Phase Field Models and Continuous Data Assimilation

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Outline of Talk

1. Phase Field Models
2. Continuous Data Assimilation
3. Future Work and Thanks

PHASE FIELD MODELS

- Ubiquitous in mathematical modeling of multiphase processes.

- Two basic models:
  - Allen-Cahn Equation
    - Models phase separation and evolution of a two component system that eventually becomes homogeneous.
  - Cahn-Hilliard Equation
    - Models phase separation and evolution of a two component system that preserves volume fractions.

- Each of these can be understood as a gradient flow of the following energy:

$$E(\varphi) = \int_\Omega \left\{ F(\varphi) + \frac{\varepsilon^2}{2} |\nabla \varphi|^2 \right\} d\mathbf{x},$$

  - φ represents an order parameter or concentration,
  - $\varepsilon > 0$ is known as the interfacial width parameter, and
  - $F(\varphi)$ is a double-well potential (here we will consider $F(\varphi) = \frac{1}{4}\left(\varphi^2 - 1\right)^2$).

The Allen-Cahn and Cahn-Hilliard Equations

Recall:

$$E(\varphi) = \int_\Omega \left\{ \frac{1}{4}\left(\varphi^2 - 1\right)^2 + \frac{\varepsilon^2}{2}\left|\nabla\varphi\right|^2 \right\} d\mathbf{x},$$

- The Allen-Cahn equation can be considered as an L^2 gradient flow of E [(Allen and Cahn, 1979)]:

$$\partial_t\varphi = \varepsilon^2\Delta\varphi - \left(\varphi^3 - \varphi\right),$$

where we assume homogeneous Neumann boundary conditions.

- The Cahn-Hilliard equation can be considered as an H^{-1} gradient flow of E [(Cahn and Hilliard, 1958)]:

$$\partial_t\varphi = -\Delta\left(\varepsilon^2\Delta\varphi - \left(\varphi^3 - \varphi\right)\right),$$

where we once again assume homogeneous Neumann boundary conditions.

Key Properties

- Energy Dissipation
  - Allen-Cahn Equation
    - Weak solutions dissipate the energy at the rate

$$E(\varphi(s)) + \int_0^s \|\mu\|_{L^2}^2 \, dt = E(\varphi(0)), \quad \left(d_t E(\varphi) = -\|\mu\|_{L^2}^2 \right),$$

where $\mu := \frac{\delta E}{\delta \varphi}$.

  - Cahn-Hilliard Equation
    - Weak solutions dissipate the energy at the rate

$$E(\varphi(s)) + \int_0^s \|\nabla \mu\|_{L^2}^2 \, dt = E(\varphi(0)), \quad \left(d_t E(\varphi) = -\|\nabla \mu\|_{L^2}^2 \right).$$

- Volume ratio preservation for the Cahn-Hilliard Equation:

$$\int_\Omega (\varphi(\mathbf{x}, t) - \varphi(\mathbf{x}, 0)) \, d\mathbf{x} = 0, \text{ a.e. } t > 0, \quad \left(d_t \int_\Omega \varphi(\mathbf{x}, t) \, d\mathbf{x} = 0 \right).$$

CONTINUOUS DATA ASSIMILATION

Continuous Data Assimilation

Motivating Question: Could incorporating known solution values consistently throughout time but at only a few points in space into a numerical simulation allow for more stable and accurate numerical approximations?

Continuous Data Assimilation based on the AOT formulation [Azouani, Olson, and Titi, 2014]:

- Uses a spacial interpolation operator for 'nudging'.
- Provides rigorous mathematical justification for:
  - exponentially fast in time convergence to 'true' solutions,
  - long time accuracy and stability of the numerical solutions.
- Most successful implementations have been focused on fluid flow models.

Set-up

Consider the following PDE:

$$\partial_t u = G(u),$$

- $u(x,t)$ represents a state variable at spatial position x and time t,
- the initial data $u_0(x) := u(x,0)$ is missing.

Now let v represent an approximation of the state variable u. A continuous data assimilation formulation for the problem above is:

$$\begin{aligned} \partial_t v &= G(v) - \omega I_H(v) + \omega I_H(u), \\ v(x,0) &= v_0(x), \end{aligned}$$

- v_0 is taken to be arbitrary,
- $\omega > 0$ is a relaxation (or nudging) parameter,
- H is the resolution of the coarse spatial grid representing the locations where measurements of observable data are taken,
- the operator I_H is an interpolation operator.

Interpolant Properties

For a given mesh $\mathscr{T}_H$ with $H \leq 1$ and associated finite element space Y_H,

$$\begin{gathered}\left\|I_H(w) - w\right\|_{L^2} \leq C_I H \left\|\nabla w\right\|_{L^2}, \\ \left\|I_H(w)\right\|_{L^2} \leq C_I \left\|w\right\|_{L^2},\end{gathered}$$

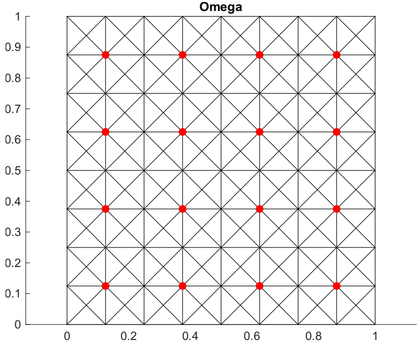
where C_I is independent of w, for any $w \in H^1(\Omega)$.

Examples of such I_H are:

- the L^2 projection onto Y_H where Y_H consists of piecewise constants over $\mathscr{T}_H$, and
- the Scott-Zhang interpolant.

Coarse Grid H

An example of a triangulation of Ω where points $\mathscr{T}_H$ are shown in red.



- Mesh size: $h = \frac{1}{8}$
- Coarse Grid Size: $H = \frac{2}{8}$
- Number of Known Data Points: 16
- Number of Fine Mesh Nodes: 8321
- Mesh produced using the FELICITY MATLAB/C++ Toolbox

A CDA Scheme for the Allen-Cahn Equation

Recall the Allen-Cahn Equation:

$$\partial_t \varphi = \varepsilon^2 \Delta \varphi - \left(\varphi^3 - \varphi\right).$$

Then a CDA scheme is simply stated as:

$$\begin{aligned} \partial_t \phi - \varepsilon^2 \Delta \phi + \left(\phi^3 - \phi\right) + \omega I_H(\phi) - \omega I_H(\varphi) = 0, &\quad \text{in } \Omega, \\ \partial_n \phi = 0, &\quad \text{on } \partial\Omega, \end{aligned}$$

where

- φ is the true concentration,
- ϕ is an approximation to the true concentration,
- $\varepsilon > 0$ is known as the interfacial width parameter,
- $\omega > 0$ is known as a nudging parameter,
- H is the resolution of the coarse spatial grid which represents the locations where measurements are taken, and
- I_H is the interpolation operator.

A CDA FEM for the Allen-Cahn Equation

Let M be a positive integer and $0 = t_0 < t_1 < \cdots < t_M = T$ be a uniform partition of $[0, T]$, with $\tau = T/M$. Define $V_h := \{v_h \in C(\Omega) \mid v_h|_K \in P_q(K),\, K \in \mathscr{T}_h\}$. Given $\phi_h^{m-1} \in V_h$ and true solution $\varphi \in L^\infty(0, T; H^1(\Omega))$, find $\phi_h^m \in V_h$ such that

$$\left(\frac{\phi_h^m - \phi_h^{m-1}}{\tau}, \psi_h\right) + \varepsilon^2(\nabla\phi_h^m, \nabla\psi_h) + \left(\left((\phi_h^m)^3 - \phi_h^{m-1}\right), \psi_h\right) \\ + \omega\left(I_H\left(\phi_h^m - \varphi^m\right), I_H\psi_h\right) = 0, \quad \forall \psi_h \in V_h.$$

Previous Works:

- A. Azouani, E.S. Titi. *Feedback control of nonlinear dissipative systems by finite determining parameters - A reaction-diffusion paradigm.* Evolution Equations and Control Theory, 2014, 3(4): 579-594.
- A. Larios, C. Victor. *Continuous Data Assimilation with a Moving Cluster of Data Points for a Reaction Diffusion Equation: A Computational Study.* Communications in Computational Physics, 2021, 29 (4): 1273-1298.

Existence and Uniqueness

Lemma

Let $\phi_h^{m-1} \in V_h$ and $\varphi \in L^\infty(0,T;H^1(\Omega))$ be given. For all $\xi_h \in V_h$, define the nonlinear functional

$$G_h(\xi_h) := \frac{\tau}{2}\left\|\frac{\xi_h - \phi_h^{m-1}}{\tau}\right\|_{L^2}^2 + \frac{\varepsilon^2}{2}\left\|\nabla\xi_h\right\|_{L^2}^2 + \frac{1}{4}\left\|\xi_h\right\|_{L^4}^4 + \frac{\omega}{2}\left\|I_H\xi_h\right\|_{L^2}^2 - \left(\phi_h^{m-1}, \xi_h\right) - \frac{\omega}{2}\left(I_H\varphi^m, I_H\xi_h\right).$$

G_h is strictly convex and coercive on the linear subspace V_h. Consequently, G_h has a unique minimizer, call it $\phi_h^m \in V_h$. Moreover, $\phi_h^m \in V_h$ is the unique minimizer of G_h if and only if it is the unique solution to the CDA FEM for the Allen-Cahn equation above.

Remarks:

- Proof follows standard proof for convex-splitting schemes.
- But, only if 'variational crime', $\left(I_H\left(\phi_h^m - \varphi^m\right), I_H\psi_h\right)$ is utilized.

Long-time Stability

Lemma

Let $\varphi \in L^\infty(0,\infty; H^1(\Omega))$ represent the true solution and H and ω be chosen so that

$$H^2 < \frac{2\varepsilon^2}{5C_I^2} \text{ and } \omega > \max\left\{1, \frac{2\varepsilon^2}{C_I^2 H^2} - 2\right\}, \tag{1}$$

i.e. H sufficiently small and ω sufficiently large. Then, for any $m, h, \Delta t > 0$, solutions to the CDA-FEM for the Allen-Cahn equation satisfy

$$\|\phi_h^m\|_{L^2}^2 \leq \left\|\phi_h^0\right\|_{L^2}^2 \left(\frac{1}{1 + \Delta t\left(\frac{\lambda_0 - 2}{1 + 2\Delta t}\right)}\right)^m + \frac{\omega\, C_I^2}{\lambda_0 - 2}\Phi \leq C_{data},$$

where $\Phi := \|\varphi\|_{L^\infty(0,\infty;L^2(\Omega))}^2$ and $\lambda_0 = \frac{\varepsilon^2}{C_I^2 H^2} - \frac{1}{2} > 2$.

- $H = \mathcal{O}(\varepsilon) \implies \omega = \mathcal{O}(1)$

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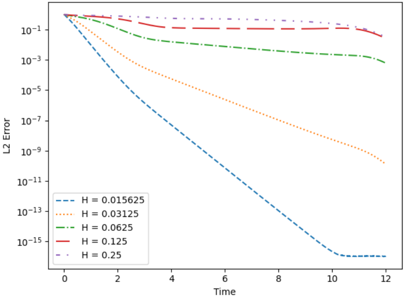
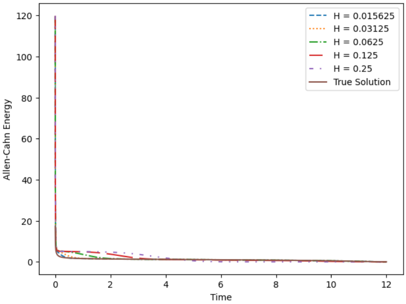
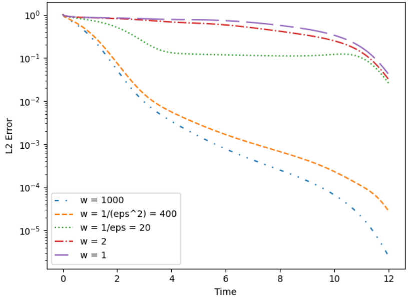
Effectiveness of the CDA-FEM for Various Grid Sizes

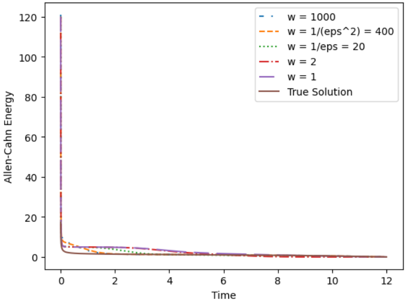




- True solution grid points: 4,096, 1,024, 256, 64 and 16
- Fine mesh nodes: 8321 nodes
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$
- Nudging parameter: $\omega = 1/\varepsilon^2 = 400$

Effectiveness of the CDA-FEM for Various Nudging Parameters





- True solution grid points: 1,024
- Fine mesh nodes: 8321 nodes
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$

A CDA Scheme for the Cahn-Hilliard Equation

Recall the Cahn-Hilliard Equation:

$$\partial_t \phi - \Delta\left(\phi^3 - \phi\right) + \varepsilon^2 \Delta^2 \phi = 0.$$

Then a CDA scheme is simply stated as:

$$\begin{aligned} \partial_t \phi - \Delta\left(\phi^3 - \phi\right) + \varepsilon^2 \Delta^2 \phi + \omega I_H(\phi - \varphi) &= 0, \quad \text{in } \Omega, \\ \partial_n \phi = \partial_n \Delta \phi &= 0, \quad \text{on } \partial\Omega. \end{aligned}$$

Previous Work:

- B. You and Q. Xia. *Continuous data assimilation algorithm for the two dimensional Cahn–Hilliard–Navier–Stokes system.* Applied Mathematics & Optimization, 2002, 85(2), 5.

Ours:

- "Continuous data assimilation and long-time accuracy in a C0 interior penalty method for the Cahn-Hilliard equation." Applied Mathematics and Computation, 2002, 424: 127042.

A C^0 Interior Penalty Method - Preliminaries

- C^0 interior penalty methods were originally developed as an innovative method for solving the fourth-order plate bending problem. [Brenner, et.al.]
- We take a locally quasi-uniform conforming triangulation $\mathscr{T}_h \equiv \mathscr{T}_h(\Omega)$ of the computational domain.
- Define the space:

$$Z_h := \{v_h \in C(\Omega) \mid v_h|_K \in P_2(K),\, K \in \mathscr{T}_h\}.$$

- Define the average and jump terms:

$$\left\{\!\!\left\{ \frac{\partial^2 w}{\partial n_e^2} \right\}\!\!\right\} = \frac{1}{2}\left(\frac{\partial^2 w_-}{\partial n_e^2} + \frac{\partial^2 w_+}{\partial n_e^2} \right), \quad \left[\!\left[\frac{\partial v}{\partial n_e} \right]\!\right] = n_e \cdot \left(\nabla v_+ - \nabla v_-\right),$$

where e denotes the edge of a triangle.

A C0 Interior Penalty Method

Let M be a positive integer and $0 = t_0 < t_1 < \cdots < t_M = T$ be a uniform partition of $[0, T]$. Given $\phi_h^{m-1} \in Z_h$ and true solution $\varphi \in L^\infty(0, T; H_N^2(\Omega))$, find $\phi_h^m \in Z_h$ such that

$$(\delta_\tau \phi_h^m, \psi) + \left(\nabla \left((\phi_h^m)^3 - \phi_h^{m-1}\right), \nabla\psi\right) + \varepsilon^2 a_h^{IP}(\phi_h^m, \psi) + \omega\left(I_H\left(\phi_h^m - \varphi^m\right), \psi\right) = 0$$

for all $\psi \in Z_h$, where $\delta_\tau \phi_h^m := \dfrac{\phi_h^m - \phi_h^{m-1}}{\tau}$ with $\tau = T/M$,

$$\begin{aligned} a_h^{IP}(w, v) = &\sum_{T \in \mathscr{T}_h} \int_T \left(\nabla^2 w : \nabla^2 v\right) dx + \sum_{e \in \mathscr{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 w}{\partial n_e^2} \right\}\!\!\right\} \left[\!\left[\frac{\partial v}{\partial n_e} \right]\!\right] ds \\ &+ \sum_{e \in \mathscr{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 w}{\partial n_e^2} \right\}\!\!\right\} \left[\!\left[\frac{\partial v}{\partial n_e} \right]\!\right] ds + \sum_{e \in \mathscr{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 v}{\partial n_e^2} \right\}\!\!\right\} \left[\!\left[\frac{\partial w}{\partial n_e} \right]\!\right] ds \\ &+ \sigma \sum_{e \in \mathscr{E}_h} \frac{1}{|e|} \int_e \left[\!\left[\frac{\partial w}{\partial n_e} \right]\!\right] \left[\!\left[\frac{\partial v}{\partial n_e} \right]\!\right] ds, \end{aligned}$$

and where $\sigma > 0$ is a penalty parameter.

Solvability and Stability

- Regarding Solvability
  - Unconditionally solvable
  - Conditionally unique solutions: $\frac{1}{\tau} + \omega > \left(\frac{C_I^2 C_P^2 H^2 \omega^2 + 18(C_{inf})^4}{C_{coer}\varepsilon^2} \right)$
- Unconditionally long-time stable
  - Let $\varphi \in L^\infty(0,\infty; H_N^2(\Omega))$ represent the true solution and H and ω be chosen so that

$$\lambda_0 := \frac{\omega C_{coer}\varepsilon^2 - 2\omega^2 C_I^2 C_P^2 H^2 - 4}{C_{coer}\varepsilon^2 + 4\tau} > 0,$$

i.e. H sufficiently small and ω sufficiently large, then

$$\|\phi_h^m\|_{L^2}^2 \leq \left\|\phi_h^0\right\|_{L^2}^2 \left(\frac{1}{1+\lambda_0\tau}\right)^m + \frac{\omega\,\varepsilon^2 C_I^2}{\omega\varepsilon^2 - 2\omega^2 C_I^2 C_P^2 H^2 - 4}\Phi \leq C_{data},$$

where $\Phi := \|\varphi\|_{L^\infty(0,\infty;L^2(\Omega))}^2$.

Important Remarks

- The following geometric series bound was pivotal to the proofs for stability and convergence.
  Suppose the constants r and B satisfy $r > 1$ and $B \geq 0$. Then if the sequence of real numbers $\{a_m\}$ satisfies

$$r\, a_{m+1} \leq a_m + B, \quad \text{we have that} \quad a_{m+1} \leq a_0 \left(\frac{1}{r}\right)^{m+1} + \frac{B}{r-1}.$$

- Stability is satisfied if the nudging parameter ω is $\mathcal{O}(\varepsilon^{-2})$ which would then require H to be $\mathcal{O}(\varepsilon^2)$. However, our numerical experiments suggest that H can be taken much larger than that.
- Since CH solutions generally converge quickly to a steady state solution, we expect the condition required in the proof for uniqueness is not necessary in practice.

Error Estimates

Theorem

Let φ^m represent the true solution to the CH equation at time t_m and suppose that φ satisfies the appropriate regularities and that H and ω are chosen so that

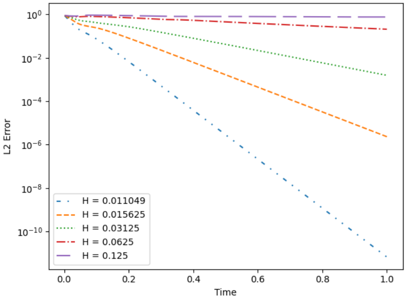
$$\lambda_1 := \frac{C_{coer}\varepsilon^2\omega - 4C_I^2 C_P^2 H^2\omega^2 - 72\left((C_{inf})^2 + (C'_{data})^2\right)^2 - 16}{C_{coer}\varepsilon^2 + 16\tau} > 0,$$

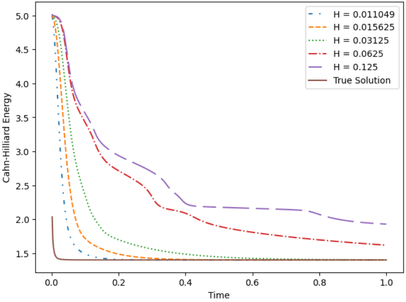
i.e. H sufficiently small and ω sufficiently large. Then we have

$$\|\varphi^m - \phi_h^m\|_{L^2}^2 \leq \left\|\varphi^0 - \phi_h^0\right\|_{L^2}^2 \left(\frac{1}{1+\lambda_1\tau}\right)^m + \left(\frac{C_{coer}\varepsilon^2\left(h^2 + h^5 + (\tau)^2\right)}{\omega C_{coer}\varepsilon^2 - 4C_I^2 C_P^2 H^2\omega^2 - 72\left((C_{inf})^2 + (C'_{data})^2\right)^2 - 16}\right) C^*_{data}$$

for any $m, h, \tau > 0$.

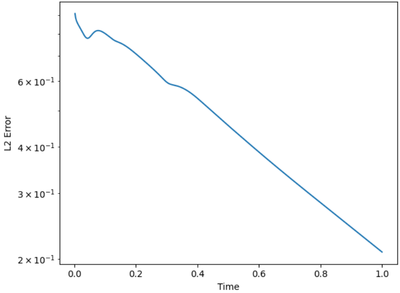
Effectiveness of the CDA-FEM for Various Grid Sizes

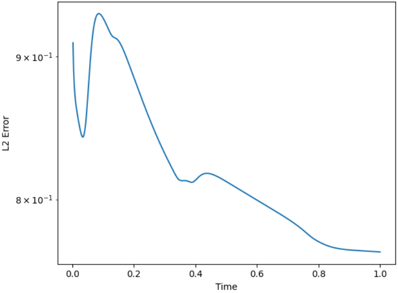




- True solution grid points: 8,100, 4,096, 1,024, 256 and 64
- Fine mesh nodes: 33,025
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$
- Nudging parameter: $\omega = {}^{1}\!/_{\varepsilon^2} = 400$

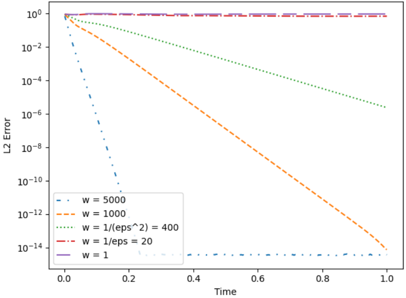
Effectiveness of the CDA-FEM for Various Grid Sizes

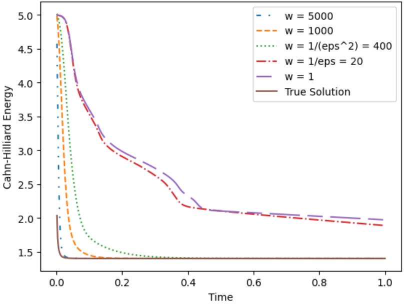




- True solution grid points: 256 and 64
- Fine mesh nodes: 33,025
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$
- Nudging parameter: $\omega = {}^{1}/_{\varepsilon^2} = 400$

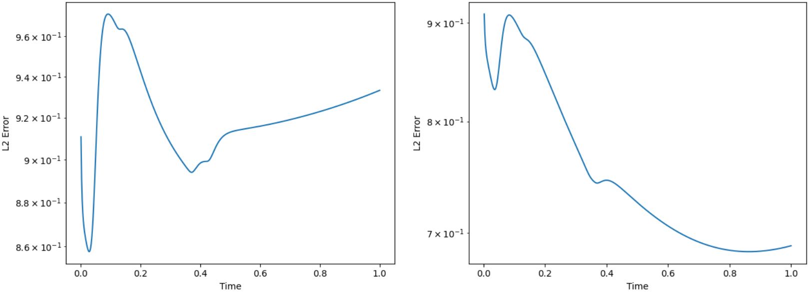
Effectiveness of the CDA-FEM for Various Nudging Parameters





- True solution grid points: 1,024
- Fine mesh nodes: 33,025
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$

Effectiveness of the CDA-FEM for Various Nudging Parameters



- True solution grid points: 1,024
- Fine mesh nodes: 33,025
- Time step size: $\tau = 0.002$
- Interfacial width parameter: $\varepsilon = 0.05$
- Left: $\omega = 1$, Right: $\omega = 20$

Cross Shape Test

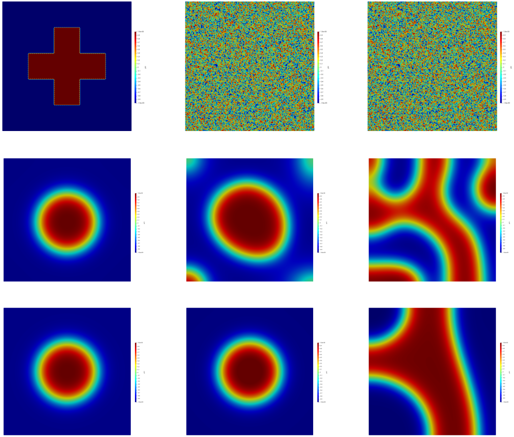
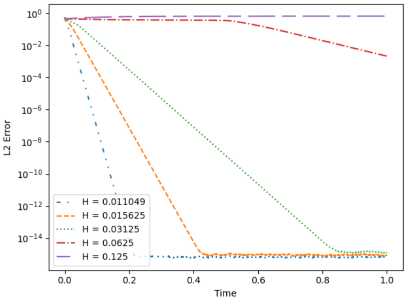
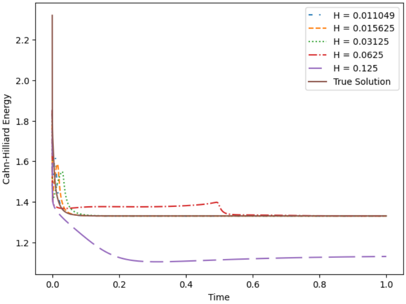


Figure: True solution (left), CDA CH (middle), CH (right) at 5 and 25 Time Steps

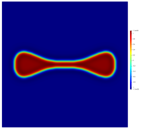
Effectiveness of the CDA-FEM - Dumbbell Test



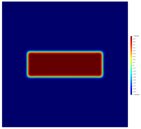


- Fine mesh nodes: 33,025
- Time step size: $\tau = 0.002/32$
- Interfacial width parameter: $\varepsilon = 0.02$
- Left: $\omega = {}^{1}/_{\varepsilon^2} = 2500$

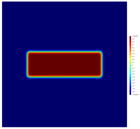
Dumbbell Test



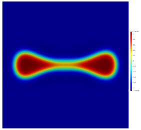
(c) $t = 0.0$



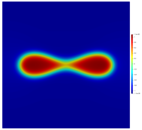
(d) $t = 0.0$



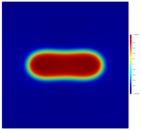
(e) $t = 0.0$



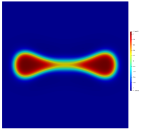
(f) $t = 0.000625$



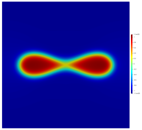
(g) $t = 0.015625$



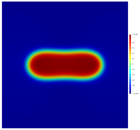
(h) $t = 0.015625$



(i) $t = 0.001$

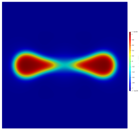


(j) $t = 0.016$

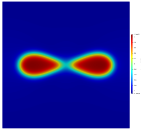


(k) $t = 0.016$

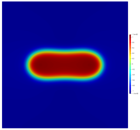
Dumbbell Test



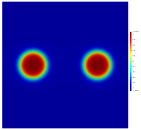
(l) $t = 0.0035$



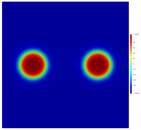
(m) $t = 0.018125$



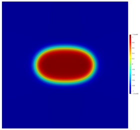
(n) $t = 0.018125$



(o) $t = 0.1$



(p) $t = 0.1$



(q) $t = 0.1$

FUTURE WORK AND THANKS

Future Work

- Current and Future Work on Data Assimilation:
  - Develop a CDA FEM for the mixed formulation of the Cahn-Hilliard equation.
  - Extend to two-phase flow equations such as the Navier-Stokes Cahn-Hilliard system of equations.
  - Extend to other gradient flows, such as the phase field crystal equation.
- Open Questions:
  - What if the data involves an element of stochasticity?
  - Could CDA help correct for too large of an interfacial width parameter?
  - How does CDA effect efficient solvers?
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