A Continuous Interior Penalty Method Framework for Sixth Order Cahn-Hilliard-type Equations with applications to microstructure evolution and microemulsions

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Funding: NSF DMS-2110774
Joint work with Amanda Diegel (Mississippi State University)

FEM@LLNL Seminar Series
July 18, 2023

Sixth Order Cahn-Hilliard-type Equations

Applications

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- Microstructure evolution specifically formation of defects within microstructures.

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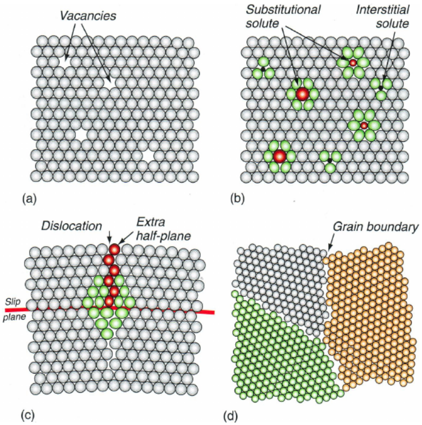
Goal: Develop a Continuous Interior Penalty Method framework to solve these Sixth-Order Phase Field Models.

Defects in Crystalline Materials



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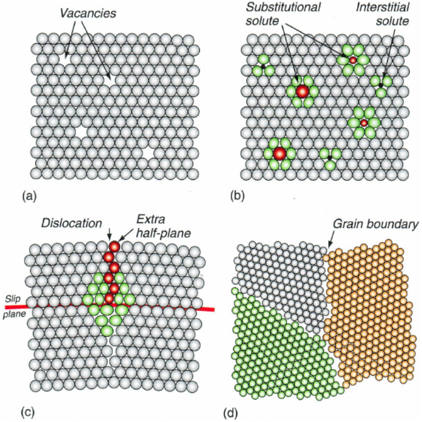

Defects control

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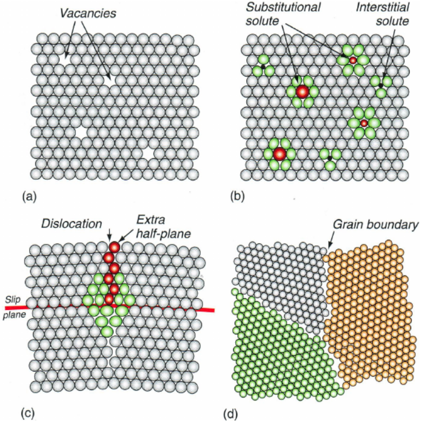

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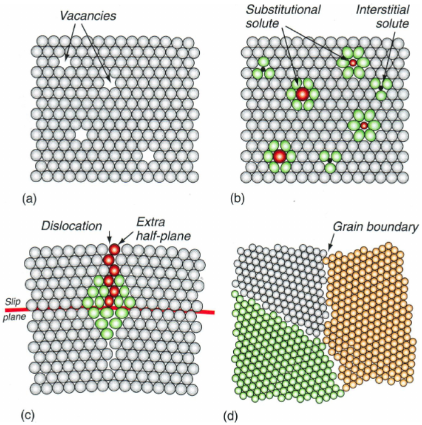

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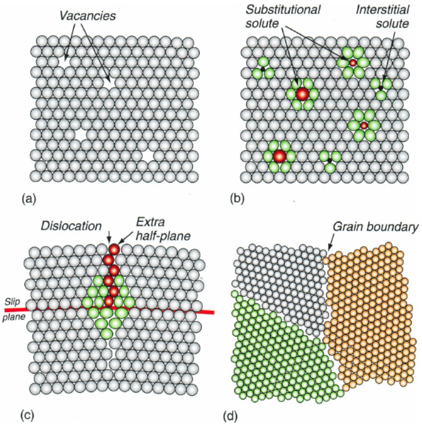

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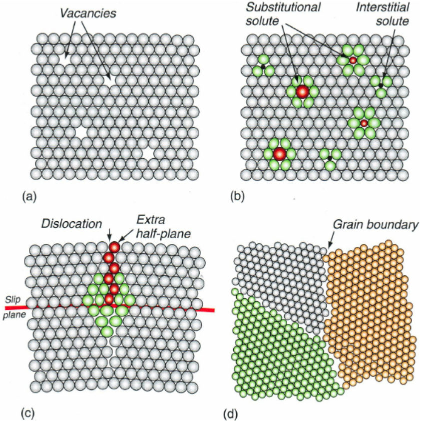

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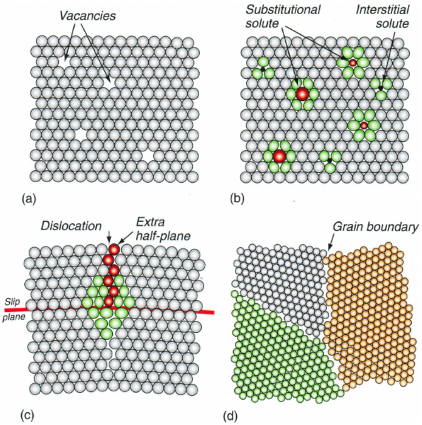

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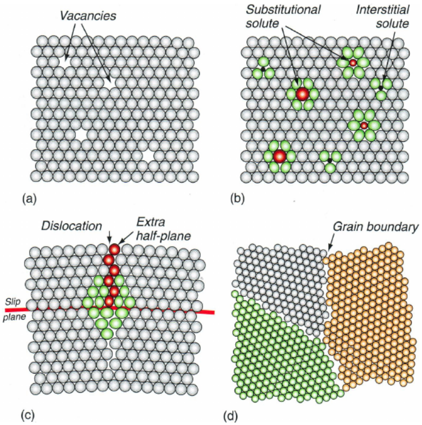

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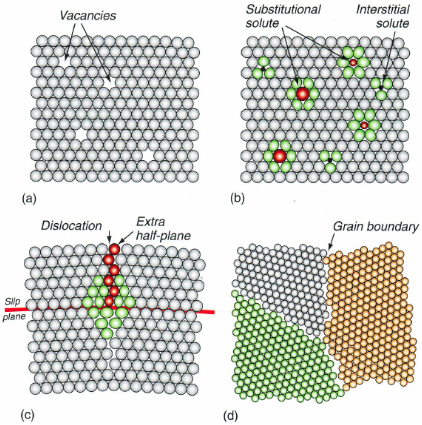

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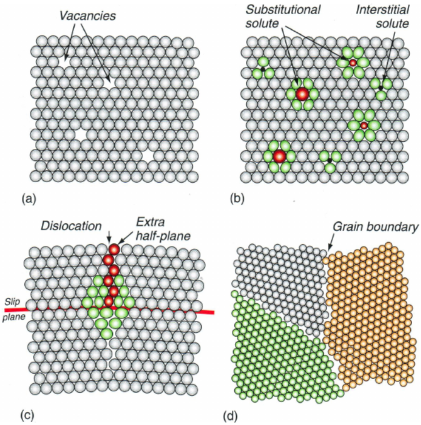

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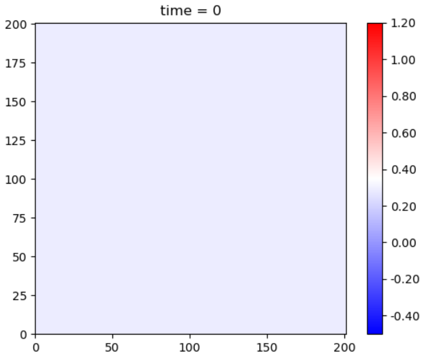
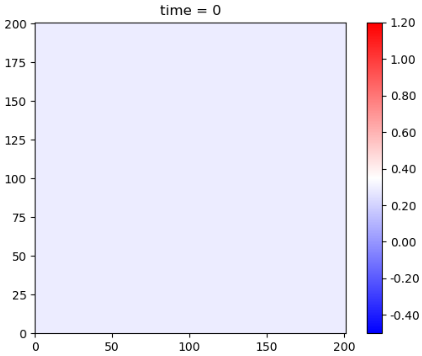
- Develop an accurate, efficient, easy-to-compute numerical scheme.

Phase Field Crystal Equation



Two-phase system



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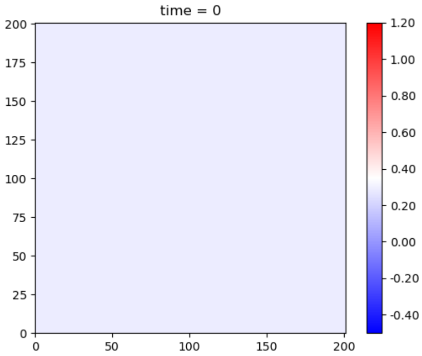

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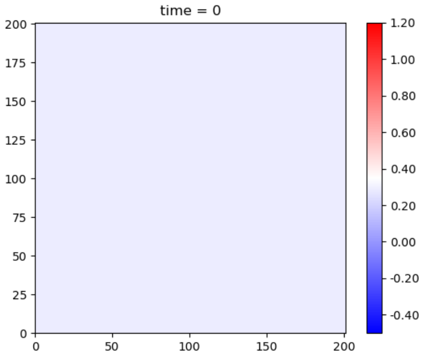

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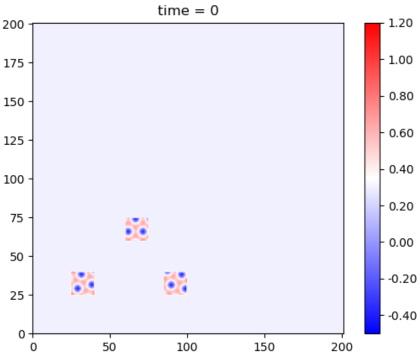
- liquid phase characterized by a constant value of φ
- solid phase characterized by a spatially varying periodic function φ that inherits the symmetry and periodicity of the crystal lattice



Phase Field Crystal Equation

Conservation Law:

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Phase Field Crystal Equation (Elder et al. 2004)

$$\frac{\partial \varphi}{\partial t} = \nabla \cdot \left(\mathcal{M} \nabla \left(\varphi^3 + 2\Delta\varphi + (1-\varepsilon)\varphi + \Delta^2 \varphi\right)\right) \quad \text{on } \Omega \times (0, T).$$

PFC equation in the mixed form

$$
\begin{aligned}
\frac{\partial \varphi}{\partial t} - \nabla \cdot (\mathcal{M} \nabla \mu) &= 0, \\
\varphi^3 + (1-\varepsilon)\varphi + 2\Delta\varphi + \Delta^2\varphi - \mu &= 0,
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with either periodic boundary conditions or natural boundary conditions

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Notation:

- $H^s(\Omega)$ denote the Sobolev spaces of order $s \geq 1$,
- $Z := \{z \in H^2(\Omega) \mid \mathrm{n}\cdot\nabla z = 0 \text{ on } \partial\Omega\}$.

Weak Formulation

Find (φ, μ) such that

$$\varphi \in L^\infty(0, T; Z) \cap L^2(0, T; H^3(\Omega)),$$
$$\partial_t \varphi \in L^2(0, T; H_N^{-1}(\Omega)),$$
$$\mu \in L^2(0, T; H^1(\Omega)),$$

and for almost all $t \in (0, T)$

$$\langle \partial_t \varphi, \nu \rangle + (\mathcal{M} \nabla \mu, \nabla \nu) = 0 \quad \forall\, \nu \in H^1(\Omega)$$
$$\Big((\varphi)^3 + (1 - \epsilon)\varphi, \psi \Big) - 2\,(\nabla \varphi, \nabla \psi) + \ a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall\, \psi \in Z$$

with $a(u, v) := \displaystyle\int_\Omega \left(\nabla^2 u : \nabla^2 v \right)\ dx,$

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with $a(u, v) := \displaystyle\int_\Omega \left(\nabla^2 u : \nabla^2 v\right)\, dx$, $\varphi(0) = \varphi_0 \in H^4(\Omega)$ such that φ_0 satisfies the boundary conditions.

[Pawlow et al., 2013]

Numerical Schemes: Challenges

Phase Field Crystal Equation

$$\frac{\partial \varphi}{\partial t} - \nabla \cdot (\mathcal{M} \nabla \mu) = 0,$$
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- Space discretization: Choose a suitable discretization for the higher order term.

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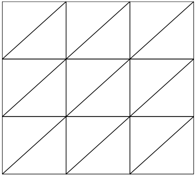
- Fourier-spectral Method: Li and Shen, 2020 (Scalar Auxiliary Variable approach) Yang and Han, 2017 (Invariant Energy Quadratization)

Numerical Schemes: Our Approach

- Space discretization: Relax the C^1-continuity, use C^0-Interior Penalty Method
- Time discretization: Use Eyre's convex splitting scheme known to be uniquely solvable and unconditionally stable

Spatial Discretization



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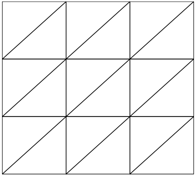

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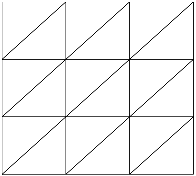

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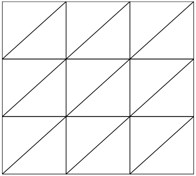

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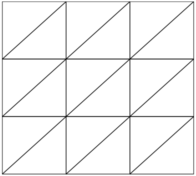

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- $\mathscr{E}_h$: collection of all edges e wrt $\mathscr{T}_h$

Classical C^1 Finite Element Method

Find $(\varphi, \mu) : [0, T] \to Z \times H^1(\Omega)$ s.t. for almost all $t \in (0, T)$

$$\langle \partial_t \varphi, \nu \rangle + (\mathcal{M} \nabla \mu, \nabla \nu) = 0 \qquad \forall\, \nu \in H^1(\Omega)$$
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$$Z_h \subset H^1(\Omega)$$

$(\varphi_h, \mu_h) : [0, T] \to Z_h \times V_h$:

$$\begin{aligned} \langle \partial_t \varphi_h, \nu\rangle + (\mathcal{M}\nabla\mu_h, \nabla\nu) &= 0, \\ \left((\varphi_h)^3 + (1-\epsilon)\varphi_h, \psi\right) - 2\left(\nabla\varphi_h, \nabla\psi\right) + a_h^{IP}(\varphi_h, \psi) - (\mu_h, \psi) &= 0 \end{aligned}$$

$\forall \nu \in V_h,\ \psi \in Z_h$ holds for almost all $t \in (0, T)$.

Spatial Discretization using C^0-IP Method

$$V_h := \{v \in C(\overline{\Omega}) |\ v|_K \in P_1(K)\ \forall K \in \mathscr{T}_h\}$$

Spatial Discretization using C^0-IP Method

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$$Z_h := \{v \in C(\overline{\Omega}) |\ v|_K \in P_2(K)\ \forall K \in \mathscr{T}_h\},$$

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$R_h : H^1(\Omega) \to V_h$ is a Ritz projection operator such that

$$\left(\nabla \left(R_h\mu - \mu\right), \nabla\xi\right) = 0 \quad \forall\, \xi \in V_h, \quad (R_h\mu - \mu, 1) = 0.$$

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$P_h : Z \to Z_h$ is a Ritz projection operator such that

$$a_h^{IP}\left(P_h\varphi - \varphi, \xi\right) + (1-\epsilon)\left(P_h\varphi - \varphi, \xi\right) = 0 \quad \forall\, \xi \in Z_h, \quad \left(P_h\varphi - \varphi, 1\right) = 0.$$

Spatial Discretization using C^0-IP Method

$a_h^{IP} : Z_h \times Z_h \to \mathbb{R}$ according to

$$a_h^{IP}(\xi_h, \psi_h) := \sum_{K \in \mathcal{T}_h} \int_K \nabla^2 \xi_h : \nabla^2 \psi_h \, dx \; + J(\xi_h, \psi_h), \quad \xi_h, \psi_h \in Z_h$$

where

$$J(\xi_h, \psi_h) := \sum_{e \in \mathcal{E}_h} \int_e \Big([\mathrm{n}_e \cdot \nabla \xi_h]_e \, \{\mathrm{n}_e \cdot \nabla^2 \psi_h \mathrm{n}_e\}_e + \{\mathrm{n}_e \cdot \nabla^2 \xi_h \mathrm{n}_e\}_e \, [\mathrm{n}_e \cdot \nabla \psi_h]_e \Big) ds$$
$$+ \sum_{e \in \mathcal{E}_h} \int_e \frac{\alpha}{h_e} \, [\mathrm{n}_e \cdot \nabla \xi_h]_e \, [\mathrm{n}_e \cdot \nabla \psi_h]_e \, ds, \quad \xi_h, \psi_h \in Z_h$$

and $\alpha > 0$ is a penalty parameter.

Boundedness of $a_h^{IP}(\cdot,\cdot)$

Lemma (Boundedness of $a_h^{IP}(\cdot,\cdot)$)

There exists positive constants C_{cont} and C_{coer} such that for choices of the penalty parameter α large enough we have

$$a_h^{IP}(w_h, v_h) \leq C_{cont} \|w_h\|_{2,h} \|v_h\|_{2,h} \quad \forall\, w_h, v_h \in Z_h,$$
$$C_{coer} \|w_h\|_{2,h}^2 \leq a_h^{IP}(w_h, w_h) \quad \forall\, w_h \in Z_h,$$

where the constants C_{cont} and C_{coer} depend only on the shape regularity of $\mathscr{T}_h$.

where the C^0-IP Norm is:

$$\|\xi_h\|_{2,h}^2 := \sum_{K\in\mathscr{T}_h} |\xi_h|_{H^2(K)}^2 + \sum_{e\in\mathscr{E}_h} \alpha \| h_e^{-\frac{1}{2}} [\mathrm{n}_e \cdot \nabla \xi_h]_e \|_{L^2(e)}^2.$$

Time Discretization

We introduce a partition of (0,T)

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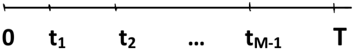

into M sub-intervals (t_{m-1}, t_m):

$$t_m = t_{m-1} + \tau, \text{ for } 1 \leq m \leq M$$

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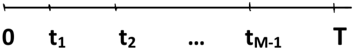

into M sub-intervals (t_{m-1}, t_m):

$$t_m = t_{m-1} + \tau, \text{ for } \ 1 \leq m \leq M$$

Notation: φ^m approximate φ at time t_m.

Numerical time derivative w.r.t. τ:

$$\delta_\tau \varphi^m := \frac{\varphi^{m+1} - \varphi^m}{\tau}$$

Convex Time Splitting Scheme

- Basic Idea:

$$\mu = \delta_\varphi E(\varphi) = \delta_\varphi \big(\underbrace{E^+(\varphi)}_{\text{convex}} + \underbrace{E^-(\varphi)}_{\text{concave}} \big)$$

$$\Longrightarrow \ \mu^m = \underbrace{(\varphi^m)^3 + (1-\epsilon)\varphi^m + \Delta^2\varphi^m}_{\delta_\varphi E^+(\varphi^m)} + \underbrace{2\Delta\varphi^{m-1}}_{\delta_\varphi E^-(\varphi^{m-1})}$$

where $E(\varphi) = \displaystyle\int_\Omega \left(\frac{\varphi^4}{4} + \frac{1-\varepsilon}{2}\varphi^2 + \frac{1}{2}(\Delta\varphi)^2 - |\nabla\varphi|^2 \right) dx.$

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where $E(\varphi) = \displaystyle\int_\Omega \left(\frac{\varphi^4}{4} + \frac{1-\varepsilon}{2}\varphi^2 + \frac{1}{2}(\Delta\varphi)^2 - |\nabla\varphi|^2\right) dx.$

Given φ^0, find (φ^m, μ^m) for $1 \le m \le M$ by

$$\delta_\tau\varphi^m - \nabla\cdot(\mathcal{M}\nabla\mu^m) = 0,$$
$$(\varphi^m)^3 + (1-\epsilon)\varphi^m + \Delta^2\varphi^m + 2\Delta\varphi^{m-1} - \mu^m = 0,$$

with boundary conditions

$$\partial_n\varphi^m = \partial_n\Delta\varphi^m = \partial_n\mu^m = 0.$$

Fully Discrete C^0-IP Method

Given $\varphi_h^{m-1} \in Z_h$, find $\varphi_h^m, \mu_h^m \in Z_h \times V_h$ such that for all $\nu_h \in V_h,\ \psi_h \in Z_h$ it holds

$$(\delta_\tau \varphi_h^m, \nu_h) + (\mathcal{M}\nabla \mu_h^m, \nabla \nu_h) = 0$$

$$\left((\varphi_h^m)^3 + (1-\epsilon)\varphi_h^m, \psi_h\right) + a_h^{IP}(\varphi_h^m, \psi_h) - 2\left(\nabla \varphi_h^{m-1}, \nabla \psi_h\right) - (\mu_h^m, \psi_h) = 0,$$

where $\varphi_h^0 := P_h \varphi_0$ and $\mu_h^0 \in V_h$ is defined as $\mu_h^0 := R_h \mu_0$.

Remark

The scheme satisfies the discrete conservation property

$$(\varphi_h^m, 1) = \left(\varphi_h^0, 1\right) = (\varphi_0, 1) \ \textit{ for any } 1 \leq m \leq M.$$

Properties of Scheme

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$$F(\varphi_h^m) := \frac{1}{4}\|\varphi_h^m\|_{L^4}^4 + \frac{1-\epsilon}{2}\|\varphi_h^m\|_{L^2}^2 - \|\nabla\varphi_h^m\|_{L^2}^2 + \frac{1}{2}a_h^{IP}(\varphi_h^m, \varphi_h^m)$$

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3. Optimal error estimates: Main Result!

Unconditional Unique Solvability

Definition

Define the functional $G_h : \mathring{Z}_h \to \mathbb{R}$

$$G_h(\varphi_h) := \frac{\tau}{2} \left\| \frac{\varphi_h - \varphi_h^{m-1}}{\tau} \right\|_{-1,h}^2 + \frac{1}{2} a_h^{IP}\left(\varphi_h, \varphi_h\right) + \frac{1}{4} \left\|\varphi_h + \overline{\varphi}_0\right\|_{L^4(\Omega)}^4$$
$$+ \frac{1-\epsilon}{2} \left\|\varphi_h + \overline{\varphi}_0\right\|_{L^2(\Omega)}^2 - 2\left(\nabla \varphi_h^{m-1}, \nabla \varphi_h\right),$$

where

$$\|v_h\|_{-1,h} = \left(\nabla \mathrm{T}_h v_h, \nabla \mathrm{T}_h v_h\right)^{1/2} = \left(v_h, \mathrm{T}_h v_h\right)^{1/2} = \left(\mathrm{T}_h v_h, v_h\right)^{1/2},$$

with $\mathrm{T}_h : \mathring{Z}_h \to \mathring{Z}_h$ defined as: given $\zeta_h \in \mathring{Z}_h$, find $\mathrm{T}_h \zeta_h \in \mathring{Z}_h$:

$$\left(\nabla \mathrm{T}_h \zeta_h, \nabla \chi_h\right) = \left(\zeta_h, \chi_h\right) \qquad \forall\, \chi_h \in \mathring{Z}_h.$$

Unconditional Unique Solvability

Theorem

The fully discrete C^0-IP scheme is uniquely solvable for any mesh parameters: τ and h and for any $\varepsilon < 1$.

Proof.

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1. Shown through the **zero mean formulation** corresponding to our scheme

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The fully discrete C^0-IP scheme is uniquely solvable for any mesh parameters: τ and h and for any $\varepsilon < 1$.

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2. Prove the one-to-one correspondence between solution of our scheme with the solution to the **zero mean formulation**
3. Existence of the unique solution to the **zero mean formulation** proved through existence of a minimizer for a functional G_h.

□

Unconditional Stability

Lemma (Discrete Energy Law)

Let $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ be a solution of the C^0-IP method. Then the following energy law holds for any $h, \tau > 0$:

$$
\begin{aligned}
& F\left(\varphi_h^\ell\right) + \tau \sum_{m=1}^{\ell} \left\| \mathcal{M}^{1/2} \nabla \mu_h^m \right\|_{L^2(\Omega)}^2 \\
& \quad + \tau^2 \sum_{m=1}^{\ell} \left\{ \frac{(1-\epsilon)}{2} \left\| \delta_\tau \varphi_h^m \right\|_{L^2(\Omega)}^2 + \left\| \nabla \delta_\tau \varphi_h^m \right\|_{L^2(\Omega)}^2 \right. \\
& \qquad \left. + \frac{1}{4} \left\| \delta_\tau (\varphi_h^m)^2 \right\|_{L^2(\Omega)}^2 + \frac{1}{2} \left\| \varphi_h^m \delta_\tau \varphi_h^m \right\|_{L^2(\Omega)}^2 + \frac{1}{2} a_h^{IP}\left(\delta_\tau \varphi_h^m, \delta_\tau \varphi_h^m \right) \right\} \\
& \quad = F\left(\varphi_h^0\right), \quad 1 \le \ell \le M.
\end{aligned}
$$

Uniform *a priori* estimates

Lemma

Let $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ be the unique solution of C^0-IP scheme. Suppose that $F(\varphi_h^0) \le C$ independent of h and $\epsilon < \frac{C_{coer}-4}{C_{coer}} < 1$. For any $h, \tau > 0$:

$$\max_{0\le m\le M}\left[\|\varphi_h^m\|_{L^4(\Omega)}^2 + \|\varphi_h^m\|_{L^2(\Omega)}^2 + \|\varphi_h^m\|_{2,h}^2\right] \le C$$

$$\max_{0\le m\le M}\|\varphi_h^m\|_{H^1}^2 \le C$$

$$\tau\sum_{m=1}^{\ell}\left\|\mathcal{M}^{1/2}\nabla\mu_h^m\right\|_{L^2(\Omega)}^2 \le C$$

$$\tau^2\sum_{m=1}^{\ell}\left\{\|\nabla\delta_\tau\varphi_h^m\|_{L^2(\Omega)}^2 + \left\|(\varphi_h^m)^2\delta_\tau(\varphi_h^m)^2\right\|_{L^2(\Omega)}^2 + \|\delta_\tau\varphi_h^m\|_{2,h}^2\right\} \le C$$

for some constant C that is independent of h, τ, and T.

Error Estimates

Assume additional regularites:

$$\begin{aligned}
\varphi &\in L^\infty\left(0, T; H^3(\Omega)\right) \cap L^2\left(0, T; H^3(\Omega)\right), \\
\partial_t \varphi &\in L^2\left(0, T; H^3(\Omega)\right) \cap L^2(0, T; H_N^{-1}(\Omega)), \\
\partial_{tt} \varphi &\in L^2\left(0, T; L^2(\Omega)\right), \\
\mu &\in L^2\left(0, T; H^2(\Omega)\right), \\
\partial_t \mu &\in L^2\left(0, T; L^2(\Omega)\right).
\end{aligned}$$

C^0-IP Norm:

$$\|\xi_h\|_{2,h}^2 := \sum_{K \in \mathscr{T}_h} |\xi_h|_{H^2(K)}^2 + \sum_{e \in \mathscr{E}_h} \alpha \| h_e^{-\frac{1}{2}} [\mathrm{n}_e \cdot \nabla \xi_h]_e \|_{L^2(e)}^2.$$

Notation:

$$e^{\varphi,m} := \varphi^m - \varphi_h^m, \quad e^{\mu,m} := \mu^m - \mu_h^m.$$

Assumption: $\mathcal{M} \equiv 1$.

Error Analysis: Error Equation

Weak Form:

$$\langle \partial_t \varphi^m, \nu \rangle + (\nabla \mu^m, \nabla \nu) = 0 \ \forall \, \nu \in H^1(\Omega) \tag{1}$$

$$\left((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi\right) - 2\left(\nabla \varphi^m, \nabla \psi\right) + a(\varphi^m, \psi) - (\mu^m, \psi) = 0 \ \forall \, \psi \in Z. \tag{2}$$

Fully Discrete C^0-IP Form:

$$(\delta_\tau \varphi_h^m, \nu) + (\nabla \mu_h^m, \nabla \nu) = 0 \ \forall \nu \in V_h \tag{3}$$

$$\left((\varphi_h^m)^3 + (1-\epsilon)\varphi_h^m, \psi\right) - 2\left(\nabla \varphi_h^{m-1}, \nabla \psi\right) + a_h^{IP}\left(\varphi_h^m, \psi\right) - (\mu_h^m, \psi) = 0, \forall \psi \in Z_h \tag{4}$$

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- (1) and (3) $\implies$ $(\delta_\tau e^{\varphi,m}, \nu_h) + (\nabla e^{\mu,m}, \nabla \nu_h) = (\delta_\tau \varphi^m - \partial_t \varphi^m, \nu_h)$, $\nu_h \in V_h \subset H^1(\Omega)$.

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- Error equation based on (2) and (4) is not well-defined since $Z_h \not\subset Z$!

Error Analysis: Error Equation

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$$\left((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi\right) - 2\,(\nabla\varphi^m, \nabla\psi) + a(\varphi^m, \psi) - (\mu^m, \psi) = 0 \;\forall\, \psi \in Z.$$

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$$\left((\varphi^m)^3 - (\varphi_h^m)^3 + (1-\epsilon)e^{\varphi,m}, \psi\right) - 2\left(\nabla e^{\varphi,m}, \nabla\psi\right) + a(\varphi^m, \psi) - a_h^{IP}\left(\varphi_h^m, \psi\right)$$
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Problem: $\psi \in Z$ is not in $H^{2+1/2}$ locally! $\psi \in Z_h$ is not in H^2 globally!

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Problem: $\psi \in Z$ is not in $H^{2+1/2}$ locally! $\psi \in Z_h$ is not in H^2 globally!
Remedy: Lift $\psi \in Z_h$ into a finite dimensional subspace of Z.

Error Analysis

- Remedy: Introduce $W_h \subset Z$ to be the Hsieh-Clough-Tocher micro finite element space associated with $\mathscr{T}_h$.

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- **Weak Form with correction term:** find $(\varphi^m, \mu^m) \in Z \times H^1(\Omega)$:

$$
\begin{aligned}
&(\partial_t \varphi^m, \nu_h) + (\nabla \mu^m, \nabla \nu_h) = 0 \quad \forall\, \nu_h \in V_h, \\
&a_h^{IP}(\varphi^m, \psi_h) + \Big((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi_h\Big) - 2\,(\nabla \varphi^m, \nabla \psi_h) - (\mu^m, \psi_h) \\
&= \mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h\psi_h) \qquad \forall\, \psi_h \in Z_h
\end{aligned}
$$

where

$$
\begin{aligned}
\mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h\psi_h) &:= a_h^{IP}(\varphi^m, \psi_h - E_h\psi_h) - (\mu^m, \psi_h - E_h\psi_h) \\
&+ \left((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi_h - E_h\psi_h\right) - 2\,(\nabla \varphi^m, \nabla \psi_h - \nabla E_h\psi_h)\,.
\end{aligned}
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\begin{aligned}
&(\partial_t \varphi^m, \nu_h) + (\nabla \mu^m, \nabla \nu_h) = 0 \quad \forall\, \nu_h \in V_h, \\
&a_h^{IP}(\varphi^m, \psi_h) + \Big((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi_h\Big) - 2\,(\nabla \varphi^m, \nabla \psi_h) - (\mu^m, \psi_h) \\
&= \mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h \psi_h) \qquad \forall\, \psi_h \in Z_h
\end{aligned}
$$

where

$$
\begin{aligned}
\mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h\psi_h) &:= a_h^{IP}(\varphi^m, \psi_h - E_h\psi_h) - (\mu^m, \psi_h - E_h\psi_h) \\
&+ \left((\varphi^m)^3 + (1-\epsilon)\varphi^m, \psi_h - E_h\psi_h\right) - 2\,(\nabla\varphi^m, \nabla\psi_h - \nabla E_h\psi_h)\,.
\end{aligned}
$$

- Solutions to weak form are consistent since $a_h^{IP}(\varphi, E_h\psi) = a(\varphi, E_h\psi)$ for all $\psi \in Z_h$.

Error Equation

Subtracting fully discrete form from the weak form with the correction term gives:

$$(\delta_\tau e^{\varphi,m}, \nu_h) + (\nabla e^{\mu,m}, \nabla \nu_h) = (\delta_\tau \varphi^m - \partial_t \varphi^m, \nu_h)\,, \tag{5}$$

$$\begin{aligned} & a_h^{IP}\left(e^{\varphi,m}, \psi_h\right) + ((1-\epsilon)e^{\varphi,m}, \psi_h) - 2\left(\nabla e^{\varphi,m-1}, \nabla \psi_h\right) - (e^{\mu,m}, \psi_h) = \\ & -\left((\varphi^m)^3 - \left(\varphi_h^m\right)^3, \psi_h\right) - 2\left(\nabla \varphi^{m-1} - \nabla \varphi^m, \nabla \psi_h\right) + \mathcal{L}(\varphi^m, \mu_h^m; \psi_h - E_h \psi_h). \end{aligned} \tag{6}$$

Notation:

$$\begin{aligned} e^{\varphi,m} &= e_P^{\varphi,m} + e_h^{\varphi,m}, \quad e_P^{\varphi,m} := \varphi^m - P_h \varphi^m, \quad e_h^{\varphi,m} := P_h \varphi^m - \varphi_h^m, \\ e^{\mu,m} &= e_R^{\mu,m} + e_h^{\mu,m}, \quad e_R^{\mu,m} := \mu^m - R_h \mu^m, \quad e_h^{\mu,m} := R_h \mu^m - \mu_h^m. \end{aligned}$$

Error Equation

Subtracting fully discrete form from the weak form with the correction term gives:

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$$\begin{aligned} &a_h^{IP}\,(e^{\varphi,m}, \psi_h) + ((1-\epsilon)e^{\varphi,m}, \psi_h) - 2\left(\nabla e^{\varphi,m-1}, \nabla \psi_h\right) - (e^{\mu,m}, \psi_h) = \\ &-\left((\varphi^m)^3 - (\varphi_h^m)^3\,, \psi_h\right) - 2\left(\nabla \varphi^{m-1} - \nabla \varphi^m, \nabla \psi_h\right) + \mathcal{L}(\varphi^m, \mu_h^m; \psi_h - E_h\psi_h). \end{aligned} \tag{6}$$

Notation:

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Set $\nu_h = e_h^{\mu,m}$ in (5) and $\psi_h = \delta_\tau e_h^{\varphi,m}$ in (6).

Error Equation

$$
\begin{aligned}
&\|\nabla e_h^{\mu,m}\|_{L^2}^2 + a_h^{IP}\left(e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) + \left((1-\epsilon)e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) - 2\left(\nabla e_h^{\varphi,m-1}, \nabla \delta_\tau e_h^{\varphi,m}\right) \\
&\quad = \left(\delta_\tau \varphi^m - \partial_t \varphi^m, e_h^{\mu,m}\right) - \left(\delta_\tau e_P^{\varphi,m}, e_h^{\mu,m}\right) + \left(e_R^{\mu,m}, \delta_\tau e_h^{\varphi,m}\right) \\
&\qquad + 2\left(\nabla \varphi^m - \nabla \varphi^{m-1}, \nabla \delta_\tau e_h^{\varphi,m}\right) - \left(\left(\varphi^m\right)^3 - \left(\varphi_h^m\right)^3, \delta_\tau e_h^{\varphi,m}\right) \\
&\qquad + 2\left(\nabla e_P^{\varphi,m-1}, \nabla \delta_\tau e_h^{\varphi,m}\right) \; + \; \mathcal{L}(\varphi^m, \mu_h^m; \psi_h - E_h\psi_h)
\end{aligned}
$$

Error Analysis

Lemma

Let (φ^m, μ^m) be a weak solution with the additional regularities. Then for any $h, \tau > 0$ and any $0 \le m \le M$, we have

$$\|\delta_\tau e_h^{\varphi,m}\|_{-1,h}^2 \le 4\,\|\nabla e_h^{\mu,m}\|_{L^2}^2 + \frac{Ch^2}{\tau}\int_{t_{m-1}}^{t_m} \|\partial_s \varphi(s)\|_{H^2}^2\, ds + C\tau \int_{t_{m-1}}^{t_m} \|\partial_{ss}\varphi(s)\|_{H^1}^2\, ds$$

where the constant C may depend upon a Poincaré constant but does not depend on h or τ.

where $\|v_h\|_{-1,h} = (\nabla \mathrm{T}_h v_h, \nabla \mathrm{T}_h v_h)^{1/2} = (v_h, \mathrm{T}_h v_h)^{1/2} = (\mathrm{T}_h v_h, v_h)^{1/2}$ and T_h is the discrete inverse Laplacian.

Error Analysis: LHS

$$
\begin{aligned}
&\|\nabla e_h^{\mu,m}\|_{L^2}^2 + a_h^{IP}\left(e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) + \left((1-\epsilon)e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) - 2\left(\nabla e_h^{\varphi,m-1}, \nabla\delta_\tau e_h^{\varphi,m}\right)\\
&\quad = \left(\delta_\tau\varphi^m - \partial_t\varphi^m, e_h^{\mu,m}\right) - \left(\delta_\tau e_P^{\varphi,m}, e_h^{\mu,m}\right) + \left(e_R^{\mu,m}, \delta_\tau e_h^{\varphi,m}\right)\\
&\qquad + 2\left(\nabla\varphi^m - \nabla\varphi^{m-1}, \nabla\delta_\tau e_h^{\varphi,m}\right) - \left(\left(\varphi^m\right)^3 - \left(\varphi_h^m\right)^3, \delta_\tau e_h^{\varphi,m}\right)\\
&\qquad + 2\left(\nabla e_P^{\varphi,m-1}, \nabla\delta_\tau e_h^{\varphi,m}\right) \; + \; \mathcal{L}(\varphi^m, \mu_h^m; \psi_h - E_h\psi_h)
\end{aligned}
$$

Polarization Property:

$$
\begin{aligned}
a_h^{IP}\left(e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) &= \frac{1}{2}\delta_\tau\, a_h^{IP}\left(e_h^{\varphi,m}, e_h^{\varphi,m}\right) + \frac{\tau}{2} a_h^{IP}\left(\delta_\tau e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right)\\
\left((1-\epsilon)e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) &= \frac{(1-\epsilon)}{2}\delta_\tau\left\|e_h^{\varphi,m}\right\|_{L^2}^2 + \frac{(1-\epsilon)}{2}\left\|\delta_\tau e_h^{\varphi,m}\right\|_{L^2}^2\\
-2\left(\nabla e_h^{\varphi,m-1}, \nabla\delta_\tau e_h^{\varphi,m}\right) &= \tau\left\|\nabla\delta_\tau e_h^{\varphi,m}\right\|_{L^2}^2 - \delta_\tau\left(\nabla e_h^{\varphi,m}, \nabla e_h^{\varphi,m}\right)
\end{aligned}
$$

Error Analysis: First 3 RHS terms

$$(\delta_\tau \varphi^m - \partial_t \varphi^m, e_h^{\mu,m}) \leq C\tau \int_{t_{m-1}}^{t_m} \|\partial_{ss}\varphi(s)\|_{L^2}^2 \, ds + \frac{1}{12} \|\nabla e_h^{\mu,m}\|_{L^2}^2 \,,$$

$$\begin{aligned}
(\delta_\tau e_P^{\varphi,m}, e_h^{\mu,m}) &\leq C \|\delta_\tau e_P^{\varphi,m}\|_{L^2}^2 + \frac{1}{12} \|\nabla e_h^{\mu,m}\|_{L^2}^2 \\
&\leq \frac{C}{\tau} \int_{t_{m-1}}^{t_m} \|P_h \partial_s \varphi(s) - \partial_s \varphi(s)\|_{L^2}^2 \, ds + \frac{1}{12} \|\nabla e_h^{\mu,m}\|_{L^2}^2 \\
&\leq \frac{C}{\tau} \int_{t_{m-1}}^{t_m} \|\partial_s \varphi(s) - P_h \partial_s \varphi(s)\|_{2,h}^2 \, ds + \frac{1}{12} \|\nabla e_h^{\mu,m}\|_{L^2}^2 \,, \\
(e_R^{\mu,m}, \delta_\tau e_h^{\varphi,m}) &\leq C \|\nabla e_R^{\mu,m}\|_{L^2}^2 + \frac{1}{36} \|\delta_\tau e_h^{\varphi,m}\|_{-1,h}^2 \,,
\end{aligned}$$

Error Analysis: next two RHS terms

$$
\begin{aligned}
2\left(\nabla\varphi^m - \nabla\varphi^{m-1}, \nabla\delta_\tau e_h^{\varphi,m}\right) &= -2\left(\tau\Delta\delta_\tau\varphi^m, \delta_\tau e_h^{\varphi,m}\right) \\
&\le 2\left\|\tau\nabla\Delta\delta_\tau\varphi^m\right\|_{L^2}\left\|\delta_\tau e_h^{\varphi,m}\right\|_{-1,h} \\
&\le C\tau\int_{t_{m-1}}^{t_m}\left\|\partial_s\varphi(s)\right\|_{H^3}^2\,ds + \frac{1}{36}\left\|\delta_\tau e_h^{\varphi,m}\right\|_{-1,h}^2 .
\end{aligned}
$$

$$
\begin{aligned}
\left(\left(\varphi^m\right)^3 - \left(\varphi_h^m\right)^3, \delta_\tau e_h^{\varphi,m}\right) &\le \left\|\nabla\left(\left(\varphi^m\right)^3 - \left(\varphi_h^m\right)^3\right)\right\|_{L^2}\left\|\delta_\tau e_h^{\varphi,m}\right\|_{-1,h} \\
&= \left\|3\left(\varphi^m\right)^2\nabla\varphi^m - 3\left(\varphi_h^m\right)^2\nabla\varphi_h^m\right\|_{L^2} \\
&\quad\times\left\|\delta_\tau e_h^{\varphi,m}\right\|_{-1,h} \\
&= 3\left\|\left(\varphi^m + \varphi_h^m\right)\nabla\varphi^m e^{\varphi,m} + \left(\varphi_h^m\right)^2\nabla e^{\varphi,m}\right\|_{L^2} \\
&\quad\times\left\|\delta_\tau e_h^{\varphi,m}\right\|_{-1,h}
\end{aligned}
$$

Error Analysis: next two RHS terms

$$
\begin{aligned}
&\left((\varphi^m)^3 - (\varphi_h^m)^3, \delta_\tau e_h^{\varphi,m}\right) \\
&\qquad \le 3\left(\|\varphi^m + \varphi_h^m\|_{L^6} \|\nabla \varphi^m\|_{L^6} \|e^{\varphi,m}\|_{L^6} + \|\varphi_h^m\|_{L^6}^2 \|\nabla e^{\varphi,m}\|_{L^6}\right) \\
&\qquad\quad \times \|\delta_\tau e_h^{\varphi,m}\|_{-1,h} \\
&\qquad \le C\left(\|\nabla e_P^{\varphi,m}\|_{L^2} + \|\nabla e_h^{\varphi,m}\|_{L^2} + \|e_P^{\varphi,m}\|_{2,h} + \|e_h^{\varphi,m}\|_{2,h}\right) \\
&\qquad\quad \times \|\delta_\tau e_h^{\varphi,m}\|_{-1,h} \\
&\qquad \le C\left(\|\nabla e_P^{\varphi,m}\|_{L^2} + \|\nabla e_h^{\varphi,m}\|_{L^2} + \|e_P^{\varphi,m}\|_{2,h} + \|e_h^{\varphi,m}\|_{2,h}\right) \\
&\qquad\quad \times \|\delta_\tau e_h^{\varphi,m}\|_{-1,h} \\
&\qquad \le C\|e_P^{\varphi,m}\|_{2,h}^2 + C\|e_h^{\varphi,m}\|_{2,h}^2 + \frac{1}{36}\|\delta_\tau e_h^{\varphi,m}\|_{-1,h}^2 .
\end{aligned}
$$

Error Analysis: second last term

Using discrete product rule:

$$
\begin{aligned}
\left(a^{m-1}, \frac{b^m - b^{m-1}}{\tau}\right) &= \frac{1}{\tau}\left[(a^m, b^m) - \left(a^{m-1}, b^{m-1}\right)\right] - \left(\frac{a^m - a^{m-1}}{\tau}, b^m\right) \\
&= \delta_\tau \left(a^m, b^m\right) - \left(\delta_\tau a^m, b^m\right),
\end{aligned}
$$

we have the following bound

$$
\begin{aligned}
2\left(\nabla e_P^{\varphi,m-1}, \nabla \delta_\tau e_h^{\varphi,m}\right) &= 2\delta_\tau \left(\nabla e_P^{\varphi,m}, \nabla e_h^{\varphi,m}\right) - 2\left(\nabla \delta_\tau e_P^{\varphi,m}, \nabla e_h^{\varphi,m}\right) \\
&\le 2\delta_\tau \left(\nabla e_P^{\varphi,m}, \nabla e_h^{\varphi,m}\right) + C\left\|\delta_\tau e_P^{\varphi,m}\right\|_{L^2}^2 + C\left\|e_h^{\varphi,m}\right\|_{2,h}^2 \\
&\le 2\delta_\tau \left(\nabla e_P^{\varphi,m}, \nabla e_h^{\varphi,m}\right) + \frac{C}{\tau}\int_{t_{m-1}}^{t_m} \left\|\partial_s \varphi(s) - P_h \partial_s \varphi(s)\right\|_{2,h}^2 ds \\
&\quad + C\left\|e_h^{\varphi,m}\right\|_{2,h}^2 .
\end{aligned}
$$

Error Analysis: last term

Lemma

Suppose (φ^m, μ^m) is a weak solution to the PFC equation, with the additional regularities. Then for any $h, \tau > 0$ and any $0 \le m \le M$ and any $\beta > 0$,

$$a_h^{IP}\left(\varphi^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right) + \left((\varphi^m)^3 + (1-\epsilon)\varphi^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right)$$
$$- 2\left(\nabla\varphi^m, \nabla\left(e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right)\right) - \left(\mu^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right) \le C\left[Osc_j(\mu^m)\right]^2 +$$
$$C\left\|e_P^{\varphi,m}\right\|_{2,h}^2 + \frac{C_{coer}}{4\beta}\left\|e_h^{\varphi,m}\right\|_{2,h}^2$$

and

$$a_h^{IP}\left(\delta_\tau\varphi^m, e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1}\right) + \left(\delta_\tau\left((\varphi^m)^3 + (1-\epsilon)\varphi^m\right), e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1}\right)$$
$$- 2\left(\delta_\tau\nabla\varphi^m, \nabla\left(e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1}\right)\right) - \left(\delta_\tau\mu^m, e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1}\right)$$
$$\le C\left[Osc_j(\mu_t(t^*))\right]^2 + C\left\|e_P^{\varphi,m}\right\|_{2,h}^2$$

$$
\begin{aligned}
&\|\nabla e_h^{\mu,m}\|_{L^2}^2 + \frac{1}{2}\delta_\tau\, a_h^{IP}\left(e_h^{\varphi,m}, e_h^{\varphi,m}\right) + \frac{\tau}{2} a_h^{IP}\left(\delta_\tau e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) \\
&\quad + \frac{(1-\epsilon)}{2}\delta_\tau \left\|e_h^{\varphi,m}\right\|_{L^2}^2 + \frac{(1-\epsilon)\tau}{2}\left\|\delta_\tau e_h^{\varphi,m}\right\|_{L^2}^2 + \tau\left\|\nabla\delta_\tau e_h^{\varphi,m}\right\|_{L^2}^2 \\
&\leq \delta_\tau\left(\nabla e_h^{\varphi,m}, \nabla e_h^{\varphi,m}\right) + 2\delta_\tau\left(\nabla e_P^{\varphi,m}, \nabla e_h^{\varphi,m}\right) + \frac{6}{12}\left\|\nabla e_h^{\mu,m}\right\|_{L^2}^2 + C\left\|e_h^{\varphi,m}\right\|_{2,h}^2 \\
&\quad + C\left\|e_h^{\varphi,m-1}\right\|_{2,h}^2 + C\left\|\nabla e_R^{\mu,m}\right\|_{L^2}^2 + C\left\|e_P^{\varphi,m}\right\|_{2,h}^2 + C\left[\mathrm{Osc}_j(\mu_t(t^*))\right]^2 \\
&\quad + C\tau\int_{t_{m-1}}^{t_m}\left[\|\partial_s\varphi(s)\|_{H^3}^2 + \|\partial_{ss}\varphi(s)\|_{L^2}^2\right] ds + \frac{C}{\tau}\int_{t_{m-1}}^{t_m}\|\partial_s\varphi(s) - P_h\partial_s\varphi(s)\|_{2,h}^2\, ds \\
&\quad + \delta_\tau a_h^{IP}\left(\varphi^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right) + \delta_\tau\left(\left(\varphi^m\right)^3 + (1-\epsilon)\varphi^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right) \\
&\quad - 2\delta_\tau\left(\nabla\varphi^m, \nabla\left(e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right)\right) - \delta_\tau\left(\mu^m, e_h^{\varphi,m} - E_h e_h^{\varphi,m}\right).
\end{aligned}
$$

Applying $2\tau \sum_{m=1}^{\ell}$, using the fact that $e_h^{\varphi,0} = 0$ we obtain

$$
\begin{aligned}
& a_h^{IP}\left(e_h^{\varphi,\ell}, e_h^{\varphi,\ell}\right) + (1-\epsilon)\left\|e_h^{\varphi,\ell}\right\|_{L^2}^2 + \tau \sum_{m=1}^{\ell} \|\nabla e_h^{\mu,m}\|_{L^2}^2 \\
& + \tau^2 \sum_{m=1}^{\ell} \left[a_h^{IP}\left(\delta_\tau e_h^{\varphi,m}, \delta_\tau e_h^{\varphi,m}\right) + (1-\epsilon)\|\delta_\tau e_h^{\varphi,m}\|_{L^2}^2 + 2\|\nabla \delta_\tau e_h^{\varphi,m}\|_{L^2}^2\right] \\
\leq & \frac{C_{coer}}{2\beta}\left\|e_h^{\varphi,\ell}\right\|_{2,h}^2 + \frac{8\beta}{C_{coer}}\left\|e_h^{\varphi,\ell}\right\|_{L^2}^2 + C\left\|e_P^{\varphi,\ell}\right\|_{2,h}^2 + C\tau \sum_{m=1}^{\ell} \|e_h^{\varphi,m}\|_{2,h}^2 \\
& + C\tau \sum_{m=1}^{\ell} \left[\|\nabla e_R^{\mu,m}\|_{L^2}^2 + \|e_P^{\varphi,m}\|_{2,h}^2 + [\mathrm{Osc}_j(\mu_t(t^*))]^2\right] \\
& + C\tau^2 \int_{t_0}^{t_\ell} \left[\|\partial_s \varphi(s)\|_{H^3}^2 + \|\partial_{ss}\varphi(s)\|_{L^2}^2\right] ds + C\int_{t_0}^{t_\ell} \|\partial_s\varphi(s) - P_h\partial_s\varphi(s)\|_{2,h}^2\, ds \\
& + 2\Big[C\left[\mathrm{Osc}_j(\mu^\ell)\right]^2 + C\left\|e_P^{\varphi,\ell}\right\|_{2,h}^2 + \frac{C_{coer}}{4\beta}\left\|e_h^{\varphi,\ell}\right\|_{2,h}^2\Big],
\end{aligned}
$$

Error Estimates: Main Result

Theorem

Suppose (φ^m, μ^m) *is a weak solution to the weak form of the PFC equation, with the additional regularities. Then for any* $\tau, h > 0, \epsilon < \frac{C_{coer} - 16}{C_{coer}} < 1$ *and any* $0 \leq \tau \leq M$,

$$\left\| e_h^{\varphi,\ell} \right\|_{2,h}^2 + C \left\| e_h^{\varphi,\ell} \right\|_{L^2}^2 + C\tau \sum_{m=1}^{\ell} \|\nabla e_h^{\mu,m}\|_{L^2}^2 +$$

$$C\tau^2 \sum_{m=1}^{\ell} \left[\left\| \delta_\tau e_h^{\varphi,\ell} \right\|_{2,h}^2 + (1-\epsilon) \|\delta_\tau e_h^{\varphi,m}\|_{L^2}^2 + \|\nabla \delta_\tau e_h^{\varphi,m}\|_{L^2}^2 \right] \leq C^*(h^2 + \tau^2)$$

where C^* *may depend on the oscillations of* μ *and* $\partial_t \mu$ *and the final stopping time* T *but does not depend upon the spacial step size* h *or the time step size* τ.

Our Numerical Scheme

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- Project $\varphi_h^0 := P_h \varphi_0$

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- Project $\varphi_h^0 := P_h\varphi_0$
- Given $\varphi_h^{m-1} \in Z_h$, solve for $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$: Given $\varphi_h^{m-1} \in Z_h$, find $\varphi_h^m, \mu_h^m \in Z_h \times V_h$ such that for all $\nu_h \in V_h,\ \psi_h \in Z_h$ it holds

$$(\delta_\tau \varphi_h^m, \nu_h) + (\mathcal{M}\nabla\mu_h^m, \nabla\nu_h) = 0$$
$$\left((\varphi_h^m)^3 + (1-\epsilon)\varphi_h^m, \psi_h\right) + a_h^{IP}\left(\varphi_h^m, \psi_h\right) - 2\left(\nabla\varphi_h^{m-1}, \nabla\psi_h\right) - (\mu_h^m, \psi_h) = 0,$$

where $\varphi_h^0 := P_h\varphi_0$ and $\mu_h^0 \in V_h$ is defined as $\mu_h^0 := R_h\mu_0$.
model parameters: $\varepsilon = 0.025$ and $\mathcal{M} = 1$, penalty parameter: $\alpha = 20$.

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- Project $\varphi_h^0 := P_h\varphi_0$
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$$(\delta_\tau \varphi_h^m, \nu_h) + (\mathcal{M}\nabla\mu_h^m, \nabla\nu_h) = 0$$
$$\Big((\varphi_h^m)^3 + (1-\epsilon)\varphi_h^m, \psi_h\Big) + a_h^{IP}\left(\varphi_h^m, \psi_h\right) - 2\left(\nabla\varphi_h^{m-1}, \nabla\psi_h\right) - \left(\mu_h^m, \psi_h\right) = 0,$$

  where $\varphi_h^0 := P_h\varphi_0$ and $\mu_h^0 \in V_h$ is defined as $\mu_h^0 := R_h\mu_0$.
  model parameters: $\varepsilon = 0.025$ and $\mathcal{M} = 1$, penalty parameter: $\alpha = 20$.
- We use Newton iteration method to solve the discrete nonlinear system with tolerance of the Newton iteration is set to 10^{-6}.
  The initial guess at each time step is taken as the numerical solution at the previous time level.
  One to three Newton's iterative steps are involved at each time step.

Numerical Experiment I: Accuracy Test

Example (Hu, Wise, Wang, Lowengrub, 2009)

$$\varphi_0(x, y) = 0.07 - 0.02\cos\left(\frac{2\pi(x-12)}{32}\right)\sin\left(\frac{2\pi(y-1)}{32}\right) + 0.02\cos^2\left(\frac{\pi(x+10)}{32}\right)\cos^2\left(\frac{\pi(y+3)}{32}\right) - 0.01\sin^2\left(\frac{4\pi x}{32}\right)\sin^2\left(\frac{4\pi(y-6)}{32}\right)$$

$\Omega = (0, 32) \times (0, 32)$, $T = 10$.
$\mathcal{M} \equiv 1$, $\varepsilon = 0.025$, and the penalty parameter $\alpha = 20$.

Numerical Experiment I: Accuracy Test

$$\|\xi_h\|_{2,h}^2 := \sum_{K\in\mathcal{T}_h} |\xi_h|_{H^2(K)}^2 + \sum_{e\in\mathcal{E}_h} \alpha \| h_e^{-\frac{1}{2}} [\mathrm{n}_e \cdot \nabla \xi_h]_e \|_{L^2(e)}^2.$$

Mesh $h = 32/512$ with τ with $\tau = 0.05h$ and $T = 10$ as the 'exact' solution, φ_{exact}.

$$error_\varphi := \varphi_h - \varphi_{exact}$$

where φ_h indicates the solution on the mesh size h.

h	$\|error_\varphi\|_{2,h}$	rate	$\|error_\mu\|_{H^1}$	rate
$32/8$	0.08412	N/A	0.00522	N/A
$32/16$	0.05896	0.71329	0.00242	1.07627
$32/32$	0.03466	0.85058	0.00157	0.76970
$32/64$	0.01568	1.10514	0.00103	0.76082
$32/128$	0.00601	1.30482	0.00041	1.25840
$32/256$	0.00255	1.17707	0.00016	1.27362

Numerical Experiment I: Unconditional Stability

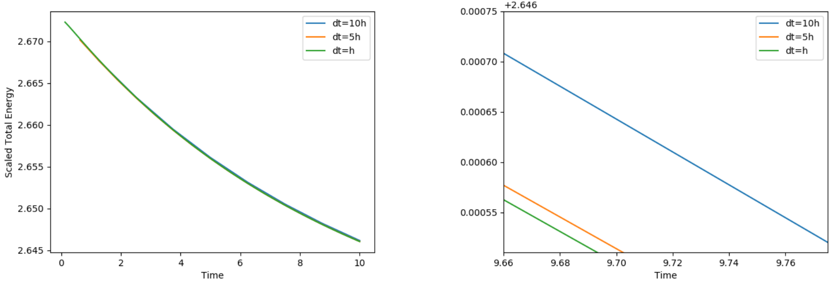


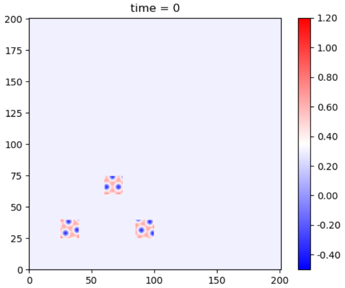
Figure: Unconditional stability demonstrated through the time evolution of the scaled total energy ${}^{F}\!/_{32^2}$ for time step sizes $dt = 10h,\ 5h, h$ with the spacial step size $h = {}^{32}\!/_{256}$.

Numerical Experiment II: Crystal growth

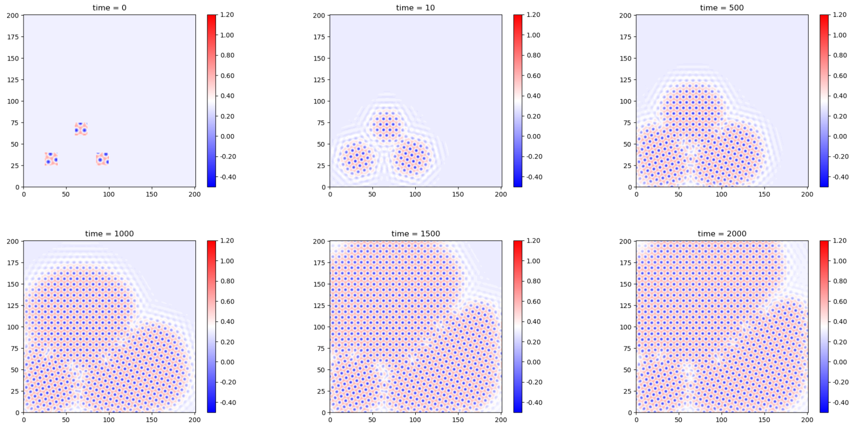
Example (Gomez, Nogueira, 2012)

$$\varphi_0(x,y) = \bar{\varphi} + C\left[\cos\left(\frac{q}{\sqrt{3}}y\right)\cos(qx) - 0.5\cos\left(\frac{2q}{\sqrt{3}}y\right)\right]$$

where $\bar{\varphi} = 0.285,\ C = 0.466,\ q = 0.66,\ \Omega = (0,201)\times(0,201), h = {}^{201}\!/_{402}$.

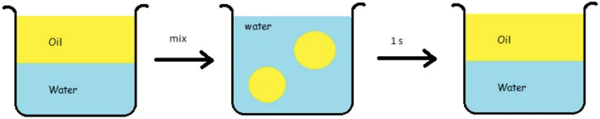


Motion of liquid-crystal interfaces and grain boundaries



Phase Field Model for Microemulsions: Motivation

No surfactants



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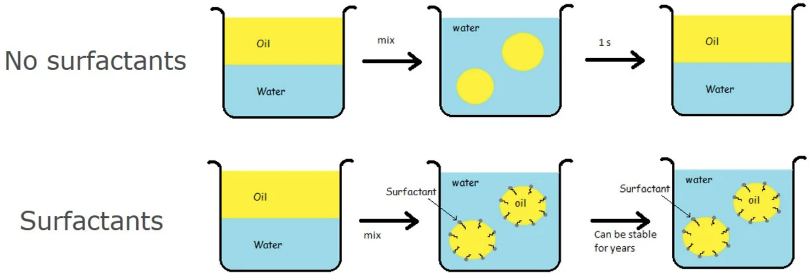

[Picture Courtesy: Biolin Scientific]

Motivation: Microemulsion systems as skin drug delivery systems

[Source: Walgreens]

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- **Issue:** Topical cream formulations contain petrochemical ingredients (such as petrolatum, silicones).
- **Goal:** Develop skin drug delivery systems that contain natural and renewable sourced alternatives to these ingredients without compromising on the functionality.
- **Approach:** Provide computational tools to predict and assess the properties of novel and more sustainable alternatives to the toxic ingredients.

[Source: The Nabi Laboratory of Bioengineered Therapeutics,UTEP]

Mathematical Model for Microemulsions

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- φ : the scalar order parameter indicating the local difference between oil and water concentrations.
- $\varphi = -1$ (water phase), $\varphi = 1$ (oil phase) and $\varphi = 0$ (microemulsions phase)
- $E(\varphi)$: (Ginzburg-Landau free energy)

$$\underbrace{\int_\Omega \left\{ \frac{(\varphi^2 - a_0)}{2} |\nabla \varphi|^2 + \frac{\lambda}{2} (\Delta \varphi)^2 \right\} \, dx}_{\text{tendency to mix}} + \underbrace{\frac{\beta}{2} \int_\Omega (\varphi + 1)^2 (\varphi^2 + 0.5)(\varphi - 1)^2 \, dx}_{\text{tendency to separate}}$$

[Gompper et. al. 90]

Mathematical Model for Microemulsions

Conservation Law:

$$\partial_t \varphi + \nabla \cdot \mathrm{j} = 0$$

- φ : the scalar order parameter
- $\mathrm{j} = -\mathcal{M}\nabla\mu$: mass flux
- $\mathcal{M}$: mobility coefficient, $\mu = \delta_\varphi E$: chemical potential

$$E(\varphi) = \int_\Omega \left\{ \frac{(\varphi^2 - a_0)}{2}|\nabla\varphi|^2 + \frac{\lambda}{2}(\Delta\varphi)^2 + \frac{\beta}{2}(\varphi+1)^2(\varphi^2+0.5)(\varphi-1)^2 \right\} dx$$

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$$\partial_t\varphi - \mathcal{M}\Delta\Big(3\beta(\varphi^5 - \varphi^3) + \varphi|\nabla\varphi|^2 - \nabla\cdot((\varphi^2 - 4)\nabla\varphi) + \lambda\Delta^2\varphi\Big) = 0.$$

Mathematical Model for Microemulsions

Compliment

$$\frac{\partial\varphi}{\partial t} - \nabla\cdot(\mathcal{M}\nabla\mu) = 0, \quad \text{in } \Omega^T := \Omega\times(0,T),$$
$$3\beta(\varphi^5-\varphi^3) + \varphi|\nabla\varphi|^2 - \nabla\cdot((\varphi^2-a_0)\nabla\varphi) + \lambda\Delta^2\varphi - \mu = 0, \quad \text{in } \Omega^T$$

with natural boundary conditions

$$\partial_n\varphi = \lambda\partial_n\,\Delta\varphi = \partial_n\mu = 0, \quad \text{on } \partial\Omega^T$$

and the initial value:

$$\varphi(0) = \varphi_0.$$

Notation:

- $H^s(\Omega)$ denote the Sobolev spaces of order $s\geq 1$,
- $Z := \{z\in H^2(\Omega) \mid \partial_n z = 0 \text{ on } \partial\Omega\}$. [Pawlow et al., 2011]

Numerical Schemes: Existing Literature

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- Hoppe/Linsemnann 2019: Fully implicit backward Euler and C^0-IP Method quasi-optimal error estimates without any discrete energy law
- Diegel/Sharma 2022: Closely related literature is the C^0-IP framework developed for the Phase Field Crystal Equation based on Eyre's convex splitting scheme.

Fully Discrete Scheme

Given $\varphi_h^{m-1} \in Z_h$, find $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ which satisfies

$$(\delta_\tau \varphi_h^m, \nu_h) + (M\nabla \mu_h^m, \nabla \nu_h) = 0, \qquad \forall \quad \nu_h \in V_h$$

$$3\beta \left((\varphi_h^m)^5 - (\varphi_h^{m-1})^3, \psi_h\right) + \left((\varphi_h^m)^2 \nabla \varphi_h^m, \nabla \psi_h\right) + \left(\varphi_h^m |\nabla \varphi_h^{m-1}|^2, \psi_h\right)$$
$$-a_0 \left(\nabla \varphi_h^{m-1}, \nabla \psi_h\right) + \lambda\, a_h^{IP}\left(\varphi_h^m, \psi_h\right) - (\mu_h^m, \psi_h) = 0 \qquad \forall \quad \psi_h \in Z_h$$

with initial data taken to be $\varphi_h^0 := P_h \varphi_0$.

Existence of a solution

Theorem

Let $\lambda \geq \dfrac{3\beta|\overline{\varphi_0}|^4 C_{P,1}}{2C_{coer}}$, *where* $C_{P,1}$ *depends upon a Poincarè constant but does not depend upon* h *or* τ. *Then, there exists a solution* $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ *to the scheme.*

Unconditional Energy Stability

$$F(\varphi) := \frac{\beta}{2}\|\varphi\|_{L^6}^6 - \frac{3\beta}{4}\|\varphi\|_{L^4}^4 + \frac{\beta|\Omega|}{4} + \frac{1}{2}\|\varphi\nabla\varphi\|_{L^2}^2 - \frac{a_0}{2}\|\nabla\varphi\|_{L^2}^2 + \frac{\lambda}{2}a_h^{IP}(\varphi,\varphi).$$

Theorem (Discrete Energy Law)

Let $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ be a solution. Then the following energy law holds for any $h, \tau > 0$:

$$F\left(\varphi_h^\ell\right) + \tau\sum_{m=1}^{\ell}\left\|\sqrt{\mathcal{M}}\nabla\mu_h^m\right\|_{L^2}^2 \le F\left(\varphi_h^0\right),$$

for all $1 \le \ell \le M$.

Uniform *A Priori* Estimates

Theorem

Let $(\varphi_h^m, \mu_h^m) \in Z_h \times V_h$ *be the* C^0 *IP approximation. Suppose that* $F(\varphi_h^0) \leq C$ *independent of* h *and that* $\lambda > \max\left\{\frac{3\beta|\overline{\varphi_0}|^4 C_{P,1}}{2C_{coer}}, \frac{a_0 C_{P,2}}{C_{coer}}\right\} > 0$ *where* $C_{P,1}, C_{P,2}$ *are Poincarè constants and do not depend on* h *or* τ*. Then the following estimates hold for any* $\tau, h > 0$*:*

$$\max_{0\leq m\leq M} \|\varphi_h^m\|_{2,h}^2 \leq C$$

$$\max_{0\leq m\leq M} \left[\|\varphi_h^m\|_{L^2}^2 + \|\nabla\varphi_h^m\|_{L^2}^2 + \|\varphi_h^m\nabla\varphi_h^m\|_{L^2}^2 + \|\varphi_h^m\|_{L^\infty}^2\right] \leq C^*$$

$$\tau\sum_{m=1}^{\ell} \left\|\sqrt{\mathcal{M}}\nabla\mu_h^m\right\|_{L^2}^2 \leq C$$

for some constants C^*, C *that is independent of* $h, \tau,$ *and* T.

Unique Solvability

Theorem

Let $\varphi_h^{m-1} \in Z_h$ be given and

$$\lambda > \max\left\{ \frac{3\beta|\overline{\varphi_0}|^4 C_{P,1}}{2C_{coer}}, \frac{a_0 C_{P,2}}{C_{coer}}, \frac{C^* C_{P,3}}{2C_{coer}} \right\} > 0,$$

where C^* is the constant from uniform a priori bounds and $C_{P,1}, C_{P,2}, C_{P,3}$ are all Poincarè constants and do not depend on h or τ.
The solution to the fully discrete scheme is unique for all $h, \tau > 0$.

Our Numerical Scheme

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- We use Newton iteration method to solve the discrete nonlinear system with tolerance of the Newton iteration is set to 10^{-6}.
  The initial guess at each time step is taken as the numerical solution at the previous time level.
  One to three Newton's iterative steps are involved at each time step.

Numerical Experiment I: Accuracy Test

Example

$$\varphi_0(x, y) = 0.3\cos(3x) + 0.5\cos(y)$$

$$\Omega = [0, 2\pi]^2,\ T = 0.4.$$

$\mathcal{M} = 10^{-3}$, $\lambda = 1$

Numerical Experiment I: First Order Convergence

- φ_{256}: "exact" solution

N	$\|\varphi_{256} - \varphi_N\|_{2,h}$	rate	$\|\varphi_{256} - \varphi_N\|_{L^2}$	rate
8	6.1911	–	0.2625	–
16	1.9293	1.6045	0.0624	2.1039
32	0.5601	1.7221	0.0151	2.0685
64	0.1599	1.7516	0.0035	2.1336
128	0.0461	1.7354	0.0008	2.1887

Table: Errors and convergence rates of the C^0-IP method with $\mathcal{M} = 10^{-3}$, $\lambda = 1$, $h = {}^{2\sqrt{2}\pi}/_{N}$, $\tau = {}^{0.05}/_{N}$.

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Numerical Experiment II: Energy Dissipation

Example

$$\varphi_0(x,y) = 0.3\cos(3x) + 0.5\cos(y)$$

$$\Omega := [0,10]^2,\ T = 5.$$

$\mathcal{M} = 10^{-3}$, $\lambda = 1$, penalty parameter $\alpha = 8$

$$F(\varphi) = \frac{\beta}{2}\|\varphi\|_{L^6}^6 - \frac{3\beta}{4}\|\varphi\|_{L^4}^4 + \frac{\beta|\Omega|}{4} + \frac{1}{2}\|\varphi\nabla\varphi\|_{L^2}^2 - \frac{a_0}{2}\|\nabla\varphi\|_{L^2}^2 + \frac{\lambda}{2}a_h^{IP}(\varphi,\varphi).$$

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Track the scaled energy $F(\varphi) - \frac{\beta|\Omega|}{4}$ for time step sizes $\tau = 0.5, 0.25, 0.0125,$ and 0.0625.

Numerical Experiment II: Energy Dissipation

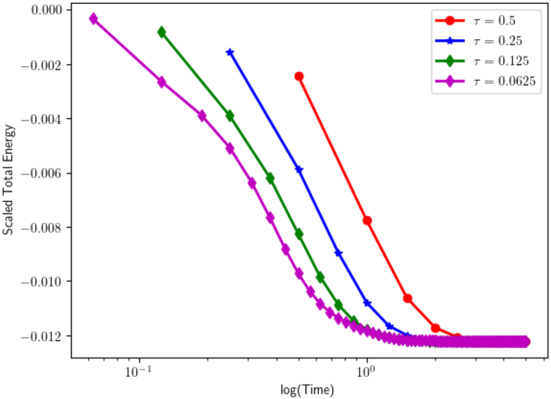
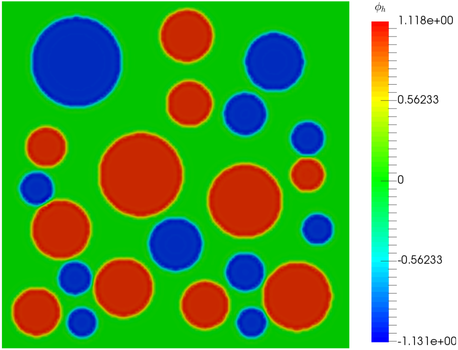


Figure: The time evolution of the scaled total energy $F(\varphi) - \frac{\beta|\Omega|}{4}$, $h = {}^{10\sqrt{2}}/_{128}$

Numerical Experiment III: Microemulsions Simulation

Example

$\Omega = (-5,5)^2, T = 0.1,\ \tau = 1.1 \times 10^{-4},\ h = 10\sqrt{2}/128,\ \mathcal{M} = 10,\ \lambda = 10^{-2}.$



Evolution of the profile

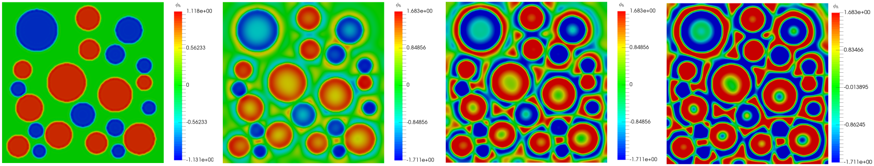


Figure: Profiles at $m = 0, 1,\ 2$ and 3.

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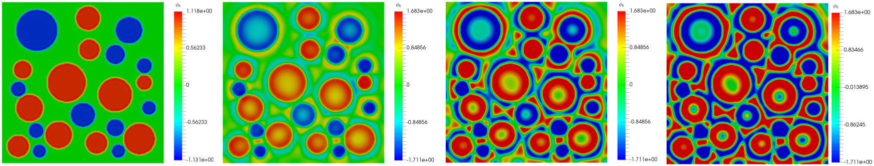

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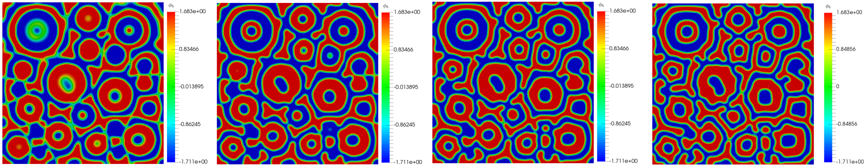

Figure: Profiles at $m = 4, 11,\ 20$ and 25.

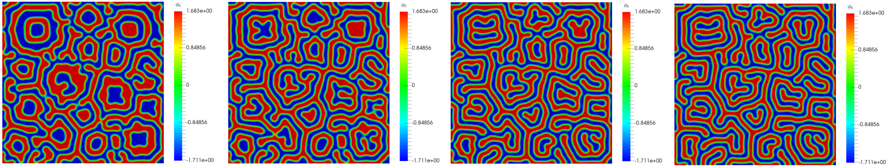

Figure: Profiles at $m = 37, 74,\ 158$ and 511.

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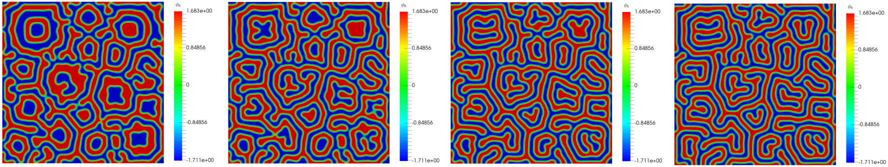

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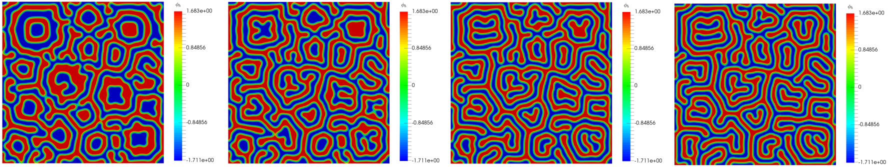

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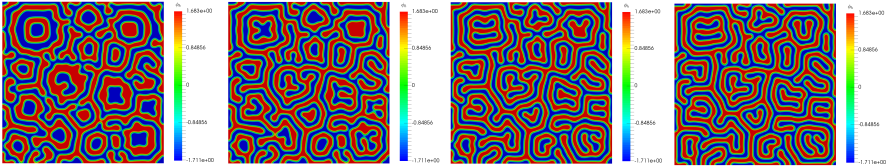

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Conclusions and Ongoing Work

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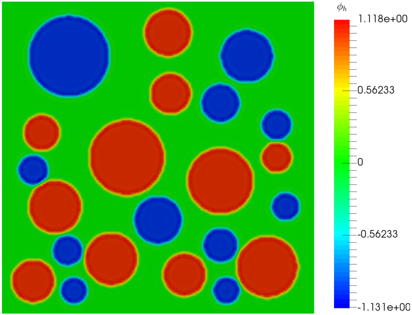
Thank you for your attention!

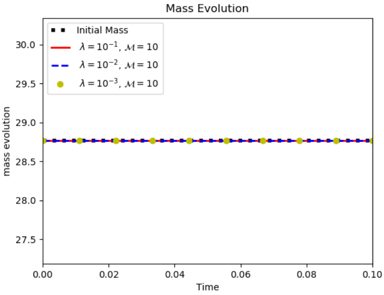
Numerical Experiment: Discrete Mass Conservation

Initial Conditions:

Example

$\Omega = (-5,5)^2, T = 0.1,\ \tau = 1.1 \times 10^{-4},\ h = 10\sqrt{2}/128,\ \mathcal{M} = 10,$
$\lambda = 10^{-1}, 10^{-2}, 10^{-3}.$





Effect of the decreasing λ

Theory suggests that increasing λ guarantees the existence and stability of the solution.

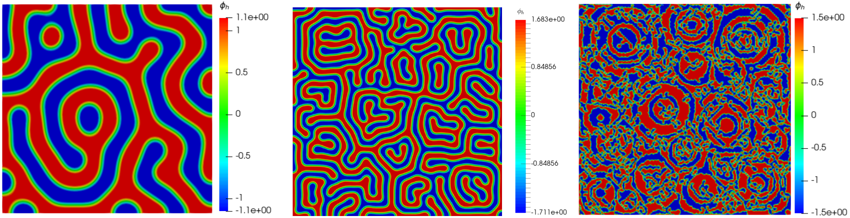


Figure: $\lambda = 10^{-1}, 10^{-2}, 10^{-3}$

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