A bound-preserving upwind DG scheme for the convective Cahn-Hilliard model





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Section 1

Linear convection

Linear convection problem

We consider the linear convection problem:

$$v_t + \nabla \cdot (\beta v) = 0$$
 in $\Omega \times (0, T)$, (1a)
 $v(0) = v_0$ in Ω , (1b)

where

- $\beta \colon \overline{\Omega} \to \mathbb{R}^d$ is continuous and incompressible, i.e, $\nabla \cdot \beta = 0$ in Ω ,
- $\boldsymbol{\beta} \cdot \boldsymbol{n} = 0$ on $\partial \Omega$.

Properties:

- Existence and uniqueness of the solution.
- Mass conservation: $\frac{d}{dt} \int_{\Omega} v = 0$.
- Maximum principle: $\min_{\overline{\Omega}} v_0 \leq v \leq \max_{\overline{\Omega}} v_0$ in $\overline{\Omega} \times (0, T)$.

Discontinuous Galerkin methods

$$\mathbb{P}^{\mathsf{disc}}_{k}(\mathscr{T}_{h}) \coloneqq \left\{ v_{h} \in L^{2}(\Omega) \colon v_{h|_{K_{i}}} \in \mathbb{P}_{k}(K_{i}) \text{ with } K_{i} \in \mathscr{T}_{h}, \forall i \in \{1, 2, \dots, N_{\mathscr{T}_{h}}\} \right\}$$

with a basis $\{\phi_i\}_{i\in\{1,2,\ldots,N_h\}}$.

Notation:

- Average: $\{v\}$:= $\begin{cases} \frac{v_K + v_L}{2} & \text{if } e = \partial K \cap \partial L \in \mathscr{C}_h^i \\ v_K & \text{if } e = \partial K \in \mathscr{C}_h^b \end{cases}$
- Jump: $\llbracket v \rrbracket := \begin{cases} v_K v_L & \text{if } e = \partial K \cap \partial L \in \mathscr{C}_h^i \\ v_K & \text{if } e = \partial K \in \mathscr{C}_h^b \end{cases}$
- Positive part: $v_{\oplus} \coloneqq \frac{|v| + v}{2} = \max\{v, 0\},$
- Negative part: $v_{\ominus} := \frac{|v| v}{2} = -\min\{v, 0\},$
- $v = v_{\oplus} v_{\ominus}$.

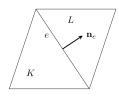


Figure: Orientation of unit normal vector.

DG upwind method

$$\begin{split} \bullet \ \ & a_h^{\mathsf{upw}} : \mathbb{P}_k^{\mathsf{disc}}(\mathscr{T}_h) \times \mathbb{P}_k^{\mathsf{disc}}(\mathscr{T}_h) \to \mathbb{R}, \\ & a_h^{\mathsf{upw}}(\boldsymbol{\beta}; \boldsymbol{v}, \overline{\boldsymbol{v}}) \coloneqq - \sum_{K \in \mathscr{T}_h} \int_K \boldsymbol{v}(\boldsymbol{\beta} \cdot \nabla \overline{\boldsymbol{v}}) \\ & + \sum_{e \in \mathscr{E}_h^i, e = K \cap L} \int_e ((\boldsymbol{\beta} \cdot \boldsymbol{n}_e)_{\oplus} \boldsymbol{v}_K - (\boldsymbol{\beta} \cdot \boldsymbol{n}_e)_{\ominus} \boldsymbol{v}_L) \left[\!\left[\overline{\boldsymbol{v}} \right]\!\right] \end{split}$$

Properties of the scheme for k = 0

Given $v^m \in \mathbb{P}_0^{\mathrm{disc}}(\mathscr{T}_h)$, find $v^{m+1} \in \mathbb{P}_0^{\mathrm{disc}}(\mathscr{T}_h)$ such that

$$\left(\frac{v^{m+1}-v^m}{\Delta t},\overline{v}\right)_{L^2(\Omega)}+a_h^{\mathsf{upw}}(\beta;v^{m+1},\overline{v})=0$$

for every $\overline{v} \in \mathbb{P}_0^{\mathsf{disc}}(\mathscr{T}_h)$.

Properties:

- Existence and uniqueness of the solution.
- Mass conservation: $\int_{\Omega} v^{m+1} = \int_{\Omega} v^m$.
- Maximum principle: $\min_{\overline{\Omega}} v^m \leq v^{m+1} \leq \max_{\overline{\Omega}} v^m$ in $\overline{\Omega}$.

Section 2

Convective Cahn-Hilliard model

Cahn-Hilliard equation

Fourth order problem:

$$u_t = \nabla \cdot \left(M(u) \nabla \left(-\varepsilon^2 \Delta u + F'(u) \right) \right) \qquad \text{in } \Omega \times (0, T),$$

$$\nabla u \cdot \mathbf{n} = \nabla \left(-\varepsilon^2 \Delta u + F'(u) \right) \cdot \mathbf{n} = 0 \qquad \text{on } \partial \Omega \times (0, T),$$

$$u(0) = u_0 \qquad \text{in } \Omega.$$

- $F(u) = \frac{1}{4}u^2(1-u)^2$ Ginzburg-Landau double well functional.
- M(u) = u(1 u) degenerate mobility function.
- *u* minimizes energy functional:

$$E(u(t)) := \frac{\varepsilon^2}{2} \int_{\Omega} |\nabla u(t)|^2 dx + \int_{\Omega} F(u(t)) dx.$$

 Applications: tumor tissues, image processing, multi-phase fluid systems, etc.

Convective Cahn-Hilliard model

$$\begin{split} \partial_t u &= \nabla \cdot (M(u) \nabla \mu) - \nabla \cdot (u \mathbf{v}) & \text{in } \Omega \times (0, T), \\ \mu &= F'(u) - \varepsilon^2 \Delta u & \text{in } \Omega \times (0, T), \\ \nabla u \cdot \mathbf{n} &= (M(u) \nabla \mu - u \mathbf{v}) \cdot \mathbf{n} = 0 & \text{on } \partial \Omega \times (0, T), \\ u(0) &= u_0 & \text{in } \Omega. \end{split}$$

where

- $\mathbf{v} : \overline{\Omega} \times (0, T) \to \mathbb{R}^d$ is continuous and incompressible, i.e, $\nabla \cdot \mathbf{v} = 0$ in Ω ,
- $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial \Omega$.

Properties:

- Mass conservation: $\frac{d}{dt} \int_{\Omega} u = 0$.
- Maximum principle: $u \in [0,1]$ in $\overline{\Omega} \times (0,T)$ if $u_0 \in [0,1]$ in $\overline{\Omega}$.

Nonlinear flux direction

Notice that

$$\nabla \cdot (M(u)\nabla \mu) = M'(u)\nabla \mu \cdot \nabla u + M(u)\Delta \mu.$$

Hence, M'(u) determines the direction of the flux.

• If $u \in [0,1]$ then $M(u) = M(u)_{\oplus}$.

Consider:

- Increasing part of $M(u)_{\oplus}$: $M^{\uparrow}(u) = \begin{cases} M(u)_{\oplus} & \text{if } u \leq \frac{1}{2} \\ M(\frac{1}{2}) & \text{if } u > \frac{1}{2} \end{cases}$.
- Decreasing part of $M(u)_{\oplus}$: $M^{\downarrow}(u) = \begin{cases} 0 & \text{if } u \leq \frac{1}{2} \\ M(u)_{\oplus} M(\frac{1}{2}) & \text{if } u > \frac{1}{2} \end{cases}$.

Notice that $M(u)_{\oplus}=M^{\uparrow}(u)+M^{\downarrow}(u)$.

Generalized upwind method

• $a_h^{\mathsf{upw}}: \mathbb{P}_k^{\mathsf{disc}}(\mathscr{T}_h) \times \mathbb{P}_k^{\mathsf{disc}}(\mathscr{T}_h) \to \mathbb{R}$,

$$\begin{split} a_h^{\text{upw}}(\boldsymbol{\beta}; \boldsymbol{\mathit{M}}(\boldsymbol{\mathit{u}})_{\oplus}, \overline{\boldsymbol{\mathit{u}}}) &:= -\int_{\Omega} (\boldsymbol{\beta} \cdot \nabla \overline{\boldsymbol{\mathit{u}}}) \boldsymbol{\mathit{M}}(\boldsymbol{\mathit{u}})_{\oplus} \\ &+ \sum_{e \in \mathcal{E}_h^i, e = K \cap L} \int_e \left((\{\!\!\{\boldsymbol{\beta}\}\!\!\} \cdot \boldsymbol{\mathit{n}}_e)_{\oplus} (\boldsymbol{\mathit{M}}^{\uparrow}(\boldsymbol{\mathit{u}}_K) + \boldsymbol{\mathit{M}}^{\downarrow}(\boldsymbol{\mathit{u}}_L)) \right. \\ & \left. - (\{\!\!\{\boldsymbol{\beta}\}\!\!\} \cdot \boldsymbol{\mathit{n}}_e)_{\ominus} (\boldsymbol{\mathit{M}}^{\uparrow}(\boldsymbol{\mathit{u}}_L) + \boldsymbol{\mathit{M}}^{\downarrow}(\boldsymbol{\mathit{u}}_K)) \right) [\![\overline{\boldsymbol{\mathit{u}}}]\!], \end{split}$$

where $\beta \colon \overline{\Omega} \to \mathbb{R}^d$ can be discontinuous over \mathscr{E}_h^i .

Fully discrete scheme

Given $u^m \in \mathbb{P}_0^{\mathsf{disc}}(\mathcal{T}_h)$ with $u^m \in [0,1]$, find $u^{m+1} \in \mathbb{P}_0^{\mathsf{disc}}(\mathcal{T}_h)$, with $\mu^{m+1}, w^{m+1} \in \mathbb{P}_1^{\mathsf{cont}}(\mathcal{T}_h)$, solving

$$\begin{split} \left(\frac{u^{m+1}-u^m}{\Delta t},\overline{u}\right)_{L^2(\Omega)} + a_h^{\mathsf{upw}}(-\nabla\mu^{m+1};M(u^{m+1})_{\oplus},\overline{u}) + a_h^{\mathsf{upw}}(\boldsymbol{v}(t_{m+1});u^{m+1},\overline{u}) = 0, \\ \left(\mu^{m+1},\overline{\mu}\right)_{L^2(\Omega)} &= \varepsilon^2 \left(\nabla w^{m+1},\nabla\overline{\mu}\right)_{L^2(\Omega)} + \left(f(u^{m+1},u^m),\overline{\mu}\right)_{L^2(\Omega)}, \\ \left(w^{m+1},\overline{w}\right)_{L^2(\Omega)}^h &= \left(u^{m+1},\overline{w}\right)_{L^2(\Omega)}, \end{split}$$

for all $\overline{u} \in \mathbb{P}_0^{\mathsf{disc}}(\mathscr{T}_h)$ and $\overline{\mu}, \overline{w} \in \mathbb{P}_1^{\mathsf{cont}}(\mathscr{T}_h)$.

 $(\cdot,\cdot)_{L^2(\Omega)}^h$ denotates the scalar product with mass-lumping.

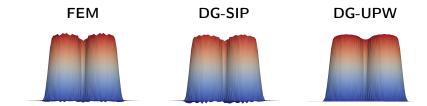
Properties:

- Existence of a solution.
- Mass conservation: $\int_{\Omega} u^{m+1} = \int_{\Omega} u^m$, $\int_{\Omega} w^{m+1} = \int_{\Omega} w^m$.
- Maximum principle: $u^{m+1}, w^{m+1} \in [0, 1]$ in $\overline{\Omega}$ if $u^m, w^m \in [0, 1]$.

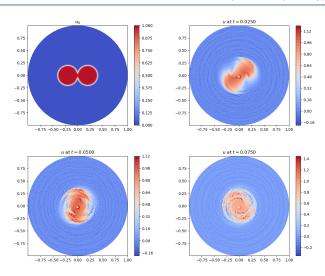
Section 3

Numerical tests

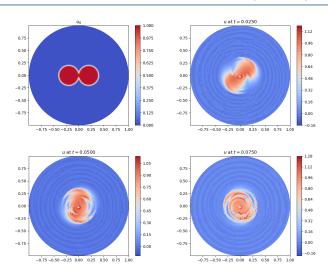
Non-convective Cahn-Hilliard ($\nu = 0$)



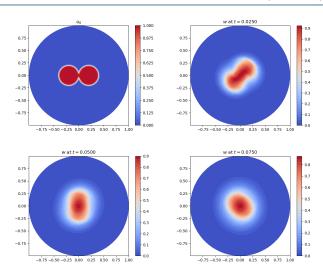
Convective Cahn-Hilliard with FEM (v = 100(y, -x))



Convective Cahn-Hilliard with DG-SIP (v = 100(y, -x))



Convective Cahn-Hilliard with DG-UPW ($\mathbf{v} = 100(y, -x)$)



Convective Cahn-Hilliard ($\mathbf{v} = 100(y, -x)$)

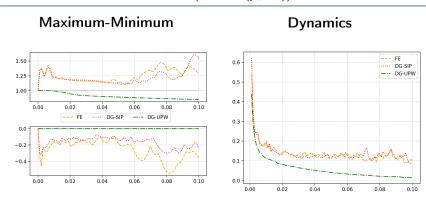
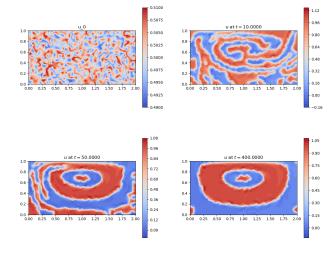


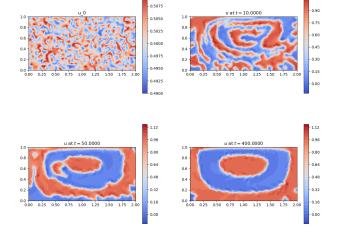
Figure: On the left, maximum and minimum of the phase field variable over time. On the right, we plot $\frac{\left\|u^{m+1}-u^m\right\|_{L^\infty(\Omega)}}{\left\|u^m\right\|_{L^\infty(\Omega)}}$ to observe the dynamics of the approximations.

Stokes-Cahn-Hilliard with FEM (cavity test)



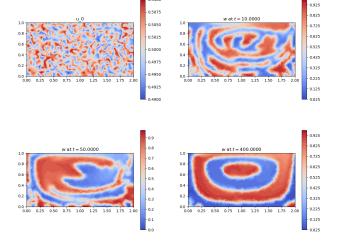
Stokes-Cahn-Hilliard with DG-SIP (cavity test)

0.5100



Stokes-Cahn-Hilliard with DG-UPW (cavity test)

0.5100



Stokes-Cahn-Hilliard (cavity test)

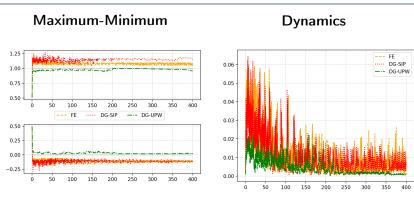


Figure: On the left, maximum and minimum of the phase field variable over time. On the right, we plot $\frac{\left\|u^{m+1}-u^m\right\|_{L^\infty(\Omega)}}{\left\|u^m\right\|_{L^\infty(\Omega)}}$ to observe the dynamics of the approximations.

Convergence order: non-convective Cahn-Hilliard

Table: Errors and convergence orders at T=0.001 without convection (v=0).

		$h \approx 2.8284 \cdot 10^{-2}$	$h/2 \approx 1.4142 \cdot 10^{-2}$		$h/3 \approx 9.428 \cdot 10^{-3}$		$h/4 \approx 7.071 \cdot 10^{-3}$	
Scheme	Norm	Error	Error	Order	Error	Order	Error	Order
	· _2	8.5268 · 10 ⁻³	3.0933 · 10 ⁻³	1.46	1.7645 · 10 -3	1.38	1.2134 · 10 -3	1.30
DG-UPW	$ \cdot _{H^{1}}$	8.0000 · 10 -1	4.0199 · 10 -1	0.99	2.6081 · 10 -1	1.07	1.8849 · 10 -1	1.13
	· ,2	5.3224 · 10 ⁻³	1.5679 · 10 -3	1.76	6.9944 · 10-4	1.99	4.0191 · 10-4	1.93
FEM	· _H 1	8.9963 · 10 -1	4.1080 · 10 -1	1.13	2.5252 · 10 -1	1.2	1.7799 · 10 -1	1.22
	$\ \cdot \ _{L^{2}}$	4.6466 · 10 ⁻³	1.3023 · 10 -3	1.84	5.8945 · 10 ⁻⁴	1.96	3.2710 · 10 ⁻⁴	2.05
DG-SIP	$\ \cdot \ _{H^{1}}$	1.1784	5.8331 · 10 -1	1.01	3.6254 · 10 -1	1.17	2.6024 · 10 -1	1.15

Convergence order: convective Cahn-Hilliard

Table: Errors and convergence orders at T=0.001 with convection ($\mathbf{v}=(y,-x)$).

		$h \approx 4 \cdot 10^{-2}$	$h/2 \approx 2 \cdot 10^{-2}$		$h/3 \approx 1.3333 \cdot 10^{-2}$		$h/4 \approx 1 \cdot 10^{-2}$	
Scheme	Norm	Error	Error	Order	Error	Order	Error	Order
	· _12	1.7288 · 10 -2	6.9446 · 10 ⁻³	1.32	3.3102 · 10 -3	1.83	2.0578 · 10 -3	1.65
DG-UPW	· _H 1	1.4549	6.0305 · 10 -1	1.27	3.0204 · 10 -1	1.71	2.0315 · 10 -1	1.38
	· 2	6.8347 · 10 ⁻³	2.1213 · 10 -3	1.69	9.7749 · 10 -4	1.91	5.3883 · 10 ⁻⁴	2.07
FEM	$\ \cdot \ _{H^{1}}$	8.3104 · 10 -1	3.8060 · 10 -1	1.13	2.1887 · 10 -1	1.36	1.4991 · 10 -1	1.32
	· _L 2	6.5242 · 10 -3	1.9557 · 10 -3	1.74	8.9471 · 10 ⁻⁴	1.93	5.0257 · 10 -4	2.00
DG-SIP	$\ \cdot \ _{H^{1}}$	1.1980	6.1624 · 10 -1	0.96	3.8451 · 10 -1	1.16	2.7439 · 10 -1	1.17

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Thanks for your attention!

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