interface terms

$\rightarrow$ natural parallelizable structure and high efficiency

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$$\partial_t \boldsymbol{\rho} - \nabla \circ (A(\boldsymbol{\rho})\nabla\boldsymbol{\rho}) = \boldsymbol{f}(\boldsymbol{\rho}) \quad \text{in } Q_T$$

entropy variable $\quad \boldsymbol{w} := s'(\boldsymbol{\rho}), \quad \boldsymbol{\rho} = (s')^{-1}(w) = \boldsymbol{u}(\boldsymbol{w})$

chain rule $\quad \nabla \boldsymbol{w} = \nabla(s'(\boldsymbol{\rho})) = s''(\boldsymbol{\rho})\nabla\boldsymbol{\rho}$ [Jüngel & Zurek, 2021]

auxiliary variables & re-formulation (recall: $\boldsymbol{\rho} = \boldsymbol{u}(\boldsymbol{w})$)

$$\underline{\boldsymbol{\zeta}} := -\nabla \boldsymbol{w}$$

$$\underbrace{A(\boldsymbol{\rho})^T s''(\boldsymbol{\rho})}_{\text{pos. def.}}\underline{\boldsymbol{\sigma}} := -\underbrace{A(\boldsymbol{\rho})^T s''(\boldsymbol{\rho})}_{\text{pos. def.}}\nabla\boldsymbol{\rho} \overset{\text{ch.r.}}{=} A(\boldsymbol{\rho})^T \underline{\boldsymbol{\zeta}} \quad \sim \quad \underline{\boldsymbol{\sigma}} = -\nabla\boldsymbol{\rho}$$

$$\underline{\boldsymbol{q}} := A(\boldsymbol{\rho})\underline{\boldsymbol{\sigma}} \quad \sim \quad \underline{\boldsymbol{q}} = -A(\boldsymbol{\rho})\nabla\boldsymbol{\rho}$$

$$\partial_t \boldsymbol{\rho} + \nabla \circ \underline{\boldsymbol{q}} = \boldsymbol{f}(\boldsymbol{\rho})$$

with boundary and initial conditions:

$$\underline{\boldsymbol{q}} \circ \underline{n}_\Omega = \boldsymbol{0} \ \text{ on } \partial\Omega \times (0,T), \qquad \boldsymbol{\rho} = \boldsymbol{\rho}_0 \ \text{ on } \Omega \times \{0\}$$

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re-formulation

$$\underline{\zeta} = -\nabla \boldsymbol{w}$$
$$A\left(\boldsymbol{u}(\boldsymbol{w})\right)^T s''\left(\boldsymbol{u}(\boldsymbol{w})\right) \underline{\boldsymbol{\sigma}} = A\left(\boldsymbol{u}(\boldsymbol{w})\right)^T \underline{\zeta}$$
$$\underline{\boldsymbol{q}} = A\left(\boldsymbol{u}(\boldsymbol{w})\right) \underline{\boldsymbol{\sigma}}$$
$$\partial_t \left(\boldsymbol{u}(\boldsymbol{w})\right) + \nabla \circ \underline{\boldsymbol{q}} = \boldsymbol{f}\left(\boldsymbol{u}(\boldsymbol{w})\right)$$

with boundary and initial conditions

- introduce a triangular mesh $\mathcal{T}_h$ of Ω, multiply by discontinuous $\mathbb{P}^p$ test functions
- the 1st equation is linear → standard DG discretization $(\widehat{\boldsymbol{w}}_h = \{\!\{\boldsymbol{w}_h\}\!\})$
- the 4th equation is linear in $\underline{\boldsymbol{q}}$ → standard DG discretization of $\nabla \circ \underline{\boldsymbol{q}}$ $(\widehat{\underline{\boldsymbol{q}}}_h = \{\!\{\underline{\boldsymbol{q}}_h\}\!\} + \eta_F [\![\boldsymbol{w}_h]\!]_{\mathsf{N}})$

nonlinearities do not appear within spatial differential operators

↓

nonlinearities do not appear within interface (coupling) terms

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$$\begin{aligned} \underline{\zeta} &= -\nabla \boldsymbol{w} \\ A(\boldsymbol{u}(\boldsymbol{w}))^T s''(\boldsymbol{u}(\boldsymbol{w}))\,\underline{\boldsymbol{\sigma}} &= A(\boldsymbol{u}(\boldsymbol{w}))^T \underline{\zeta} \\ \underline{\boldsymbol{q}} &= A(\boldsymbol{u}(\boldsymbol{w}))\,\underline{\boldsymbol{\sigma}} \\ \partial_t(\boldsymbol{u}(\boldsymbol{w})) + \nabla \circ \underline{\boldsymbol{q}} &= \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{w})) \end{aligned}$$

- the 2nd equation is linear in $\underline{\boldsymbol{\sigma}}$ and local $\rightarrow$ given $\boldsymbol{w}_h$, $\underline{\boldsymbol{\sigma}}_h$ is computed by solving independent (naturally parallelizable) linear problems on each mesh element
- the 3rd equation is linear in $\underline{\boldsymbol{q}}$ and local $\rightarrow$ same as above

semidiscrete formulation in operator form

$$\begin{aligned} (I_N \otimes \boldsymbol{M})\boldsymbol{Z}_h &= (I_N \otimes B)\mathbf{W}_h \\ \widehat{\underline{\boldsymbol{\mathcal{N}}}}_h(\mathbf{W}_h)\boldsymbol{\Sigma}_h &= \widehat{\underline{\boldsymbol{\mathcal{A}}}_h}(\mathbf{W}_h)^T \boldsymbol{Z}_h \\ (I_N \otimes \boldsymbol{M})\mathbf{Q}_h &= \widehat{\underline{\boldsymbol{\mathcal{A}}}_h}(\mathbf{W}_h)\boldsymbol{\Sigma}_h \end{aligned}$$

$$\frac{d}{dt}\boldsymbol{\mathcal{U}}_h(\mathbf{W}_h) + (I_N \otimes B^T)\mathbf{Q}_h + (I_N \otimes S)\mathbf{W}_h = \boldsymbol{\mathcal{F}}_h(\mathbf{W}_h)$$

where I_N denotes the identity matrix of size N and $\otimes$ the Kronecker product

- the blue matrices are block diagonal
- the only non-block-diagonal matrices are B and S (standard LDG matrices)
- $\boldsymbol{M}$ block-diagonal mass matrix $\rightarrow$ eliminate $\boldsymbol{Z}_h$ and $\mathbf{Q}_h$

$$
\begin{aligned}
(I_N \otimes \boldsymbol{M}) \boldsymbol{Z}_h &= (I_N \otimes B) \mathbf{W}_h \\
\widehat{\boldsymbol{\mathcal{N}}}_h(\mathbf{W}_h) \boldsymbol{\Sigma}_h &= \widehat{\boldsymbol{\mathcal{A}}_h}(\mathbf{W}_h)^T \boldsymbol{Z}_h \\
(I_N \otimes \boldsymbol{M}) \mathbf{Q}_h &= \widehat{\boldsymbol{\mathcal{A}}_h}(\mathbf{W}_h) \boldsymbol{\Sigma}_h \\
\frac{d}{dt} \boldsymbol{\mathcal{U}}_h(\mathbf{W}_h) + (I_N \otimes B^T) \mathbf{Q}_h + (I_N \otimes S) \mathbf{W}_h &= \boldsymbol{\mathcal{F}}_h(\mathbf{W}_h)
\end{aligned}
$$

eliminate $\boldsymbol{Z}_h$ and $\mathbf{Q}_h$

↓

system in $(\mathbf{W}_h, \boldsymbol{\Sigma}_h)$

theoretical results

- given $\mathbf{W}_h$, the 2nd equation defines $\boldsymbol{\Sigma}_h$ in a unique way

$$
\boldsymbol{\Sigma}_h = \widehat{\boldsymbol{\mathcal{N}}}_h(\mathbf{W}_h)^{-1} \widehat{\boldsymbol{\mathcal{A}}_h}(\mathbf{W}_h)^T \underbrace{(I_N \otimes \boldsymbol{M}^{-1} B) \mathbf{W}_h}_{\boldsymbol{Z}_h}
$$

- any solution $(\boldsymbol{w}_h, \boldsymbol{\sigma}_h)$ satisfies a space-semidiscrete version of the entropy inequality

semidiscrete formulation: compact form

$$\frac{d}{dt}\boldsymbol{\mathcal{U}}_h(\mathbf{W}_h) + \widehat{\underline{\boldsymbol{\mathcal{B}}}_h}(\mathbf{W}_h)\mathbf{W}_h = \boldsymbol{\mathcal{F}}_h(\mathbf{W}_h)$$

with $\widehat{\underline{\boldsymbol{\mathcal{B}}}_h} := (I_N \otimes B^T \boldsymbol{M}^{-1})\, \underbrace{\widehat{\underline{\boldsymbol{\mathcal{A}}}_h}(\mathbf{W}_h)\widehat{\underline{\boldsymbol{\mathcal{N}}}}_h(\mathbf{W}_h)^{-1}\widehat{\underline{\boldsymbol{\mathcal{A}}}_h}(\mathbf{W}_h)^T}_{} (I_N \otimes \boldsymbol{M}^{-1}B) + (I_N \otimes S)$

- backward Euler time discretization with time steps τ_n, $1 \le n \le N_t$
- initialization with the L^2 projection of $\boldsymbol{\rho}_0$ onto the discrete space
- additional regularization term

$$\varepsilon(I_N \otimes C)\mathbf{W}_h$$

with $\varepsilon > 0$ and C corresponding to a spatial H^ℓ-type DG inner product ($\ell = 1$ or 2) to provide control of $\boldsymbol{w}_h$ in the corresponding norm

fully discrete formulation

- $\mathbf{R}_h^0 :=$ vector representation of $\Pi_p^0 \boldsymbol{\rho}_0$; compute $\mathbf{W}_h^{\varepsilon,1}, \boldsymbol{\Sigma}_h^{\varepsilon,1}$ by solving

$$\varepsilon(I_N \otimes C)\mathbf{W}_h^{\varepsilon,1} + \frac{1}{\tau_1}\Big(\boldsymbol{\mathcal{U}}_h(\mathbf{W}_h^{\varepsilon,1}) - \mathbf{R}_h^0\Big) + \widehat{\boldsymbol{\mathcal{B}}_h}(\mathbf{W}_h^{\varepsilon,1})\mathbf{W}_h^{\varepsilon,1} = \boldsymbol{\mathcal{F}}_h(\mathbf{W}_h^{\varepsilon,1})$$

- for $n = 1, \ldots, N_t - 1$, compute $\mathbf{W}_h^{\varepsilon,n+1}, \boldsymbol{\Sigma}_h^{\varepsilon,n+1}$ by solving

$$\varepsilon(I_N \otimes C)\mathbf{W}_h^{\varepsilon,n+1} + \frac{1}{\tau_{n+1}}\Big(\boldsymbol{\mathcal{U}}_h(\mathbf{W}_h^{\varepsilon,n+1}) - \boldsymbol{\mathcal{U}}_h(\mathbf{W}_h^{\varepsilon,n})\Big) + \widehat{\boldsymbol{\mathcal{B}}_h}(\mathbf{W}_h^{\varepsilon,n+1})\mathbf{W}_h^{\varepsilon,n+1} = \boldsymbol{\mathcal{F}}_h(\mathbf{W}_h^{\varepsilon,n+1})$$

- any solution $\{\boldsymbol{w}_h^{\varepsilon,n}\}_{n=1}^{N_t}$ satisfies a discrete version of the entropy inequality
- for $n = 0, \dots, N_t - 1$, there exists a solution $\boldsymbol{w}_h^{\varepsilon,n+1}$ (Leray-Schauder/Schaefer)
- h-convergence: for any $n = 1, \dots, N_t$, there exists $\boldsymbol{w}^{\varepsilon,n} \in H^\ell(\Omega)^N$ with $\boldsymbol{u}(\boldsymbol{w}^{\varepsilon,n}) \in H^1(\Omega)^N$ such that, up to a subsequence, as $h \to 0$,

$$\boldsymbol{\rho}_h^{\varepsilon,n} := \boldsymbol{u}\left(\boldsymbol{w}_h^{\varepsilon,n}\right) \to \boldsymbol{\rho}^{\varepsilon,n} := \boldsymbol{u}\left(\boldsymbol{w}^{\varepsilon,n}\right) \qquad \text{strongly in } L^r(\Omega)^N \text{ for all } r \in [1, \infty)$$

  where $\{\boldsymbol{w}^{\varepsilon,n}\}_{n=1}^{N_t}$ solves an ε-perturbed time-semidiscrete problem and satisfies a time-discrete entropy inequality

- this limit problem is the one used in the analysis of [Jüngel, 2015]
- $\boldsymbol{\rho}^{(\varepsilon,\tau)} :=$ piecewise linear reconstruction in time of $\{\boldsymbol{\rho}^{\varepsilon,n}\}_{n=0}^{N_t}$
- (ε, τ)-convergence: there exists a *continuous weak solution* $\boldsymbol{\rho}$ to the cross-diffusion problem such that, up to a subsequence, as $(\varepsilon,\tau) \to (0,0)$,

$$
\begin{aligned}
\boldsymbol{\rho}^{(\varepsilon,\tau)} &\to \boldsymbol{\rho} \quad \text{strongly in } L^r(0,T;L^r(\Omega)^N) \text{ for any } r<\infty \text{ \& a.e. in } \Omega\times(0,T] \\
\nabla\boldsymbol{\rho}^{(\varepsilon,\tau)} &\rightharpoonup \nabla\boldsymbol{\rho} \quad \text{weakly in } L^2(0,T;[L^2(\Omega)^d]^N) \\
\frac{\boldsymbol{\rho}^{(\varepsilon,\tau)} - \mathbf{s}_\tau\boldsymbol{\rho}^{(\varepsilon,\tau)}}{\tau} &\rightharpoonup \partial_t\boldsymbol{\rho} \quad \text{weakly in } L^2(0,T;[H^\ell(\Omega)^N]')
\end{aligned}
$$

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continuous weak solution:

- $\boldsymbol{\rho} \in L^2(0,T;H^1(\Omega)^N) \cap H^1(0,T;[H^1(\Omega)^N]') \cap L^r(0,T;L^r(\Omega)^N)$ for all $r < \infty$
- $\boldsymbol{\rho}(\boldsymbol{x},t) \in \overline{\mathcal{D}}$ a.e. in $\Omega \times (0,T]$
- $\boldsymbol{\rho}(\cdot,t) = \boldsymbol{\rho}_0(\cdot)$ in the sense of $[H^1(\Omega)^N]'$
- $\int_0^T \langle\partial_t\boldsymbol{\rho},\boldsymbol{\lambda}\rangle \mathrm{d}t + \int_0^T\int_\Omega A(\boldsymbol{\rho})\nabla\boldsymbol{\rho} : \nabla\boldsymbol{\lambda}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_0^T\int_\Omega \boldsymbol{f}(\boldsymbol{\rho})\cdot\boldsymbol{\lambda}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \quad \forall\boldsymbol{\lambda} \in L^2(0,T;H^1(\Omega)^N)$

- H^1-type DG inner product if $d = 1$ or $d = 2, 3$ and $s'' A \in \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^{N\times N}\right)$

$$(w_h, v_h)_C := \int_\Omega w_h v_h \mathrm{d}\boldsymbol{x} + \int_\Omega \nabla_{\mathsf{DG}} w_h \cdot \nabla_{\mathsf{DG}} v_h \mathrm{d}\boldsymbol{x} + \int_{\mathcal{F}_h^{\mathcal{I}}} \mathsf{h}^{-1} [\![w_h]\!]_{\mathsf{N}} \cdot [\![v_h]\!]_{\mathsf{N}} \mathrm{d}S$$

properties from [Buffa & Ortner, 2009]

- H^2-type DG inner product otherwise

$$(w_h, v_h)_C := \int_\Omega w_h v_h \mathrm{d}\boldsymbol{x} + \int_\Omega \nabla_{\mathsf{DG}} w_h \cdot \nabla_{\mathsf{DG}} v_h \mathrm{d}\boldsymbol{x} + \int_\Omega \mathcal{H}_{\mathsf{DG}} w_h : \mathcal{H}_{\mathsf{DG}} v_h \mathrm{d}\boldsymbol{x} + \int_{\mathcal{F}_h^{\mathcal{I}}} \mathsf{h}^{-1} [\![\nabla_h w_h]\!] \cdot [\![\nabla_h v_h]\!] \mathrm{d}S + \int_{\mathcal{F}_h^{\mathcal{I}}} \mathsf{h}^{-3} [\![w_h]\!]_{\mathsf{N}} \cdot [\![v_h]\!]_{\mathsf{N}} \mathrm{d}S$$

properties from [Bonito, Guignard, Nochetto, Yang, 2023]

- auxiliary result (needed if $s'' A \notin \mathcal{C}^0\left(\overline{\mathcal{D}}; \mathbb{R}^{N\times N}\right)$)

  DG Sobolev embedding $\qquad \|w_h\|_{L^\infty(\Omega)} \lesssim \|w_h\|_C$

- the assumption that $\mathcal{D}$ is bounded can be removed

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One-dimensional porous medium equation ($N = 1$)

$$\partial_t \rho - \Delta \rho^m = 0 \quad \text{in } Q_T \qquad (A(\rho) = m\rho^{m-1},\ f \equiv 0\,;\ m \in (1, 2])$$

- $\mathcal{D} = (0, 1)$, $s : \overline{\mathcal{D}} \to (0, \infty)$

$$s(\rho) := \rho \log(\rho) + (1 - \rho) \log(1 - \rho) + \log(2)$$

- $s'(\rho) = \log\left(\frac{\rho}{1-\rho}\right)$, $s''(\rho) = \frac{1}{\rho(1-\rho)}$, $u(w) = \frac{e^w}{1+e^w}$
- "coer$A$" with $\gamma = m$, "cont$\boldsymbol{f}$" with $C_f = 0$

test with exact solution

$$\rho(x,t) = \frac{(x-2)^2}{12(5-t)} \qquad (m = 2,\ \Omega = (0,1))$$

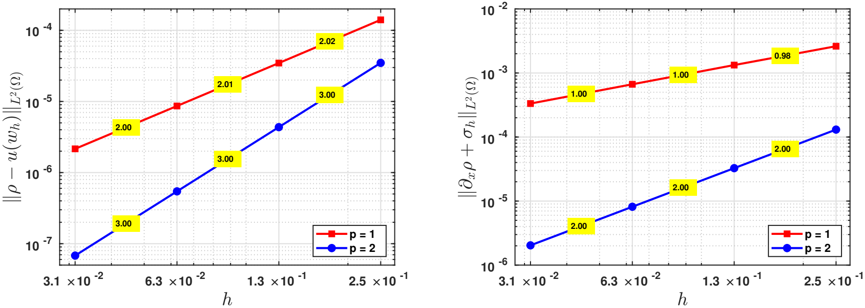

Figure: h-convergence of the errors at time $T = 1$ with $\varepsilon = 0$ ($\tau = \mathcal{O}(h^{p+1})$)

test with $\Omega = (-\pi/4, 5\pi/4)$, $m = 2$, initial datum

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

exact solution supported in $[0, \pi]$ until the waiting time $t^* = (m-1)/(2m(m+1))$

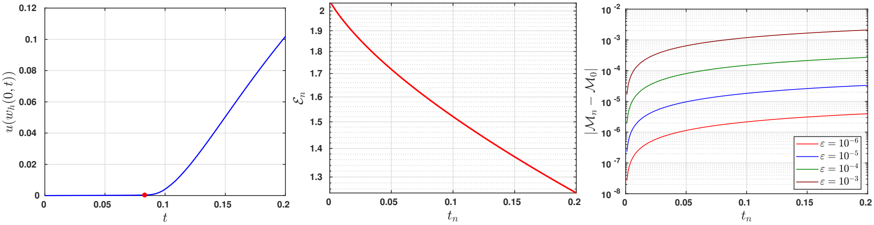

Figure: Evolution of $\rho_h := u(w_h)$ at $x = 0$, $t^* = 0.8\overline{3}$ (left); entropy values (center); error in the mass conservation, due to the regularization (right); $\varepsilon = 10^{-6}$, $p = 5$, $h \approx 0.04$, $\tau = 10^{-3}$.

Two-dimensional Shigesada-Kawasaki-Teramoto system ($N = 2$)

$$\begin{cases} \dfrac{\partial \rho_1}{\partial t} - a_{10}\Delta\rho_1 - \nabla \cdot \Big(\rho_1(2a_{11}\nabla\rho_1 + a_{12}\nabla\rho_2) + a_{12}\rho_2\nabla\rho_1\Big) = \rho_1(b_{10} - b_{11}\rho_1 - b_{12}\rho_2) \\ \dfrac{\partial \rho_2}{\partial t} - a_{20}\Delta\rho_2 - \nabla \cdot \Big(\rho_2(a_{21}\nabla\rho_1 + 2a_{22}\nabla\rho_2) + a_{21}\rho_1\nabla\rho_2\Big) = \rho_2(b_{20} - b_{21}\rho_1 - b_{22}\rho_2) \end{cases}$$

- $N = 2$, $\mathcal{D} = (0, +\infty)$, $s : (0,\infty)^2 \to (0,\infty)$

$$s(\boldsymbol{\rho}) := \pi_1\,(\rho_1(\log\rho_1 - 1) + 1) + \pi_2\,(\rho_2(\log\rho_2 - 1) + 1)$$

- $s'(\boldsymbol{\rho}) = (\pi_1 \log\rho_1, \pi_2\log\rho_2)$, $s''(\boldsymbol{\rho}) = \mathrm{diag}(\pi_i/\rho_i)$, $\boldsymbol{u}(\boldsymbol{w}) = (\exp(w_1/\pi_1), \exp(w_2/\pi_2))$
- "coer$A$" with $\gamma = \min\{\pi_1 a_{11}, \pi_2 a_{22}\}$, "cont$\boldsymbol{f}$" compensated with τ suff. small

test with $a_{10} = a_{20} = 0$, $a_{12} = a_{21} = 1$ ($\pi_1 = \pi_2 = 1$) and exact solution

$$\rho_1(x, y, t) = 0.25 \cos(2\pi x) \cos(\pi y) \exp(-t) + 0.5$$
$$\rho_2(x, y, t) = 0.25 \cos(\pi x) \cos(2\pi y) \exp(-t) + 0.5$$

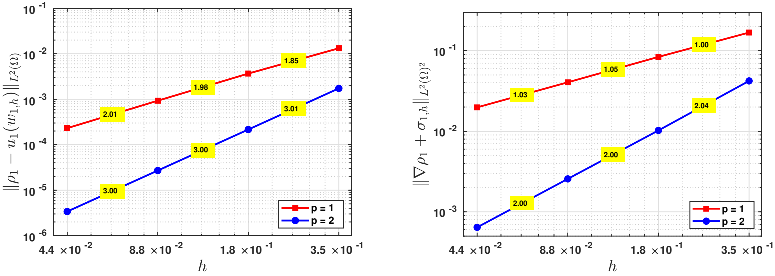

Figure: h-convergence of the errors at time $T = 0.5$ with $\varepsilon = 0$ ($\tau = \mathcal{O}(h^{p+1})$)

test with data as in [Jüngel & Zurek, 2021] ($\rho_{1|_{t=0}}$ two bumps, $\rho_{2|_{t=0}} = 0.5$)

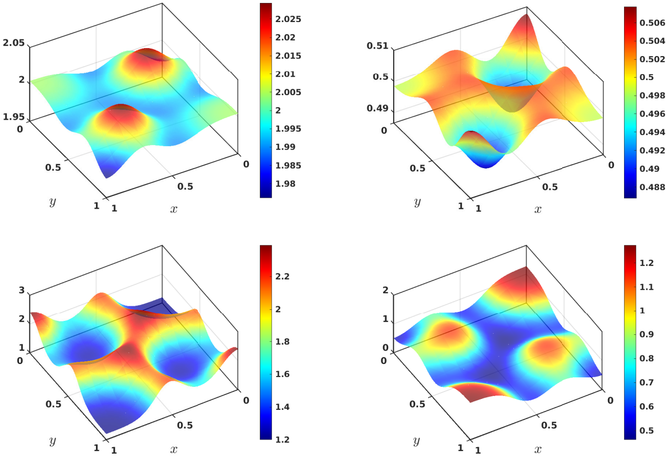

Figure: ρ_1 (left) and ρ_2 (right) at $t = 0.5$ (top) and $t = 10$ (bottom); $\varepsilon = 0$, $p = 3$, $h \approx 0.14$.

structure-preserving LDG method

- postitivity
- chain rule
- entropy stability inequality
- local nonlinear terms

[S. Gómez, A. Jüngel, and I. Perugia, Structure-preserving discretization of nonlinear cross-diffusion systems, in preparation]

ongoing work

- high-order discretization in time
- extensive numerical testing

Thank you for your attention!