Phase Field Models and Continuous Data Assimilation

Amanda E. Diegel

In Collaboration with
Leo G. Rebholz, Clemson University

Department of Mathematics and Statistics
Mississippi State University

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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:

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

- \( \varphi \) 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 \( F(\varphi) = \frac{1}{4} (\varphi^2 - 1)^2 \)).
The Allen-Cahn and Cahn-Hilliard Equations

Recall:

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

- The Allen-Cahn equation can be considered as an \( L^2 \) gradient flow of \( E \) [(Allen and Cahn, 1979)]:
  \[ \partial_t \varphi = \varepsilon^2 \Delta \varphi - (\varphi^3 - \varphi), \]
  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)]:
  \[ \partial_t \varphi = -\Delta \left( \varepsilon^2 \Delta \varphi - (\varphi^3 - \varphi) \right), \]
  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 \( \mu := \delta E / \delta \varphi \).
  - 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:
  \[
  \int_\Omega (\varphi(x, t) - \varphi(x, 0)) \, dx = 0, \text{ a.e. } t > 0, \quad \left( d_t \int_\Omega \varphi(x, t) \, dx = 0 \right).
  \]
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:

\[ \partial_t v = G(v) - \omega I_H(v) + \omega I_H(u), \]
\[ v(x, 0) = v_0(x), \]

- \( v_0 \) 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 $\mathcal{T}_H$ with $H \leq 1$ and associated finite element space $Y_H$, 

$$
\| I_H(w) - w \|_{L^2} \leq C_I H \| \nabla w \|_{L^2},
$$

$$
\| I_H(w) \|_{L^2} \leq C_I \| w \|_{L^2},
$$

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 $\mathcal{T}_H$, and
- the Scott-Zhang interpolant.
Coarse Grid $H$

An example of a triangulation of $\Omega$ where points $\mathcal{T}_H$ 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:

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

Then a CDA scheme is simply stated as:

$$\partial_t \phi - \varepsilon^2 \Delta \phi + (\phi^3 - \phi) + \omega I_H(\phi) - \omega I_H(\varphi) = 0, \quad \text{in } \Omega,$$

$$\partial_n \phi = 0, \quad \text{on } \partial \Omega,$$

where

- $\varphi$ is the true concentration,
- $\phi$ 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

$$V_h := \{ v_h \in C(\Omega) \mid v_h|_K \in P_q(K), \ K \in \mathcal{T}_h \}.$$ 

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

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

Previous Works:


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

$$G_{h}(\xi_{h}) := \frac{\tau}{2} \left\| \frac{\xi_{h} - \phi_{h}^{m-1}}{\tau} \right\|_{L^2}^2 + \frac{\varepsilon^2}{2} \left\| \nabla \xi_{h} \right\|_{L^2}^2 + \frac{1}{4} \left\| \xi_{h} \right\|_{L^4}^4 + \frac{\omega}{2} \left\| I_{H} \xi_{h} \right\|_{L^2}^2$$

$$- (\phi_{h}^{m-1}, \xi_{h}) - \frac{\omega}{2} (I_{H} \varphi^{m}, I_{H} \xi_{h}).$$

$G_{h}$ 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’, $(I_{H} (\phi_{h}^{m} - \varphi^{m}), I_{H} \psi_{h})$ is utilized.
Long-time Stability

Lemma

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

\[
H^2 < \frac{2\varepsilon^2}{5C_i^2} \quad \text{and} \quad \omega > \max \left\{ 1, \frac{2\varepsilon^2}{C_i^2 H^2} - 2 \right\},
\]

(1)
i.e. \( H \) sufficiently small and \( \omega \) sufficiently large. Then, for any \( m, h, \Delta t > 0 \), solutions to the CDA-FEM for the Allen-Cahn equation satisfy

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

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

\( H = O(\varepsilon) \implies \omega = O(1) \)
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: \( \omega = \frac{1}{\varepsilon^2} = 400 \)
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:

\[ \partial_t \phi - \Delta (\phi^3 - \phi) + \varepsilon^2 \Delta^2 \phi = 0. \]

Then a CDA scheme is simply stated as:

\[ \partial_t \phi - \Delta (\phi^3 - \phi) + \varepsilon^2 \Delta^2 \phi + \omega I_H(\phi - \varphi) = 0, \quad \text{in } \Omega, \]
\[ \partial_n \phi = \partial_n \Delta \phi = 0, \quad \text{on } \partial \Omega. \]

Previous Work:


Ours:

A C⁰ Interior Penalty Method - Preliminaries

- C⁰ 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 \( \mathcal{T}_h \equiv \mathcal{T}_h(\Omega) \) of the computational domain.
- Define the space:
  \[
  Z_h := \{ v_h \in C(\Omega) \mid v_h|_K \in P_2(K), \ K \in \mathcal{T}_h \}.
  \]
- Define the average and jump terms:
  \[
  \left\{ \frac{\partial^2 w}{\partial n_e^2} \right\} = \frac{1}{2} \left( \frac{\partial^2 w_-}{\partial n_e^2} + \frac{\partial^2 w_+}{\partial n_e^2} \right), \quad \left[ \frac{\partial v}{\partial n_e} \right] = n_e \cdot (\nabla v_+ - \nabla v_-),
  \]
  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 $\varphi \in L^\infty (0, T; H^2_N(\Omega))$, find $\phi_{h}^{m} \in Z_h$ such that

$$(\delta_{\tau} \phi_{h}^{m}, \psi) + \left( \nabla \left( (\phi_{h}^{m})^3 - \phi_{h}^{m-1} \right), \nabla \psi \right) + \varepsilon^2 a^{IP} (\phi_{h}^{m}, \psi) + \omega (l_H (\phi_{h}^{m} - \varphi^{m}), \psi) = 0$$

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

$$a^{IP} (w, v) = \sum_{T \in \mathcal{T}_h} \int_{T} \left( \nabla^2 w : \nabla^2 v \right) \, dx + \sum_{e \in \mathcal{E}_h} \int_{e} \left\{ \frac{\partial^2 w}{\partial n_e^2} \right\} \begin{bmatrix} \frac{\partial v}{\partial n_e} \end{bmatrix} \, ds$$

$$+ \sum_{e \in \mathcal{E}_h} \int_{e} \left\{ \frac{\partial^2 v}{\partial n_e^2} \right\} \begin{bmatrix} \frac{\partial w}{\partial n_e} \end{bmatrix} \, ds + \sum_{e \in \mathcal{E}_h} \int_{e} \left\{ \frac{\partial^2 w}{\partial n_e^2} \right\} \begin{bmatrix} \frac{\partial v}{\partial n_e} \end{bmatrix} \, ds$$

$$+ \sigma \sum_{e \in \mathcal{E}_h} \frac{1}{|e|} \int_{e} \left\{ \frac{\partial w}{\partial n_e} \right\} \begin{bmatrix} \frac{\partial v}{\partial n_e} \end{bmatrix} \, ds,$$

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

- **Regarding Solvability**
  - Unconditionally solvable
  - Conditionally unique solutions: \( \frac{1}{\tau} + \omega > \left( \frac{C_l^2 C_p H^2 \omega^2 + 18 (C_{inf})^4}{C_{coer} \varepsilon^2} \right) \)

- **Unconditionally long-time stable**
  - Let \( \phi \in L^\infty(0, \infty; H_N^2(\Omega)) \) represent the true solution and \( H \) and \( \omega \) be chosen so that

\[
\lambda_0 := \frac{\omega C_{coer} \varepsilon^2 - 2 \omega^2 C_l^2 C_p^2 H^2 - 4}{C_{coer} \varepsilon^2 + 4 \tau} > 0,
\]

i.e. \( H \) sufficiently small and \( \omega \) sufficiently large, then

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

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

$$r a_{m+1} \leq a_m + B,$$

we have that

$$a_{m+1} \leq a_0 \left( \frac{1}{r} \right)^{m+1} + \frac{B}{r - 1}.$$

Stability is satisfied if the nudging parameter $\omega$ is $O(\varepsilon^{-2})$ which would then require $H$ to be $O(\varepsilon^2)$. 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 $\varphi^m$ represent the true solution to the CH equation at time $t_m$ and suppose that $\varphi$ satisfies the appropriate regularities and that $H$ and $\omega$ are chosen so that

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

i.e. $H$ sufficiently small and $\omega$ sufficiently large. Then we have

$$
\| \varphi^m - \phi^m_h \|_{L^2}^2 \leq \| \varphi^0 - \phi^0_h \|_{L^2}^2 \left( \frac{1}{1 + \lambda_1 \tau} \right)^m
$$

$$
+ \left( \frac{C_{\text{coer}} \varepsilon^2 \left( h^2 + h^5 + (\tau)^2 \right)}{\omega C_{\text{coer}} \varepsilon^2 - 4 C_i^2 C_P^2 H^2 \omega^2 - 72 ((C_{\text{inf}})^2 + (C'_{\text{data}})^2)^2 - 16} \right) C^*_\text{data}
$$

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: $\omega = \frac{1}{\varepsilon^2} = 400$
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: $\omega = \frac{1}{\varepsilon^2} = 400$
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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