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

Natasha S. Sharma
Department of Mathematical Sciences
The University of Texas at El Paso
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

Microstructure evolution specifically formation of defects within microstructures.

Microemulsions capturing the dynamics of phase transitions in oil-water-surfactant mixtures with applications to designing drug delivery systems.

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

Applications
Applications

- Microstructure evolution specifically formation of defects within microstructures.
Sixth Order Cahn-Hilliard-type Equations

Applications

- Microstructure evolution specifically formation of defects within microstructures.
- Microemulsions capturing the dynamics of phase transitions in a oil-water-surfactant mixtures with applications to designing drug delivery systems.
Sixth Order Cahn-Hilliard-type Equations

Applications

- Microstructure evolution specifically formation of defects within microstructures.
- Microemulsions capturing the dynamics of phase transitions in a oil-water-surfactant mixtures with applications to designing drug delivery systems.

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

1. Defects in crystalline materials control electrical conductivity whether they make efficient solar panels.
2. Defects also control chemical reactivity and influence the tensile strength of a material.

Goal:
Control/predict the formation and evolution of defects.

Approach:
Use the phase field crystal equation as our atomistic model. Develop an accurate, efficient, easy-to-compute numerical scheme.
Defects in Crystalline Materials

Defects control whether they make efficient solar panels, chemical reactivity, or tensile strength of a material. The goal is to control/predict the formation and evolution of defects. The approach involves using the phase field crystal equation as our atomistic model and developing an accurate, efficient, easy-to-compute numerical scheme.
Defects control

1. electrical conductivity whether they make efficient solar panels,
Defects in Crystalline Materials

Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material
Defects in Crystalline Materials

Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material
Defects in Crystalline Materials

Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material

Goal: Control/predict the formation and evolution of defects.
Defects in Crystalline Materials

Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material

Goal: Control/predict the formation and evolution of defects.

Approach:
Defects in Crystalline Materials

Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material

Goal: Control/predict the formation and evolution of defects.

Approach:

- Use phase field crystal equation as our atomistic model.
Defects control

1. electrical conductivity whether they make efficient solar panels,
2. chemical reactivity
3. tensile strength of a material

Goal: Control/predict the formation and evolution of defects.

Approach:
- Use phase field crystal equation as our atomistic model.
- Develop an accurate, efficient, easy-to-compute numerical scheme.
Phase Field Crystal Equation

Two-phase system

\[ \phi \]: number density of atoms in the material occupying \( \Omega \) with

\[ \diamond \]: liquid phase characterized by a constant value of \( \phi \)

\[ \phi \]: solid phase characterized by a spatially varying periodic function

that inherits the symmetry and periodicity of the crystal lattice
Phase Field Crystal Equation

Two-phase system
Two-phase system

\( \varphi \): number density of atoms in the material occupying \( \Omega \) with
Phase Field Crystal Equation

Two-phase system

\[ \varphi: \] number density of atoms in the material occupying \( \Omega \) with

- liquid phase characterized by a constant value of \( \varphi \)
- solid phase characterized by a spatially varying periodic function
  that inherits the symmetry and periodicity of the crystal lattice
Phase Field Crystal Equation

Two-phase system

\( \varphi \): number density of atoms in the material occupying \( \Omega \) with

- liquid phase characterized by a constant value of \( \varphi \)
- solid phase characterized by a spatially varying periodic function \( \varphi \) that inherits the symmetry and periodicity of the crystal lattice
Phase Field Crystal Equation

Conservation Law:

\[ \frac{\partial \varphi}{\partial t} = \nabla \cdot (M \nabla \mu) \]

\( M \): mobility coefficient assumed to be constant

\( \mu = \delta \varphi E \):

\( E(\varphi) = \int_{\Omega} \varphi^4 - |\nabla \varphi|^2 + \frac{1}{2} - \varepsilon \varphi^2 + \frac{1}{2} (\Delta \varphi)^2 \, dx \)
Phase Field Crystal Equation

Conservation Law:

\[
\frac{\partial \varphi}{\partial t} = \nabla \cdot (M \nabla \mu)
\]

- \( M \): mobility coefficient assumed to be constant
Phase Field Crystal Equation

Conservation Law:

\[
\frac{\partial \varphi}{\partial t} = \nabla \cdot (\mathcal{M} \nabla \mu)
\]

- \(\mathcal{M}\): mobility coefficient assumed to be constant
- \(\mu = \delta \varphi E\): chemical potential
Phase Field Crystal Equation

Conservation Law:

\[
\frac{\partial \varphi}{\partial t} = \nabla \cdot (\mathcal{M} \nabla \mu)
\]

- \( \mathcal{M} \): mobility coefficient assumed to be constant
- \( \mu = \delta \varphi E \): chemical potential
- \( E(\varphi) = \int_{\Omega} \left( \frac{\varphi^4}{4} - |\nabla \varphi|^2 + \frac{1-\varepsilon}{2} \varphi^2 + \frac{1}{2} (\Delta \varphi)^2 \right) \, dx \)
Conservation Law:

\[ \frac{\partial \varphi}{\partial t} = \nabla \cdot (M \nabla \mu) \]

- \( M \): mobility coefficient assumed to be constant
- \( \mu = \delta \varphi E \): chemical potential

\[ E(\varphi) = \int_{\Omega} \frac{\varphi^4}{4} - |\nabla \varphi|^2 + \frac{1-\varepsilon}{2} \varphi^2 + \frac{1}{2} (\Delta \varphi)^2 \, dx \]

Phase Field Crystal Equation (Elder et al. 2004)

\[ \frac{\partial \varphi}{\partial t} = \nabla \cdot (M \nabla (\varphi^3 + 2\Delta \varphi + (1 - \varepsilon)\varphi + \Delta^2 \varphi)) \] on \( \Omega \times (0, T) \).
PFC equation in the mixed form

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0,
\]

\[
\varphi^3 + (1 - \varepsilon) \varphi + 2 \Delta \varphi + \Delta^2 \varphi - \mu = 0,
\]
PFC equation in the mixed form

Compliment

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot \left( \mathcal{M} \nabla \mu \right) = 0, \\
\varphi^3 + (1 - \varepsilon) \varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0,
\]

with either periodic boundary conditions or natural boundary conditions

\[
\partial_n \varphi = \partial_n \Delta \varphi = \partial_n \mu = 0,
\]
PFC equation in the mixed form

Compliment

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0, \\
\varphi^3 + (1 - \varepsilon)\varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0,
\]

with either periodic boundary conditions or natural boundary conditions

\[
\partial_n \varphi = \partial_n \Delta \varphi = \partial_n \mu = 0,
\]

and the initial value:

\[
\varphi(0) = \varphi_0.
\]
PFC equation in the mixed form

Compliment

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0, \\
\varphi^3 + (1 - \varepsilon)\varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0,
\]

with either periodic boundary conditions or natural boundary conditions

\[
\partial_n \varphi = \partial_n \Delta \varphi = \partial_n \mu = 0,
\]

and the initial value:

\[
\varphi(0) = \varphi_0.
\]

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

Find \((\varphi, \mu)\) such that

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

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

\[
\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)
\]
\[
\left( (\varphi)^3 + (1 - \epsilon)\varphi, \psi \right) - 2(\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z
\]

with \(a(u, v) := \int_{\Omega} (\nabla^2 u : \nabla^2 v) \, dx\),

\[\text{[Pawlow et al., 2013]}\]
Find \((\varphi, \mu)\) such that

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

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

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

with \(a(u, \nu) := \int_{\Omega} (\nabla^2 u : \nabla^2 \nu) \, dx\), \(\varphi(0) = \varphi_0 \in H^4(\Omega)\) such that \(\varphi_0\) satisfies the boundary conditions.

[Pawlow et al., 2013]
Phase Field Crystal Equation

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0,
\]

\[
\varphi^3 + (1 - \varepsilon)\varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0 \quad \text{on } \Omega \times (0, T).
\]

- **Space discretization:** Choose a suitable discretization for the higher order term.
Numerical Schemes: Challenges

Phase Field Crystal Equation

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

- **Space discretization:** Choose a suitable discretization for the higher order term.
- **Time discretization:** Classical methods give us *conditional* solvability and stability.
Numerical Schemes: Challenges

Phase Field Crystal Equation

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

- Space discretization: Choose a suitable discretization for the higher order term.
- Time discretization: Classical methods give us conditional solvability and stability.
Phase Field Crystal Equation

\[ \frac{\partial \varphi}{\partial t} - \nabla \cdot (\mathcal{M} \nabla \mu) = 0, \]

\[ \varphi^3 + (1 - \varepsilon) \varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0 \text{ on } \Omega \times (0, T). \]
Phase Field Crystal Equation

\[ \frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0, \]

\[ \varphi^3 + (1 - \varepsilon) \varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0 \quad \text{on } \Omega \times (0, T). \]

- Finite Element Method for a Mixed form of three second-order equations:
  Backofen, Rätz, and Voigt 2007
Numerical Schemes: Some Existing Literature

Phase Field Crystal Equation

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

- **Finite Element Method** for a Mixed form of three second-order equations: Backofen, Rätz, and Voigt 2007
- **Finite Difference Method**: Wise, Wang, and Lowengrub 2009; Dong, Feng, Wang, Wise and Zhang, 2018
Phase Field Crystal Equation

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

- **Finite Element Method for a Mixed form of three second-order equations:** Backofen, Rätz, and Voigt 2007
- **Finite Difference Method:** Wise, Wang, and Lowengrub 2009; Dong, Feng, Wang, Wise and Zhang, 2018
- **C^1 Finite Element Method:** Gomez, Nogueira, 2012
Phase Field Crystal Equation

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (\mathcal{M} \nabla \mu) = 0,
\]

\[
\varphi^3 + (1 - \varepsilon)\varphi + 2\Delta \varphi + \Delta^2 \varphi - \mu = 0 \quad \text{on } \Omega \times (0, T).
\]

- **Finite Element Method** for a Mixed form of three second-order equations: Backofen, Rätz, and Voigt 2007
- **Finite Difference Method**: Wise, Wang, and Lowengrub 2009; Dong, Feng, Wang, Wise and Zhang, 2018
- **C^1** Finite Element Method: Gomez, Nogueira, 2012
- **Local Discontinuous Galerkin Method**: Guo and Xu, 2016
Phase Field Crystal Equation

\[
\frac{\partial \phi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0,
\]
\[
\phi^3 + (1 - \varepsilon)\phi + 2\Delta \phi + \Delta^2 \phi - \mu = 0 \quad \text{on } \Omega \times (0, T).
\]

- **Finite Element Method for a Mixed form of three second-order equations:** Backofen, Rätz, and Voigt 2007
- **Finite Difference Method:** Wise, Wang, and Lowengrub 2009; Dong, Feng, Wang, Wise and Zhang, 2018
- **C\(^1\) Finite Element Method:** Gomez, Nogueira, 2012
- **Local Discontinuous Galerkin Method:** Guo and Xu, 2016
- **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

$\Omega = \bigcup_{K \in T_h} K$

Assume this partition is geometrically-conforming and shape-regular.

$T_h$: collection of all elements

$h_K = \text{diameter of triangle } K$

$E_h$: collection of all edges wrt $T_h$
Spatial Discretization

\[ \Omega = \bigcup_{K \in \mathcal{T}_h} K \]

Assume this partition is geometrically-conforming and shape-regular.

\[ \mathcal{T}_h : \text{collection of all elements} \]

\[ h_K = \text{diameter of triangle } K \]

\[ h = \max_{K \in \mathcal{T}_h} h_K \]

\[ \mathcal{E}_h : \text{collection of all edges wrt } \mathcal{T}_h \]
Spatial Discretization

\[ \Omega = \bigcup_{K \in \mathcal{T}_h} K, \]

Assume this partition is geometrically-conforming and shape-regular.

\[ \mathcal{T}_h: \text{collection of all elements } K \]
\[ \Omega = \bigcup_{K \in \mathcal{T}_h} K, \]

**Assume this partition is geometrically-conforming and shape-regular.**

\( \mathcal{T}_h \): collection of all elements \( K \)

- \( h_K = \) diameter of triangle \( K \), \( h = \max_{K \in \mathcal{T}_h} h_K \)
Spatial Discretization

\[ \Omega = \bigcup_{K \in \mathcal{T}_h} K, \]

Assume this partition is geometrically-conforming and shape-regular.

- \( \mathcal{T}_h \): collection of all elements \( K \)
- \( h_K = \text{diameter of triangle } K \), \( h = \max_{K \in \mathcal{T}_h} h_K \)
- \( \mathcal{E}_h \): collection of all edges \( e \) wrt \( \mathcal{T}_h \)
Find \((\varphi, \mu) : [0, T] \to Z \times H^1(\Omega)\) s.t. for almost all \(t \in (0, T)\)

\[
\langle \partial_t \varphi, \nu \rangle + (\mathcal{M} \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)
\]

\[
(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2 (\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z
\]
Find \((\varphi, \mu) : [0, T] \rightarrow Z \times H^1(\Omega)\) s.t. for almost all \(t \in (0, T)\)

\[
\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)
\]

\[
(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2 (\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z
\]

Find finite dimensional subspaces:

\[
V_h \subset H^1(\Omega), \; Z_h \subset Z,
\]
Classical \( C^1 \) Finite Element Method

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

\[
\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)
\]

\[
(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2(\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z
\]

Find finite dimensional subspaces:

\[V_h \subset H^1(\Omega), \quad Z_h \subset Z,\]

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

\[
\langle \partial_t \varphi_h, \nu \rangle + (M \nabla \mu_h, \nabla \nu) = 0 \quad \forall \nu \in V_h
\]

\[
\left(\left(\varphi_h\right)^3 + (1 - \epsilon)\varphi_h, \psi\right) - 2(\nabla \varphi_h, \nabla \psi) + a(\varphi_h, \psi) - (\mu_h, \psi) = 0 \quad \forall \psi \in Z_h
\]

holds for almost all \(t \in (0, T)\).
Our Approach: Relax $C^1$ continuity

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

$$\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)$$

$$(\varphi^3 + (1 - \epsilon) \varphi, \psi) - 2(\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z$$
Our Approach: Relax $C^1$ continuity

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

$$\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)$$

$$(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2(\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z$$

Find finite dimensional subspaces:

$$V_h \subset H^1(\Omega), \ Z_h \not\subset Z,$$
Our Approach: Relax $C^1$ continuity

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

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

$$(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2 (\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z$$

Find finite dimensional subspaces:

$$V_h \subset H^1(\Omega), \ Z_h \not\subset Z,$$

$$Z_h \subset H^1(\Omega)$$
Our Approach: Relax $C^1$ continuity

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

$$\langle \partial_t \varphi, \nu \rangle + (M \nabla \mu, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega)$$

$$(\varphi^3 + (1 - \epsilon)\varphi, \psi) - 2(\nabla \varphi, \nabla \psi) + a(\varphi, \psi) - (\mu, \psi) = 0 \quad \forall \psi \in Z$$

Find finite dimensional subspaces:

$$V_h \subset H^1(\Omega), \ Z_h \not\subset Z,$$

$$Z_h \subset H^1(\Omega)$$

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

$$\langle \partial_t \varphi_h, \nu \rangle + (M \nabla \mu_h, \nabla \nu) = 0,$$

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

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

Natasha S. Sharma (UTEP)
$V_h := \{ v \in C(\bar{\Omega}) | v|_K \in P_1(K) \ \forall K \in \mathcal{T}_h \}$
$V_h := \{ \nu \in C(\overline{\Omega}) \mid \nu|_K \in P_1(K) \ \forall K \in \mathcal{T}_h \}$

$Z_h := \{ \nu \in C(\overline{\Omega}) \mid \nu|_K \in P_2(K) \ \forall K \in \mathcal{T}_h \}$,
Spatial Discretization using C⁰-IP Method

\[ V_h := \{ v \in C(\overline{\Omega}) \mid v\mid_K \in P_1(K) \ \forall K \in \mathcal{T}_h \} \]

\[ Z_h := \{ v \in C(\overline{\Omega}) \mid v\mid_K \in P_2(K) \ \forall K \in \mathcal{T}_h \}, \]

\[ R_h : H^1(\Omega) \to V_h \text{ is a Ritz projection operator such that} \]

\[ (\nabla (R_h \mu - \mu), \nabla \xi) = 0 \quad \forall \xi \in V_h, \quad (R_h \mu - \mu, 1) = 0. \]
Spatial Discretization using $C^0$-IP Method

\[ V_h := \{ v \in C(\overline{\Omega}) \mid v|_K \in P_1(K) \ \forall K \in \mathcal{T}_h \} \]

\[ Z_h := \{ v \in C(\overline{\Omega}) \mid v|_K \in P_2(K) \ \forall K \in \mathcal{T}_h \}, \]

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

\[ (\nabla (R_h \mu - \mu), \nabla \xi) = 0 \ \forall \xi \in V_h, \quad (R_h \mu - \mu, 1) = 0. \]

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

\[ a_h^{IP} (P_h \varphi - \varphi, \xi) + (1 - \epsilon) (P_h \varphi - \varphi, \xi) = 0 \ \forall \xi \in Z_h, \quad (P_h \varphi - \varphi, 1) = 0. \]
Spatial Discretization using $C^0$-IP Method

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

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

where

$$J(\xi_h, \psi_h) := \sum_{e \in \mathcal{E}_h} \int_e \left( [n_e \cdot \nabla \xi_h]_e \{n_e \cdot \nabla^2 \psi_h n_e\}_e + \{n_e \cdot \nabla^2 \xi_h n_e\}_e [n_e \cdot \nabla \psi_h]_e \right) \, ds$$

$$+ \sum_{e \in \mathcal{E}_h} \int_e \frac{\alpha}{h_e} [n_e \cdot \nabla \xi_h]_e [n_e \cdot \nabla \psi_h]_e \, ds, \quad \xi_h, \psi_h \in Z_h$$

and $\alpha > 0$ is a penalty parameter.
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 $\alpha$ 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 $\mathcal{T}_h$.

where the $C^0$-IP Norm is:

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

We introduce a partition of \((0,T)\)
Time Discretization

We introduce a partition of \((0, T)\) into \(M\) sub-intervals \((t_{m-1}, t_m)\):

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

Notation: \(\phi_m\) approximate \(\phi\) at time \(t_m\).

Numerical time derivative w.r.t. \(\tau\):

\[
\delta_\tau \phi_m := \phi_{m+1} - \phi_m
\]
Time Discretization

We introduce a partition of $(0,T)$ into $M$ sub-intervals $(t_{m-1}, t_m)$:

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

Notation: $\varphi^m$ approximate $\varphi$ at time $t_m$.

Numerical time derivative w.r.t. $\tau$:

$$\delta_\tau \varphi^m := \frac{\varphi^{m+1} - \varphi^m}{\tau}$$
Convex Time Splitting Scheme

- Basic Idea:

\[ \mu = \delta \varphi E(\varphi) = \delta \varphi \left( E^+(\varphi) + E^-(\varphi) \right) \]

\[ \Rightarrow \mu^m = (\varphi^m)^3 + (1 - \epsilon)\varphi^m + \Delta^2 \varphi^m + \frac{2\Delta \varphi^{m-1}}{\delta \varphi E^+(\varphi^m)} \]

where \( E(\varphi) = \int_\Omega \left( \frac{\varphi^4}{4} + \frac{1-\epsilon}{2} \varphi^2 + \frac{1}{2} (\Delta \varphi)^2 - |\nabla \varphi|^2 \right) \, dx. \]
Convex Time Splitting Scheme

Basic Idea:

\[ \mu = \delta \varphi E(\varphi) = \delta \varphi \left( E^+(\varphi) + E^-(\varphi) \right) \]

\[ \Rightarrow \mu^m = (\varphi^m)^3 + (1 - \epsilon)\varphi^m + \Delta^2 \varphi^m + \frac{2\Delta \varphi^{m-1}}{\delta \varphi E^+(\varphi^m)} \]

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

Given \[ \varphi^0, \] find \( (\varphi^m, \mu^m) \) for \( 1 \leq m \leq M \) by

\[ \delta \tau \varphi^m - \nabla \cdot (M \nabla \mu^m) = 0, \]

\[ (\varphi^m)^3 + (1 - \epsilon)\varphi^m + \Delta^2 \varphi^m + 2\Delta \varphi^{m-1} - \mu^m = 0, \]

with boundary conditions

\[ \partial_n \varphi^m = \partial_n \Delta \varphi^m = \partial_n \mu^m = 0. \]
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

\[
\left( \delta_{T} \varphi_{h}^{m}, \nu_{h} \right) + \left( M \nabla \mu_{h}^{m}, \nabla \nu_{h} \right) = 0 \\
\left( \left( \varphi_{h}^{m} \right)^{3} + (1 - \epsilon) \varphi_{h}^{m}, \psi_{h} \right) + a_{h}^{IP} \left( \varphi_{h}^{m}, \psi_{h} \right) - 2 \left( \nabla \varphi_{h}^{m-1}, \nabla \psi_{h} \right) - \left( \mu_{h}^{m}, \psi_{h} \right) = 0,
\]

where \( \varphi_{h}^{0} := P_{h} \varphi_{0} \) and \( \mu_{h}^{0} \in V_{h} \) is defined as \( \mu_{h}^{0} := R_{h} \mu_{0} \).

**Remark**

The scheme satisfies the discrete conservation property

\[
\left( \varphi_{h}^{m}, 1 \right) = \left( \varphi_{h}^{0}, 1 \right) = \left( \varphi_{0}, 1 \right) \text{ for any } 1 \leq m \leq M.
\]
Unique Solvability:

$$f(\phi_m h) := 1 - \frac{1}{2} \| \phi_m h \|_4^4 + 1 - \frac{1}{2} \alpha \text{IP}(\phi_m h, \phi_m h)$$

Direct consequence of the convex decomposition of the energy.
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:
   \[ F(\phi_m h) := 1 - \|\phi_m h\|_4 L_4 - \|\nabla \phi_m h\|_2 L_2 + \frac{1}{2} a_{IP h}(\phi_m h, \phi_m h) \]
   Direct consequence of the convex decomposition of the energy.

3. Optimal error estimates:
   Main Result!
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:

   \[ F(\phi_m^h) := \frac{1}{4} \| \phi_m^h \|_{L^4}^4 + \frac{1}{2} \| \phi_m^h \|_{L^2}^2 - \| \nabla \phi_m^h \|_{L^2}^2 + \frac{1}{2} a_{IP}(\phi_m^h, \phi_m^h) \]

   Direct consequence of the convex decomposition of the energy.

3. Optimal error estimates:
   Main Result!
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:

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

Direct consequence of the convex decomposition of the energy.
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:

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

   Direct consequence of the convex decomposition of the energy.
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:

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

   Direct consequence of the convex decomposition of the energy.

3. Optimal error estimates:
Properties of Scheme

1. Unique Solvability:
   Relies on Convexity arguments.

2. Unconditional Stability:
   \[
   F(\varphi_h^m) := \frac{1}{4} \|\varphi_h^m\|_{L^4}^4 + \frac{1 - \epsilon}{2} \|\varphi_h^m\|_{L^2}^2 - \|\nabla \varphi_h^m\|_{L^2}^2 + \frac{1}{2} a_h^{IP}(\varphi_h^m, \varphi_h^m)
   \]
   Direct consequence of the convex decomposition of the energy.

3. Optimal error estimates: Main Result!
Unconditional Unique Solvability

Definition

Define the functional \( G_h : \tilde{Z}_h \rightarrow \mathbb{R} \)

\[
G_h(\varphi_h) := \frac{\tau}{2} \left\| \varphi_h - \frac{\varphi_h^{m-1}}{\tau} \right\|_{-1,h}^2 + \frac{1}{2} a_h^{IP} (\varphi_h, \varphi_h) + \frac{1}{4} \| \varphi_h + \overline{\varphi_0} \|^4_{L^4(\Omega)}
+ \frac{1 - \epsilon}{2} \| \varphi_h + \overline{\varphi_0} \|^2_{L^2(\Omega)} - 2 \left( \nabla \varphi_h^{m-1}, \nabla \varphi_h \right),
\]

where

\[
\| v_h \|_{-1,h} = (\nabla T_h v_h, \nabla T_h v_h)^{1/2} = (v_h, T_h v_h)^{1/2} = (T_h v_h, v_h)^{1/2},
\]

with \( T_h : \tilde{Z}_h \rightarrow \tilde{Z}_h \) defined as: given \( \zeta_h \in \tilde{Z}_h \), find \( T_h \zeta_h \in \tilde{Z}_h \):

\[
(\nabla T_h \zeta_h, \nabla \chi_h) = (\zeta_h, \chi_h) \quad \forall \chi_h \in \tilde{Z}_h.
\]
Unconditional Unique Solvability

Theorem

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

Proof.
Theorem

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

Proof.
Unconditional Unique Solvability

Theorem

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

Proof.

1. Shown through the zero mean formulation corresponding to our scheme
Unconditional Unique Solvability

Theorem

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

Proof.

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

2. Prove the one-to-one correspondence between solution of our scheme with the solution to the **zero mean formulation**
Theorem

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

Proof.

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

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 \((\varphi^m_h, \mu^m_h) \in Z_h \times V_h\) be a solution of the \(C_0\)-IP method. Then the following energy law holds for any \(h, \tau > 0\):

\[
F (\varphi^\ell_h) + \tau \sum_{m=1}^{\ell} \left\| \mathcal{M}^{1/2} \nabla \mu^m_h \right\|_{L^2(\Omega)}^2
+ \tau^2 \sum_{m=1}^{\ell} \left\{ \frac{(1 - \epsilon)}{2} \left\| \delta_\tau \varphi^m_h \right\|_{L^2(\Omega)}^2 + \left\| \nabla \delta_\tau \varphi^m_h \right\|_{L^2(\Omega)}^2
+ \frac{1}{4} \left\| \delta_\tau (\varphi^m_h)^2 \right\|_{L^2(\Omega)}^2 + \frac{1}{2} \left\| \varphi^m_h \delta_\tau \varphi^m_h \right\|_{L^2(\Omega)}^2 + \frac{1}{2} a^\text{IP}_h (\delta_\tau \varphi^m_h, \delta_\tau \varphi^m_h) \right\}
\]

\[= F (\varphi^0_h), \quad 1 \leq \ell \leq M.\]
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 
\(F(\varphi_h^0) \leq C\) independent of \(h\) and \(\epsilon < \frac{C_{\text{coer}}^{-4}}{C_{\text{coer}}} < 1\). For any \(h, \tau > 0\):

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

\[
\max_{0 \leq m \leq M} \|\varphi_h^m\|^2_{H^1} \leq C
\]

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

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

for some constant \(C\) that is independent of \(h, \tau,\) and \(T\).
Assume additional regularities:

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

C^0-IP Norm:

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

Notation:

\[ e^{\varphi,m} := \varphi^m - \varphi^m_h, \quad e^{\mu,m} := \mu^m - \mu^m_h. \]

Assumption: \( \mathcal{M} \equiv 1. \)
Error Analysis: Error Equation

Weak Form:

\[
\langle \partial_t \varphi^m, \nu \rangle + (\nabla \mu^m, \nabla \nu) = 0 \ \forall \ \nu \in H^1(\Omega)
\]

(1)

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

(2)

Fully Discrete C^0-IP Form:

\[
(\delta_T \varphi^m, \nu) + (\nabla \mu^m, \nabla \nu) = 0 \ \forall \ \nu \in V_h
\]

(3)

\[
\left( (\varphi_h^m)^3 + (1 - \epsilon)\varphi_h^m, \psi \right) - 2 (\nabla \varphi_h^{m-1}, \nabla \psi) + a^I_P (\varphi_h^m, \psi) - (\mu_h^m, \psi) = 0, \ \forall \ \psi \in Z_h
\]

(4)
**Weak Form:**

\[ \langle \partial_t \varphi^m, \nu \rangle + (\nabla \mu^m, \nabla \nu) = 0 \quad \forall \nu \in H^1(\Omega) \]  
\[ \left( (\varphi^m)^3 + (1 - \epsilon) \varphi^m, \psi \right) - 2 (\nabla \varphi^m, \nabla \psi) + a(\varphi^m, \psi) - (\mu^m, \psi) = 0 \quad \forall \psi \in Z. \]  

**Fully Discrete C^0-IP Form:**

\[ (\delta_t \varphi^m_h, \nu) + (\nabla \mu^m_h, \nabla \nu) = 0 \quad \forall \nu \in V_h \]  
\[ \left( (\varphi^m_h)^3 + (1 - \epsilon) \varphi^m_h, \psi \right) - 2 (\nabla \varphi^m_{h-1}, \nabla \psi) + a^P_h (\varphi^m_h, \psi) - (\mu^m_h, \psi) = 0, \quad \forall \psi \in Z_h \]  

- (1) and (3) \( \implies \) \( (\delta_t e^{\varphi^m}, \nu_h) + (\nabla e^{\mu^m}, \nabla \nu_h) = (\delta_t \varphi^m - \partial_t \varphi^m, \nu_h), \) \( \nu_h \in V_h \subset H^1(\Omega). \)
Error Analysis: Error Equation

Weak Form:

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

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

Fully Discrete $C^0$-IP Form:

\[
(\delta_T \varphi_h^m, \nu) + (\nabla \mu_h^m, \nabla \nu) = 0 \ \forall \nu \in V_h \tag{3}
\]

\[
\left((\varphi_h^m)^3 + (1 - \epsilon)\varphi_h^m, \psi\right) - 2 (\nabla \varphi_h^{m-1}, \nabla \psi) + a^IP_h (\varphi_h^m, \psi) - (\mu_h^m, \psi) = 0, \ \forall \psi \in Z_h \tag{4}
\]

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

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

Weak Form:

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

Fully Discrete $C^0$-IP Form:

\[
\left( (\varphi^m_h)^3 + (1 - \epsilon)\varphi^m_h, \psi \right) - 2 (\nabla \varphi^{m-1}_h, \nabla \psi) + a^IP_h (\varphi^m_h, \psi) - (\mu^m_h, \psi) = 0, \quad \forall \psi \in Z_h
\]
Error Analysis: Error Equation

Weak Form:

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

Fully Discrete \( C^0 \)-IP Form:

\[
\left( (\varphi_h^m)^3 + (1 - \epsilon)\varphi_h^m, \psi \right) - 2 (\nabla \varphi_h^{m-1}, \nabla \psi) + a^h (\varphi_h^m, \psi) - (\mu_h^m, \psi) = 0, \quad \forall \psi \in Z_h
\]

\[
\left( (\varphi^m)^3 - (\varphi_h^m)^3 + (1 - \epsilon)e^{\varphi,m}, \psi \right) - 2 (\nabla e^{\varphi,m}, \nabla \psi) + a(\varphi^m, \psi) - a^h (\varphi_h^m, \psi) - (e^{\mu,m}, \psi) = 0
\]
Error Analysis: Error Equation

Weak Form:

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

Fully Discrete C\textsuperscript{0}-IP Form:

\[
\left((\varphi^m_h)^3 + (1 - \epsilon)\varphi^m_h, \psi\right) - 2 (\nabla \varphi^{-1}_h, \nabla \psi) + a^\text{IP}_h (\varphi^m_h, \psi) - (\mu^m_h, \psi) = 0, \quad \forall \psi \in Z_h
\]

\[
\left((\varphi^m)^3 - (\varphi^m_h)^3 + (1 - \epsilon)e^{\varphi^m}, \psi\right) - 2 (\nabla e^{\varphi^m}, \nabla \psi) + a(\varphi^m, \psi) - a^\text{IP}_h (\varphi^m_h, \psi)
- (e^{\mu^m}, \psi) = 0
\]

Problem: $\psi \in Z$ is not in $H^{2+1/2}$ locally! $\psi \in Z_h$ is not in $H^2$ globally!
Error Analysis: Error Equation

Weak Form:

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

Fully Discrete C\(^0\)-IP Form:

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

\[
\left( (\varphi^m)^3 - (\varphi_h^m)^3 + (1 - \epsilon)e^{\varphi,m}, \psi \right) - 2 (\nabla e^{\varphi,m}, \nabla \psi) + a(\varphi^m, \psi) - a_h^{IP} (\varphi_h^m, \psi) - (e^{\mu,m}, \psi) = 0
\]

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

Define the enriching operator $E_h: Z_h \rightarrow W_h \cap Z$ [Brenner, Gudi, Sung '12].

Weak Form with correction term: find $(\varphi_m, \mu_m) \in Z \times H^1(\Omega)$:

$$\left( \frac{\partial t \varphi_m, \nu_h}{} + \left( \nabla \mu_m, \nabla \nu_h \right) = 0 \right) \forall \nu_h \in V_h,$$

$$a_{IP}(\varphi_m, \psi_h) + \left( (\varphi_m)^3 + (1 - \epsilon) \varphi_m, \psi_h \right) - 2 \left( \nabla \varphi_m, \nabla \psi_h \right) - (\mu_m, \psi_h) = L(\varphi_m, \mu_m; \psi_h - E_h \psi_h) \forall \psi_h \in Z_h$$

where $L(\varphi_m, \mu_m; \psi_h - E_h \psi_h) := a_{IP}(\varphi_m, \psi_h - E_h \psi_h) - (\mu_m, \psi_h - E_h \psi_h) + \left( (\varphi_m)^3 + (1 - \epsilon) \varphi_m, \psi_h - E_h \psi_h \right) - 2 \left( \nabla \varphi_m, \nabla \psi_h - \nabla E_h \psi_h \right)$. Solutions to weak form are consistent since $a_{IP}(\varphi, E_h \psi_h) = a(\varphi, E_h \psi_h)$ for all $\psi \in Z_h$. 

Natasha S. Sharma (UTEP) 07/18/23
Error Analysis

- Remedy: Introduce $W_h \subset Z$ to be the Hsieh-Clough-Tocher micro finite element space associated with $\mathcal{T}_h$.
- Define the enriching operator $E_h : Z_h \rightarrow W_h \cap Z$ [Brenner, Gudi, Sung ’12]
Remedy: Introduce $W_h \subset Z$ to be the Hsieh-Clough-Tocher micro finite element space associated with $\mathcal{T}_h$.

Define the enriching operator $E_h : Z_h \rightarrow W_h \cap Z$ [Brenner, Gudi, Sung '12]

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

\[
(\partial_t \varphi^m, \nu_h) + (\nabla \mu^m, \nabla \nu_h) = 0 \quad \forall \nu_h \in V_h,
\]

\[
a_h^{IP} (\varphi^m, \psi_h) + \left( (\varphi^m)^3 + (1 - \epsilon)\varphi^m, \psi_h \right) - 2 (\nabla \varphi^m, \nabla \psi_h) - (\mu^m, \psi_h)
\]

\[
= L(\varphi^m, \mu^m; \psi_h - E_h \psi_h) \quad \forall \psi_h \in Z_h
\]

where

\[
L(\varphi^m, \mu^m; \psi_h - E_h \psi_h) := a_h^{IP} (\varphi^m, \psi_h - E_h \psi_h) - (\mu^m, \psi_h - E_h \psi_h)
\]

\[
+ \left( (\varphi^m)^3 + (1 - \epsilon)\varphi^m, \psi_h - E_h \psi_h \right) - 2 (\nabla \varphi^m, \nabla \psi_h - \nabla E_h \psi_h).
\]
Remedy: Introduce $W_h \subset Z$ to be the Hsieh-Clough-Tocher micro finite element space associated with $\mathcal{T}_h$.

Define the enriching operator $E_h : Z_h \rightarrow W_h \cap Z$ [Brenner, Gudi, Sung '12]

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

\[
(\partial_t \varphi^m, \nu_h) + (\nabla \mu^m, \nabla \nu_h) = 0 \quad \forall \nu_h \in V_h,
\]
\[
a_h^{LP} (\varphi^m, \psi_h) + \left( (\varphi^m)^3 + (1 - \epsilon)\varphi^m, \psi_h \right) - 2 (\nabla \varphi^m, \nabla \psi_h) - (\mu^m, \psi_h) = 0
\]

\[
= \mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h \psi_h) \quad \forall \psi_h \in Z_h
\]

where

\[
\mathcal{L}(\varphi^m, \mu^m; \psi_h - E_h \psi_h) := a_h^{LP} (\varphi^m, \psi_h - E_h \psi_h) - (\mu^m, \psi_h - E_h \psi_h)
\]
\[
+ \left( (\varphi^m)^3 + (1 - \epsilon)\varphi^m, \psi_h - E_h \psi_h \right) - 2 (\nabla \varphi^m, \nabla \psi_h - \nabla E_h \psi_h).
\]

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

Natasha S. Sharma (UTEP)  
C0-IP for Sixth-Order CH Eqns  
07/18/23
Subtracting fully discrete form from the weak form with the correction term gives:

\begin{align*}
(\delta_\tau e^{\varphi,m}, \nu_h) + (\nabla e^{\mu,m}, \nabla \nu_h) &= (\delta_\tau \varphi^m - \partial_t \varphi^m, \nu_h), \quad (5) \\
a_h^{IP} (e^{\varphi,m}, \psi_h) + ((1 - \epsilon) e^{\varphi,m}, \psi_h) - 2 (\nabla e^{\varphi,m-1}, \nabla \psi_h) - (e^{\mu,m}, \psi_h) &= \\
- \left((\varphi^m)^3 - (\varphi_h^m)^3, \psi_h\right) - 2 (\nabla \varphi^{m-1} - \nabla \varphi^m, \nabla \psi_h) + \mathcal{L}(\varphi^m, \mu^m_h; \psi_h - E_h \psi_h). \quad (6)
\end{align*}

\textbf{Notation:}

\begin{align*}
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^m_h, \\
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^m_h.
\end{align*}
Subtracting fully discrete form from the weak form with the correction term gives:

\[(\delta_t e^{\varphi,m}, \nu_h) + (\nabla e^{\mu,m}, \nabla \nu_h) = (\delta_t \varphi^m - \partial_t \varphi^m, \nu_h),\]

(5)

\[a_{IP}^h (e^{\varphi,m}, \psi_h) + ((1 - \epsilon) e^{\varphi,m}, \psi_h) - 2 (\nabla e^{\varphi,m-1}, \nabla \psi_h) - (e^{\mu,m}, \psi_h) = - \left((\varphi^m)^3 - (\varphi_h^m)^3, \psi_h\right) - 2 (\nabla \varphi^{m-1} - \nabla \varphi^m, \nabla \psi_h) + \mathcal{L}(\varphi^m, \mu_h^m; \psi_h - E_h \psi_h).\]

(6)

Notation:

\[e^{\varphi,m} = e_P^{\varphi,m} + e_h^{\varphi,m}, \quad e_P^{\varphi,m} := \varphi^m - P_h \varphi^m, \quad e_h^{\varphi,m} := P_h \varphi^m - \varphi_h^m,\]

\[e^{\mu,m} = e_R^{\mu,m} + e_h^{\mu,m}, \quad e_R^{\mu,m} := \mu^m - R_h \mu^m, \quad e_h^{\mu,m} := R_h \mu^m - \mu_h^m.\]

Set \(\nu_h = e_h^{\mu,m}\) in (5) and \(\psi_h = \delta_t e_h^{\varphi,m}\) in (6).
\[ \| \nabla e_{h}^{\mu,m} \|_{L^2}^2 + a_{h}^{IP} \left( e_{h}^{\phi,m}, \delta_{\tau} e_{h}^{\phi,m} \right) + \left( (1 - \epsilon) e_{h}^{\phi,m}, \delta_{\tau} e_{h}^{\phi,m} \right) - 2 \left( \nabla e_{h}^{\phi,m-1}, \nabla \delta_{\tau} e_{h}^{\phi,m} \right) \\
= \left( \delta_{\tau} \phi^{m} - \partial_{t} \phi^{m}, e_{h}^{\phi,m} \right) - \left( \delta_{\tau} e_{P}^{\phi,m}, e_{h}^{\mu,m} \right) + \left( e_{R}^{\mu,m}, \delta_{\tau} e_{h}^{\phi,m} \right) \\
+ 2 \left( \nabla \phi^{m} - \nabla \phi^{m-1}, \nabla \delta_{\tau} e_{h}^{\phi,m} \right) - \left( (\phi^{m})^{3} - (\phi_{h}^{m})^{3}, \delta_{\tau} e_{h}^{\phi,m} \right) \\
+ 2 \left( \nabla e_{P}^{\phi,m-1}, \nabla \delta_{\tau} e_{h}^{\phi,m} \right) + \mathcal{L}(\phi^{m}, \mu_{h}^{m}; \psi_{h} - E_{h}\psi_{h}) \]
Let \((\varphi^m, \mu^m)\) be a weak solution with the additional regularities. Then for any \(h, \tau > 0\) and any \(0 \leq m \leq M\), we have

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

where the constant \(C\) may depend upon a Poincaré constant but does not depend on \(h\) or \(\tau\).

where \(\|v_h\|_{-1,h} = (\nabla T_h v_h, \nabla T_h v_h)^{1/2} = (v_h, T_h v_h)^{1/2} = (T_h v_h, v_h)^{1/2}\) and \(T_h\) is the discrete inverse Laplacian.
\[
\| \nabla e^{\mu,m}_h \|_{L^2}^2 + a_h^{IP} (e^{\varphi,m}_h, \delta_{\tau} e^{\varphi,m}_h) + ((1 - \epsilon)e^{\varphi,m}_h, \delta_{\tau} e^{\varphi,m}_h) - 2 \left( \nabla e^{\varphi,m-1}_h, \nabla \delta_{\tau} e^{\varphi,m}_h \right) \\
= (\delta_{\tau} \varphi^m - \partial_t \varphi^m, e^{\mu,m}_h) - (\delta_{\tau} e^{\varphi,m}_P, e^{\mu,m}_h) + (e^{\mu,m}_R, \delta_{\tau} e^{\varphi,m}_h) \\
+ 2 \left( \nabla \varphi^m - \nabla \varphi^{m-1}, \nabla \delta_{\tau} e^{\varphi,m}_h \right) - \left( (\varphi^m)^3 - (\varphi^m_h)^3, \delta_{\tau} e^{\varphi,m}_h \right) \\
+ 2 \left( \nabla e^{\varphi,m-1}_P, \nabla \delta_{\tau} e^{\varphi,m}_h \right) + \mathcal{L}(\varphi^m, \mu^m_h; \psi_h - E_h \psi_h)
\]

Polarization Property:

\[
a_h^{IP} (e^{\varphi,m}_h, \delta_{\tau} e^{\varphi,m}_h) = \frac{1}{2} \delta_{\tau} \ a_h^{IP} (e^{\varphi,m}_h, e^{\varphi,m}_h) + \frac{\tau}{2} a_h^{IP} (\delta_{\tau} e^{\varphi,m}_h, \delta_{\tau} e^{\varphi,m}_h) \\
((1 - \epsilon)e^{\varphi,m}_h, \delta_{\tau} e^{\varphi,m}_h) = \frac{(1 - \epsilon)}{2} \delta_{\tau} \| e^{\varphi,m}_h \|_{L^2}^2 + \frac{(1 - \epsilon)}{2} \| \delta_{\tau} e^{\varphi,m}_h \|_{L^2}^2 \\
- 2 \left( \nabla e^{\varphi,m-1}_h, \nabla \delta_{\tau} e^{\varphi,m}_h \right) = \tau \| \nabla \delta_{\tau} e^{\varphi,m}_h \|_{L^2}^2 - \delta_{\tau} \left( \nabla e^{\varphi,m}_h, \nabla e^{\varphi,m}_h \right)
\]
Error Analysis: First 3 RHS terms

\[
\begin{align*}
(\delta_\tau \varphi^m - \partial_t \varphi^m, e^{\mu,m}_h) & \leq C_T \int_{t_{m-1}}^{t_m} \|\partial_{ss} \varphi(s)\|_{L^2}^2 \, ds + \frac{1}{12} \|\nabla e^{\mu,m}_h\|_{L^2}^2, \\
(\delta_\tau e^{\varphi,m}_P, e^{\mu,m}_h) & \leq C \|\delta_\tau e^{\varphi,m}_P\|_{L^2}^2 + \frac{1}{12} \|\nabla e^{\mu,m}_h\|_{L^2}^2, \\
& \leq \frac{C}{\tau} \int_{t_{m-1}}^{t_m} \|P_h \partial_s \varphi(s) - \partial_s \varphi(s)\|_{L^2}^2 \, ds + \frac{1}{12} \|\nabla e^{\mu,m}_h\|_{L^2}^2, \\
(\delta_\tau e^{\varphi,m}_h, e^{\mu,m}_h) & \leq C \|\nabla e^{\mu,m}_R\|_{L^2}^2 + \frac{1}{36} \|\delta_\tau e^{\varphi,m}_h\|_{-1,h}^2.
\end{align*}
\]
Error Analysis: next two RHS terms

\[ 2 \left( \nabla \varphi^m - \nabla \varphi^{m-1}, \nabla \delta T e^{\varphi,m}_h \right) = -2 \left( \tau \Delta \delta T \varphi^m, \delta T e^{\varphi,m}_h \right) \]
\[ \leq 2 \left\| \tau \nabla \Delta \delta T \varphi^m \right\|_{L^2} \left\| \delta T e^{\varphi,m}_h \right\|_{-1,h} \]
\[ \leq C_T \int_{t_{m-1}}^{t_m} \left\| \partial_s \varphi(s) \right\|_{H^3}^2 \, ds + \frac{1}{36} \left\| \delta T e^{\varphi,m}_h \right\|_{-1,h}^2. \]

\[ \left( (\varphi^m)^3 - (\varphi^m_h)^3, \delta T e^{\varphi,m}_h \right) \leq \left\| \nabla \left( (\varphi^m)^3 - (\varphi^m_h)^3 \right) \right\|_{L^2} \left\| \delta T e^{\varphi,m}_h \right\|_{-1,h} \]
\[ = \left\| 3 (\varphi^m)^2 \nabla \varphi^m - 3 (\varphi^m_h)^2 \nabla \varphi^m \right\|_{L^2} \]
\[ \times \left\| \delta T e^{\varphi,m}_h \right\|_{-1,h} \]
\[ = 3 \left\| (\varphi^m + \varphi^m_h) \nabla \varphi^m e^{\varphi,m} + (\varphi^m_h)^2 \nabla e^{\varphi,m} \right\|_{L^2} \]
\[ \times \left\| \delta T e^{\varphi,m}_h \right\|_{-1,h} \]
Error Analysis: next two RHS terms

\[
\left( (\varphi^m)^3 - (\varphi_h^m)^3, \delta_T e_{h}^{\varphi,m} \right) \\
\leq 3 \left( \| \varphi^m + \varphi_h^m \|_{L^6} \| \nabla \varphi^m \|_{L^6} \| e_{h}^{\varphi,m} \|_{L^6} + \| \varphi_h^m \|_{L^6}^2 \| \nabla e_{h}^{\varphi,m} \|_{L^6} \right) \\
\times \| \delta_T e_{h}^{\varphi,m} \|_{-1,h} \\
\leq C \left( \| \nabla e_P^{\varphi,m} \|_{L^2} + \| \nabla e_{h}^{\varphi,m} \|_{L^2} + \| e_P^{\varphi,m} \|_{2,h} + \| e_{h}^{\varphi,m} \|_{2,h} \right) \\
\times \| \delta_T e_{h}^{\varphi,m} \|_{-1,h} \\
\leq C \left( \| \nabla e_P^{\varphi,m} \|_{L^2} + \| \nabla e_{h}^{\varphi,m} \|_{L^2} + \| e_P^{\varphi,m} \|_{2,h} + \| e_{h}^{\varphi,m} \|_{2,h} \right) \\
\times \| \delta_T e_{h}^{\varphi,m} \|_{-1,h} \\
\leq C \| e_P^{\varphi,m} \|_{2,h}^2 + C \| e_{h}^{\varphi,m} \|_{2,h}^2 + \frac{1}{36} \| \delta_T e_{h}^{\varphi,m} \|_{-1,h}^2. 
\]
Using discrete product rule:

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

we have the following bound

\[
2 \left( \nabla e^{\varphi,m-1}, \nabla \delta_{\tau} e^{\varphi,m} \right) = 2\delta_{\tau} (\nabla e^{\varphi,m}, \nabla e^{\varphi,m}) - 2 (\nabla \delta_{\tau} e^{\varphi,m}, \nabla e^{\varphi,m}) \\
\leq 2\delta_{\tau} (\nabla e^{\varphi,m}, \nabla e^{\varphi,m}) + C \| \delta_{\tau} e^{\varphi,m} \|_{L^2}^2 + C \| e^{\varphi,m} \|_{2,h}^2 \\
\leq 2\delta_{\tau} (\nabla e^{\varphi,m}, \nabla e^{\varphi,m}) + \frac{C}{\tau} \int_{t_{m-1}}^{t_m} \| \partial_s \varphi(s) - P_h \partial_s \varphi(s) \|_{2,h}^2 ds \\
+ C \| e^{\varphi,m} \|_{2,h}^2.
\]
Lemma

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

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

and

\[
a_h^{IP} \left( \delta_\tau \varphi^m, e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1} \right) + \left( \delta_\tau \left( (\varphi^m)^3 + (1 - \epsilon) \varphi^m \right), e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1} \right) \\
- 2 \left( \delta_\tau \nabla \varphi^m, \nabla (e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1}) \right) - \left( \delta_\tau \mu^m, e_h^{\varphi,m-1} - E_h e_h^{\varphi,m-1} \right) \\
\leq C \left[ \text{Osc}_j (\mu_t(t^*)) \right]^2 + C \left\| e_P^{\varphi,m} \right\|_{2,h}^2
\]
\[
\left\| \nabla e_{h}^{\mu,m} \right\|_{L^{2}}^{2} + \frac{1}{2} \delta \tau \ a_{h}^{IP} \left( e_{h}^{\varphi,m}, e_{h}^{\varphi,m} \right) + \frac{\tau}{2} a_{h}^{IP} \left( \delta \tau e_{h}^{\varphi,m}, \delta \tau e_{h}^{\varphi,m} \right) \\
+ \frac{(1 - \epsilon)}{2} \delta \tau \left\| e_{h}^{\varphi,m} \right\|_{L^{2}}^{2} + \frac{(1 - \epsilon) \tau}{2} \left\| \delta \tau e_{h}^{\varphi,m} \right\|_{L^{2}}^{2} + \tau \left\| \nabla \delta \tau e_{h}^{\varphi,m} \right\|_{L^{2}}^{2} \\
\leq \delta \tau \left( \nabla e_{h}^{\varphi,m}, \nabla e_{h}^{\varphi,m} \right) + 2 \delta \tau \left( \nabla e_{P}^{\varphi,m}, \nabla e_{h}^{\varphi,m} \right) + \frac{6}{12} \left\| \nabla e_{h}^{\mu,m} \right\|_{L^{2}}^{2} + C \left\| e_{h}^{\varphi,m} \right\|_{2,h}^{2} \\
+ C \left\| e_{h}^{\varphi,m-1} \right\|_{2,h}^{2} + C \left\| \nabla e_{R}^{\mu,m} \right\|_{L^{2}}^{2} + C \left\| e_{P}^{\varphi,m} \right\|_{2,h}^{2} + C \left[ \text{Osc}_{j}(\mu(t^{*})) \right]^{2} \\
+ C \tau \int_{t_{m-1}}^{t_{m}} \left[ \left\| \partial_{s} \varphi(s) \right\|_{H^{3}}^{2} + \left\| \partial_{ss} \varphi(s) \right\|_{L^{2}}^{2} \right] ds + \frac{C}{\tau} \int_{t_{m-1}}^{t_{m}} \left\| \partial_{s} \varphi(s) - P_{h} \partial_{s} \varphi(s) \right\|_{2,h}^{2} ds \\
+ \delta \tau a_{h}^{IP} \left( \varphi^{m}, e_{h}^{\varphi,m} - E_{h} e_{h}^{\varphi,m} \right) + \delta \tau \left( \left( \varphi^{m} \right)^{3} + (1 - \epsilon) \varphi^{m}, e_{h}^{\varphi,m} - E_{h} e_{h}^{\varphi,m} \right) \\
- 2 \delta \tau \left( \nabla \varphi^{m}, \nabla \left( e_{h}^{\varphi,m} - E_{h} e_{h}^{\varphi,m} \right) \right) - \delta \tau \left( \mu^{m}, e_{h}^{\varphi,m} - E_{h} e_{h}^{\varphi,m} \right). 
\]
Applying $2\tau \sum_{m=1}^{\ell}$, using the fact that $e_{h,0} = 0$ we obtain

$$a_{h}^{IP} \left( e_{h,\ell}, e_{h,\ell} \right) + (1 - \epsilon) \left\| e_{h,\ell} \right\|_{L^2}^2 + \tau \sum_{m=1}^{\ell} \left\| \nabla e_{h,\mu,m} \right\|_{L^2}^2$$

$$+ \tau^2 \sum_{m=1}^{\ell} \left[ a_{h}^{IP} \left( \delta_{\ell} e_{h,\mu,m}, \delta_{\ell} e_{h,\mu,m} \right) + (1 - \epsilon) \left\| \delta_{\ell} e_{h,\mu,m} \right\|_{L^2}^2 + 2 \left\| \nabla \delta_{\ell} e_{h,\mu,m} \right\|_{L^2}^2 \right]$$

$$\leq \frac{C_{coer}}{2\beta} \left\| e_{h,\ell} \right\|_{2,h}^2 + \frac{8\beta}{C_{coer}} \left\| e_{h,\ell} \right\|_{L^2}^2 + C \left\| e_{P,\ell} \right\|_{2,h}^2 + C_{\tau} \sum_{m=1}^{\ell} \left\| e_{h,\mu,m} \right\|_{2,h}^2$$

$$+ C_{\tau} \sum_{m=1}^{\ell} \left[ \left\| \nabla e_{\mu,R,m} \right\|_{L^2}^2 + \left\| e_{P,\mu,m} \right\|_{2,h}^2 + \left[ \text{Osc}_j(\mu_{t}(t^{*})) \right]^2 \right]$$

$$+ C_{\tau}^2 \int_{t_0}^{t_{\ell}} \left[ \left\| \partial_s \varphi(s) \right\|_{H^3}^2 + \left\| \partial_{ss} \varphi(s) \right\|_{L^2}^2 \right] ds + C \int_{t_0}^{t_{\ell}} \left\| \partial_s \varphi(s) - P_h \partial_s \varphi(s) \right\|_{2,h}^2 ds$$

$$+ 2 \left[ C \left[ \text{Osc}_j(\mu_{t}) \right]^2 + C \left\| e_{P,\ell} \right\|_{2,h}^2 + \frac{C_{coer}}{4\beta} \left\| e_{h,\ell} \right\|_{2,h}^2 \right].$$
Theorem

Suppose \((\varphi^m, \mu^m)\) 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 \(0 \leq \tau \leq M\),

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

where \(C^*\) may depend on the oscillations of \(\mu\) 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 \(\tau\).
Our Numerical Scheme

Given $\phi_{m-1}^h \in \mathbb{Z}_h$, solve for $(\phi_m^h, \mu_m^h) \in \mathbb{Z}_h \times V_h$:

$$\big( \delta \tau \phi_m^h, \nu^h \big) + \big( M \nabla \mu_m^h, \nabla \nu^h \big) = 0$$

$$\big( \phi_m^h, \psi^h \big) + a_{IP}^h \big( \phi_m^h, \psi^h \big) - 2 \big( \nabla \phi_m^h_{-1}^h, \nabla \psi^h \big) - \big( \mu_m^h, \psi^h \big) = 0,$$

where $\phi_0^h := P_h \phi_0$ and $\mu_0^h \in V_h$ is defined as $\mu_0^h := \mathcal{R}_h \mu_0$.

Model parameters: $\epsilon = 0.025$ and $M = 1$, penalty parameter: $\alpha = 20$.

We use Newton iteration method to solve the discrete nonlinear system with tolerance of the Newton iteration 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.
Our Numerical Scheme

- Project \( \varphi^0_h := \Pi_h \varphi_0 \)
Our Numerical Scheme

- 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

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

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

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: $\epsilon = 0.025$ 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.
Our Numerical Scheme

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

$$(\delta_\tau \varphi^m_h, \nu_h) + (\mathcal{M} \nabla \mu^m_h, \nabla \nu_h) = 0$$

$$\left((\varphi^m_h)^3 + (1 - \epsilon)\varphi^m_h, \psi_h\right) + a^IP_h(\varphi^m_h, \psi_h) - 2(\nabla \varphi^{m-1}_h, \nabla \psi_h) - (\mu^m_h, \psi_h) = 0,$$

where $\varphi^0_h := P_h \varphi_0$ and $\mu^0_h \in V_h$ is defined as $\mu^0_h := R_h \mu_0$.

- model parameters: $\epsilon = 0.025$ 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

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

Mesh \( h = \frac{32}{512} \) with \( \tau \) with \( \tau = 0.05h \) and \( T = 10 \) as the ‘exact’ solution, \( \varphi_{\text{exact}} \).

\[ \text{error}_{\varphi} := \varphi_h - \varphi_{\text{exact}} \]

where \( \varphi_h \) indicates the solution on the mesh size \( h \).

<table>
<thead>
<tr>
<th>( h )</th>
<th>( | \text{error}<em>{\varphi} |</em>{2,h} )</th>
<th>( \text{rate} )</th>
<th>( | \text{error}<em>{\mu} |</em>{H^1} )</th>
<th>( \text{rate} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{32}{8} )</td>
<td>0.08412</td>
<td>N/A</td>
<td>0.00522</td>
<td>N/A</td>
</tr>
<tr>
<td>( \frac{32}{16} )</td>
<td>0.05896</td>
<td>0.71329</td>
<td>0.00242</td>
<td>1.07627</td>
</tr>
<tr>
<td>( \frac{32}{32} )</td>
<td>0.03466</td>
<td>0.85058</td>
<td>0.00157</td>
<td>0.76970</td>
</tr>
<tr>
<td>( \frac{32}{64} )</td>
<td>0.01568</td>
<td>1.10514</td>
<td>0.00103</td>
<td>0.76082</td>
</tr>
<tr>
<td>( \frac{32}{128} )</td>
<td>0.00601</td>
<td>1.30482</td>
<td>0.00041</td>
<td>1.25840</td>
</tr>
<tr>
<td>( \frac{32}{256} )</td>
<td>0.00255</td>
<td>1.17707</td>
<td>0.00016</td>
<td>1.27362</td>
</tr>
</tbody>
</table>
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 spatial 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 \( \bar{\varphi} = 0.285, \ C = 0.466, \ q = 0.66, \ \Omega = (0, 201) \times (0, 201), \ h = \frac{201}{402}. \)
Motion of liquid-crystal interfaces and grain boundaries

![Graphical representation of liquid-crystal interfaces at different times](image)

Natasha S. Sharma (UTEP)
Phase Field Model for Microemulsions: Motivation

No surfactants

[Diagram showing the mixing of oil and water, followed by no separation after 1 second.]
Phase Field Model for Microemulsions: Motivation

No surfactants

[Schematic showing the process of mixing oil and water without surfactants, creating small oil droplets that eventually form larger droplets.]

Surfactants

[Schematic showing the process of mixing oil and water with surfactants, creating small, stable droplets that remain dispersed for a long time.]

[Picture Courtesy: Biolin Scientific]
Motivation: Microemulsion systems as skin drug delivery systems

[Source: Walgreens]

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]

Natasha S. Sharma (UTEP)
C0-IP for Sixth-Order CH Eqns
07/18/23
**Motivation:** Microemulsion systems as skin drug delivery systems

**Issue:** Topical cream formulations contain petrochemical ingredients (such as petrolatum, silicones).

[Source: Walgreens]
Motivation: Microemulsion systems as skin drug delivery systems

- **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.

[Source: Walgreens]
Motivation: Microemulsion systems as skin drug delivery systems

- **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]
\( \Omega \subset \mathbb{R}^2 \) be a bounded polygonal domain occupied by the ternary mixture.
\( \Omega \subset \mathbb{R}^2 \) be a bounded polygonal domain occupied by the ternary mixture.

\( \varphi \) : the scalar order parameter indicating the local difference between oil and water concentrations.
Mathematical Model for Microemulsions

- \( \Omega \subset \mathbb{R}^2 \) be a bounded polygonal domain occupied by the ternary mixture.
- \( \varphi \): 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)
Ω ⊂ \( \mathbb{R}^2 \) be a bounded polygonal domain occupied by the ternary mixture.

\( \varphi \) : 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)

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

- tendency to mix
- tendency to separate

[Gompper et. al. 90]
Mathematical Model for Microemulsions

Conservation Law:

$$\partial_t \varphi + \nabla \cdot j = 0$$

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

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

Conservation Law:

$$\partial_t \varphi + \nabla \cdot j = 0$$

- $\varphi$: the scalar order parameter
- $j = -M \nabla \mu$: mass flux
- $M$: mobility coefficient, $\mu = \delta \varphi E$: chemical potential

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

$$\mu = 3\beta (\varphi^5 - \varphi^3) + \varphi |\nabla \varphi|^2 - \nabla \cdot (\varphi^2 \nabla \varphi) + a_0 \Delta \varphi + \lambda \Delta^2 \varphi.$$
Mathematical Model for Microemulsions

Conservation Law:

\[ \partial_t \varphi + \nabla \cdot j = 0 \]

- \( \varphi \): the scalar order parameter
- \( j = -M \nabla \mu \): mass flux
- \( M \): mobility coefficient, \( \mu = \delta \varphi E \): chemical potential

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

\[
\mu = 3\beta (\varphi^5 - \varphi^3) + \varphi |\nabla \varphi|^2 - \nabla \cdot (\varphi^2 \nabla \varphi) + a_0 \Delta \varphi + \lambda \Delta^2 \varphi.
\]
Mathematical Model for Microemulsions

Conservation Law:

$$\partial_t \varphi + \nabla \cdot j = 0$$

- \(\varphi\) : the scalar order parameter
- \(j = -M \nabla \mu\): mass flux
- \(M\): mobility coefficient, \(\mu = \delta \varphi E\): chemical potential

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

$$\mu = 3\beta (\varphi^5 - \varphi^3) + \varphi |\nabla \varphi|^2 - \nabla \cdot (\varphi^2 \nabla \varphi) + a_0 \Delta \varphi + \lambda \Delta^2 \varphi.$$
Compliment

\[
\frac{\partial \varphi}{\partial t} - \nabla \cdot (M \nabla \mu) = 0, \quad \text{in } \Omega^T := \Omega \times (0, T),
\]

\[
3\beta (\varphi^5 - \varphi^3) + \varphi |\nabla \varphi|^2 - \nabla \cdot ((\varphi^2 - a_0) \nabla \varphi) + \lambda \Delta^2 \varphi - \mu = 0, \quad \text{in } \Omega^T
\]

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]
Hoppe/Linsemmann 2019: Fully implicit backward Euler and C^0-IP Method quasi-optimal error estimates without any discrete energy law
Numerical Schemes: Existing Literature

- **Hoppe/Linsemmann 2019**: Fully implicit backward Euler and C⁰-IP Method quasi-optimal error estimates without any discrete energy law.

- **Diegel/Sharma 2022**: Closely related literature is the C⁰-IP framework developed for the Phase Field Crystal Equation based on Eyre’s convex splitting scheme.
Given $\varphi_h^{m-1} \in \mathbb{Z}_h$, find $(\varphi_h^m, \mu_h^m) \in \mathbb{Z}_h \times V_h$ which satisfies

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

$$3\beta ((\varphi_h^m)^5 - (\varphi_h^{m-1})^3, \psi_h) + ((\varphi_h^m)^2 \nabla \varphi_h^m, \nabla \psi_h) + (\varphi_h^m |\nabla \varphi_h^{m-1}|^2, \psi_h)$$

$$-a_0 (\nabla \varphi_h^{m-1}, \nabla \psi_h) + \lambda a_h^{IP} (\varphi_h^m, \psi_h) - (\mu_h^m, \psi_h) = 0 \quad \forall \quad \psi_h \in \mathbb{Z}_h$$

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

**Theorem**

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

Unconditional Energy Stability

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

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 \(h, \tau > 0\):

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

for all \(1 \leq \ell \leq M\).
Uniform *A Priori* Estimates

**Theorem**

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

\[
\begin{align*}
\max_{0 \leq m \leq M} \left\| \varphi^m_h \right\|_{2,h}^2 &\leq C \\
\max_{0 \leq m \leq M} \left[ \left\| \varphi^m_h \right\|_{L^2}^2 + \left\| \nabla \varphi^m_h \right\|_{L^2}^2 + \left\| \varphi^m_h \nabla \varphi^m_h \right\|_{L^2}^2 + \left\| \varphi^m_h \right\|_{L^\infty}^2 \right] &\leq C^* \\
\tau \sum_{m=1}^\ell \left\| \sqrt{\mathcal{M}} \nabla \mu^m_h \right\|_{L^2}^2 &\leq C
\end{align*}
\]

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

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

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

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 $\tau$.

The solution to the fully discrete scheme is unique for all $h, \tau > 0$. 
Our Numerical Scheme

- Project $\varphi_h^0 := P_h\varphi_0$
Our Numerical Scheme

- Project $\varphi_h^0 := P_h \varphi_0$
Our Numerical Scheme

- Project $\phi_h^0 := P_h \phi_0$
- Given $\phi_h^{m-1} \in Z_h$, solve for $(\phi_h^m, \mu_h^m) \in Z_h \times V_h$:

\[
(\delta_T \phi_h^m, \nu_h) + (M \nabla \mu_h^m, \nabla \nu_h) = 0, \quad \forall \quad \nu_h \in V_h
\]

\[
3 \beta \left( (\phi_h^m)^5 - (\phi_h^{m-1})^3, \psi_h \right) + \left( (\phi_h^m)^2 \nabla \phi_h^m, \nabla \psi_h \right) + \left( \phi_h^m \nabla \phi_h^{m-1}, 2 \right) \psi_h
\]

\[
- a_0 \left( \nabla \phi_h^{m-1}, \nabla \psi_h \right) + \lambda a_h^{IP} (\phi_h^m, \psi_h) - (\mu_h^m, \psi_h) = 0 \quad \forall \quad \psi_h \in Z_h,
\]

model parameters: $a_0 = 4$ and $\beta = 5$, penalty parameter: $\alpha = 8$. 

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.
Our Numerical Scheme

- Project $\varphi_h^0 := P_h \varphi_0$
- Given $\varphi_{h}^{m-1} \in Z_h$, solve for $(\varphi_{h}^{m}, \mu_{h}^{m}) \in Z_h \times V_h$:

$$
(\delta_{T} \varphi_{h}^{m}, \nu_{h}) + (M \nabla \mu_{h}^{m}, \nabla \nu_{h}) = 0, \quad \forall \nu_{h} \in V_h
$$

$$
3\beta \left( (\varphi_{h}^{m})^5 - (\varphi_{h}^{m-1})^3, \psi_{h} \right) + ((\varphi_{h}^{m})^2 \nabla \varphi_{h}^{m}, \nabla \psi_{h}) + (\varphi_{h}^{m} | \nabla \varphi_{h}^{m-1} |^2, \psi_{h})
$$

$$
- a_{0} \left( \nabla \varphi_{h}^{m-1}, \nabla \psi_{h} \right) + \lambda a_{h}^{IP} (\varphi_{h}^{m}, \psi_{h}) - (\mu_{h}^{m}, \psi_{h}) = 0 \quad \forall \psi_{h} \in Z_h,
$$

model parameters: $a_{0} = 4$ and $\beta = 5$, penalty parameter: $\alpha = 8$.

- 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

\[ \varphi_0(x, y) = 0.3 \cos(3x) + 0.5 \cos(y) \]
\[ \Omega = [0, 2\pi]^2, \ T = 0.4. \]
\[ M = 10^{-3}, \ \lambda = 1 \]
Numerical Experiment I: First Order Convergence

- $\varphi_{256}$: “exact” solution

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

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

Natasha S. Sharma (UTEP)  
C0-IP for Sixth-Order CH Eqns  
07/18/23
Numerical Experiment I: First Order Convergence

- \( \varphi_{256} \): “exact” solution
- \( N \) indicates the number of sub-intervals per side of \( \Omega \)

<table>
<thead>
<tr>
<th>( N )</th>
<th>( | \varphi_{256} - \varphi_N |_{2,h} )</th>
<th>rate</th>
<th>( | \varphi_{256} - \varphi_N |_{L^2} )</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>6.1911</td>
<td>–</td>
<td>0.2625</td>
<td>–</td>
</tr>
<tr>
<td>16</td>
<td>1.9293</td>
<td>1.6045</td>
<td>0.0624</td>
<td>2.1039</td>
</tr>
<tr>
<td>32</td>
<td>0.5601</td>
<td>1.7221</td>
<td>0.0151</td>
<td>2.0685</td>
</tr>
<tr>
<td>64</td>
<td>0.1599</td>
<td>1.7516</td>
<td>0.0035</td>
<td>2.1336</td>
</tr>
<tr>
<td>128</td>
<td>0.0461</td>
<td>1.7354</td>
<td>0.0008</td>
<td>2.1887</td>
</tr>
</tbody>
</table>

Table: Errors and convergence rates of the \( C^0 \)-IP method with \( M = 10^{-3} \), \( \lambda = 1 \), \( h = 2\sqrt{2\pi}/N \), \( \tau = 0.05/N \).
Numerical Experiment I: First Order Convergence

- $\varphi_{256}$: “exact” solution
- $N$ indicates the number of sub-intervals per side of $\Omega$
- $\tau = 0.05/N$

| $N$ | $||\varphi_{256} - \varphi_N||_{2,h}$ | 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 $M = 10^{-3}$, $\lambda = 1$, $h = 2\sqrt{2\pi}/N$, $\tau = 0.05/N$. 

Natasha S. Sharma (UTEP)
Numerical Experiment II: Energy Dissipation

Example

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

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

\[ M = 10^{-3}, \ \lambda = 1, \ \text{penalty parameter} \ \alpha = 8 \]

\[ F(\varphi) = \frac{\beta}{2} \| \varphi \|_{L^6}^6 - \frac{3\beta}{4} \| \varphi \|_{L^4}^4 + \frac{\beta |\Omega|}{4} + \frac{1}{2} \| \varphi \nabla \varphi \|_{L^2}^2 - \frac{a_0}{2} \| \nabla \varphi \|_{L^2}^2 + \frac{\lambda}{2} a_{IP}^p (\varphi, \varphi). \]
Numerical Experiment II: Energy Dissipation

Example

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

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

\[ M = 10^{-3}, \ \lambda = 1, \text{ penalty parameter } \alpha = 8 \]

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

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 $F(\varphi) - \frac{\beta|\Omega|}{4}$, $h = \frac{10\sqrt{2}}{128}$
Numerical Experiment III: Microemulsions Simulation

Example

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

Figure: Profiles at $m = 0, 1, 2$ and 3.
Evolution of the profile

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

Figure: Profiles at $m = 4, 11, 20$ and $25$. 
Evolution of the profile

Figure: Profiles at $m = 37, 74, 158$ and $511$. 
Evolution of the profile

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

- Different temporal scales capture different stages of phase-field evolution.
Evolution of the profile

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

- Different temporal scales capture different stages of phase-field evolution.
- Optimal time steps for each stage can differ by several orders of magnitude.
Evolution of the profile

Different temporal scales capture different stages of phase-field evolution.
Optimal time steps for each stage can differ by several orders of magnitude.
Time-step adaptivity is crucial for accuracy and efficiency of the numerical scheme.

Figure: Profiles at $m = 37, 74, 158$ and $511$. 
Conclusions and Ongoing Work

Numerical schemes using the C0-IP framework were presented for the sixth-order phase field models. Novel contribution: provide an error analysis of the C0-IP framework. Open challenge: Little is known a priori about the dynamics of the system thus making the task of choosing optimal time step and mesh size parameters difficult. Focus: Derive a framework which automatically adapts the choice of the method parameters in response to the change in the dynamics of the problem.

Thank you for your attention!
Conclusions and Ongoing Work

Numerical schemes using the $C^0$-IP framework were presented for the sixth-order phase field models.

**Novel contribution:** provide an error analysis of the $C^0$-IP framework.
Numerical schemes using the $C^0$-IP framework were presented for the sixth-order phase field models.

**Novel contribution:** provide an error analysis of the $C^0$-IP framework.

**Open challenge:** Little is known a priori about the dynamics of the system thus making the task of choosing optimal time step and mesh size parameters difficult.
Conclusions and Ongoing Work

Numerical schemes using the $C^0$-IP framework were presented for the sixth-order phase field models.

**Novel contribution:** provide an error analysis of the $C^0$-IP framework.

**Open challenge:** Little is known a priori about the dynamics of the system thus making the task of choosing optimal time step and mesh size parameters difficult.

**Focus:** Derive a framework which automatically adapts the choice of the method parameters in response to the change in the dynamics of the problem.
Numerical schemes using the $C^0$-IP framework were presented for the sixth-order phase field models.

**Novel contribution:** provide an error analysis of the $C^0$-IP framework.

**Open challenge:** Little is known a priori about the dynamics of the system thus making the task of choosing optimal time step and mesh size parameters difficult.

**Focus:** Derive a framework which automatically adapts the choice of the method parameters in response to the change in the dynamics of the problem.

Thank you for your attention!
Numerical Experiment: Discrete Mass Conservation

Initial Conditions:

Example

\[ \Omega = (-5, 5)^2, \quad T = 0.1, \quad \tau = 1.1 \times 10^{-4}, \quad h = 10\sqrt{2}/128, \quad M = 10, \]
\[ \lambda = 10^{-1}, 10^{-2}, 10^{-3}. \]
Effect of the decreasing $\lambda$

Theory suggests that increasing $\lambda$ guarantees the existence and stability of the solution.

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

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