



Research article

An adaptive div-curl-grad least-squares finite element method for the Cahn-Hilliard equation

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Abstract: This paper develops a new least-squares finite element approach for the efficient approximation of solutions of the Cahn-Hilliard equation. We discretize in time with either implicit backward Euler or Crank-Nicolson and use a regularized Newton iteration for the nonlinearity. The innermost iteration is reformulated as a coupled first-order div-curl-grad system, which is efficiently solved by a least-squares minimization approach using standard Lagrange finite elements for each unknown. Theoretical findings include results on the optimal finite element convergence of the variational problem, convergence of the nonlinear iteration, error bounds for the time integration schemes, and discrete asymptotic mass conservation and energy dissipation in the least-squares sense. The basic iterative approach is expanded to include adaptivity in both time and space. Numerical examples are provided to confirm the theoretical results and to demonstrate effectiveness of the proposed method for a range of test problems.

Keywords: Cahn-Hilliard equation; phase separation models; least-squares finite element methods; nonlinear partial differential equations

1. Introduction and background

In this paper, we consider the Cahn-Hilliard model for binary phase separation, which is given by the following:

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} = \Delta w & \text{in } \Omega \times (0, \infty) \\ w = -\varepsilon^2 \Delta u + F'(u) & \text{in } \Omega \times (0, \infty) \\ \mathbf{n} \cdot \nabla u = \mathbf{n} \cdot \nabla w = 0 & \text{on } \partial\Omega \times (0, \infty) \\ u(\mathbf{x}, 0) = f & \text{in } \Omega, \end{array} \right. \quad (1.1)$$

where $u = u(\mathbf{x}, t)$ is the concentration field, and $w = w(\mathbf{x}, t)$ is the *chemical* potential. $F(u) = \frac{1}{4}(u^2 - 1)^2$ is a double-well energy potential that is minimized when $u = \pm 1$, which represents the two stable phases of the concentration, and ε is the characteristic phase separation length, which is typically very small relative to the size of the domain. The domain, Ω , is assumed to be a Lipschitz smooth convex domain in $\mathbb{R}^2$, and $\mathbf{n}$ is the outward unit normal to the boundary $\partial\Omega$. Neumann boundary conditions on u and w correspond to thermodynamic equilibrium and conservation of mass, respectively. The initial condition is assumed to satisfy $u(\mathbf{x}, 0) \in [-1, 1]$. While we focus on results in two dimensions in this paper, an extension to three dimensions is relatively straightforward.

The Cahn-Hilliard equation fundamentally describes the gradient flow of an energy functional and models the separation dynamics between two distinct phases, generally resulting in large regions of uniform concentration separated by thin interfacial regions [1]. In particular, it describes the process of spinodal decomposition, where small perturbations in an initial concentration of a mixture near the unstable equilibrium ($u \approx 0$) result in a fast decomposition into separate phases ($u \approx \pm 1$). This coarsening results in the formation of coherent structures that continue to evolve by decreasing the energy [2].

It is important to note that such problems have a wide range of relevant time scales, namely the so-called *fast-slow-fast* behavior, with the initial process occurring very rapidly, evolving to relatively slow changes, which can be intermittently interrupted by rapid changes as structures interact and coalesce. Similarly, solutions for u in space tend toward requiring much higher resolution in the interfacial regions than regions of uniform concentration. Thus, adaptivity in both time and space is necessary to efficiently resolve the solution.

Additionally, System (1.1) provides the fundamental framework for a wide range of problems that involve the evolution of a phase field; e.g., see survey literature [3–7]. Such applications based on interfacial dynamics include multi-phase fluid flow [8–11], diffuse-interface tumor modeling [12, 13], and image inpainting [14, 15].

The Cahn-Hilliard model may also be posed in terms of u only, where it is a nonlinear parabolic-like problem with fourth-order derivatives in space. There is a rich history and broad literature devoted to the numerical approximation of System (1.1), which remains a challenging problem in many aspects.

Explicit time discretizations generally require severe constraints on the time step size to guarantee stability, while implicit and some semi-implicit approaches allow for larger time steps [16]. The resulting stationary problem at each time step requires a compatible spatial discretization scheme, and existing methods include a wide range of finite difference methods [17], finite element methods [18–21], discontinuous Galerkin methods [22, 23], collocation methods [24], and multigrid/multiscale approaches [25, 26]. Since discretizing fourth-order derivatives is especially difficult, it is more common to examine the second-order system for u and w . The standard variational problem based on (1.1), which serves as the basis for most finite-element approaches, results in a saddle-point problem, which brings additional challenges.

In [27, 28], the authors used a space-time discretization with a least squares spectral element method based on the residual of the coupled second-order system similar to System (1.1). C^1 Hermite polynomials are used since the formulation involves second-order derivatives. This results in symmetric positive definite linear systems and benefits from many of the advantages of the least-squares finite element approach, including the use of residual-based adaptive mesh refinement.

In the proposed approach in this paper, we introduce additional flux variables to reformulate Sys-

tem (1.1) to first-order with dominant div-curl-grad operators in space. Then, the overall iterative approach employs fully implicit time stepping (backward Euler or Crank-Nicolson), a regularized Newton iteration, and a least squares closure on the first-order system. Motivated by a well-established body of work in first-order system least squares methods (see [29–32] for the fundamental theoretical framework and [33–35] for relevant examples for nonlinear problems), our approach makes use of standard C^0 finite element spaces and produces well-conditioned, symmetric positive definite linear systems at each step. Further, we describe ways of incorporating adaptive time stepping and adaptive mesh refinement into the iterative method.

The organization of the remainder of this paper is as follows: in Section 2, we briefly review notation; Section 3 lays out the overall iterative approach, including the reformulation of the system to first-order, the treatment of the nonlinearity, and the definition of the least-squares variational problem for each step; theoretical results are given in Section 4; a summary of adaptivity in both time and space is discussed in Section 5; computational results for several example problems are given in Section 6; and brief concluding remarks are given in Section 7.

2. Notation

We use standard Sobolev spaces, $L^2(\Omega)^d$ and $H^m(\Omega)^d$ for $m \geq 1$, where $d = 1, 2$, and generally omit the dimension when it is clear by context. We denote $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ as the standard L^2 norm and inner product on Ω , respectively, $\|\cdot\|_m$ as the H^m norm, and use the standard gradient and Laplacian operators, ∇ and Δ , respectively. For $V = (V_1, V_2) \in H^1(\Omega)^2$, we use the divergence and curl with $\nabla \cdot V = \partial_x(V_1) + \partial_y(V_2)$ and $\nabla \times V = \partial_x(V_2) - \partial_y(V_1)$.

Additionally, dual spaces are defined in the natural way, where $(H^1(\Omega))^*$ is the dual to $H^1(\Omega)$, and $H_0^1(\Omega) = \{v \in H^1(\Omega) : u = 0 \text{ on } \Omega\}$ has its dual denoted by $H^{-1}(\Omega)$ with norm

$$\|v\|_{-1} = \sup_{\phi \in H_0^1(\Omega)} \frac{\langle v, \phi \rangle}{\|\phi\|_1},$$

where $\langle \cdot, \cdot \rangle$ is the dual pairing in this context. Define the spaces $\mathcal{V}_1 = H^1(\Omega)$ and $\mathcal{V}_2 = \{V \in H^1(\Omega)^2 : \mathbf{n} \cdot V = 0 \text{ on } \partial\Omega\}$. Throughout this paper, the generic positive constant C is used, which may represent different values in each usage and may depend on problem parameters, the domain, or, in some cases, a current approximation of the unknown u .

3. Reformulation and iterative framework

We define the flux variables $U = \nabla u$ and $W = \nabla w$, which allows (1.1) to be reformulated as a first-order system. The definitions of U and W imply that $\nabla \times U = \nabla \times W = 0$, which is used to augment the system.

We seek to approximate the solutions $u, w \in \mathcal{V}_1$ and $U, W \in \mathcal{V}_2$ for each time step. For the discrete approximations at each step, we take $\mathcal{V}_1^h \subseteq \mathcal{V}_1$ and $\mathcal{V}_2^h \subseteq \mathcal{V}_2$ from Lagrangian finite element spaces P2 or P3 (i.e., piecewise quadratic or cubic elements) in each component, which are equipped with the appropriate boundary conditions.

We consider the use of both the backward Euler and Crank-Nicolson time discretizations, though in what follows, we generally describe the more accurate Crank-Nicolson approach. In each case, for

time values $t_0, t_1, t_2, \dots$, let δ represent the time step parameter (which may vary) and use u_0 and u as approximations at any two consecutive time steps. Similarly, W_0 and W are approximations at the previous and current time steps, respectively. The first equation in (1.1) is replaced with one of the following:

$$\begin{aligned} \text{(BE)} \quad & \frac{u - u_0}{\delta} = \nabla \cdot W, \\ \text{(CN)} \quad & \frac{u - u_0}{\delta} = \frac{1}{2} (\nabla \cdot W + \nabla \cdot W_0). \end{aligned} \quad (3.1)$$

For each time step, we linearize the second equation in (1.1) with a modified Newton's method by iterating from the previous approximation $\tilde{u}$ to the updated approximation u by the following replacement:

$$u^3 \rightarrow 3\tilde{u}^2 u - 2\tilde{u}^3 + \rho(u - \tilde{u}),$$

where ρ is a positive regularization parameter. Putting this together for the Crank-Nicolson method (backward Euler only differs in the first equation) yields the coupled div-curl-grad system

$$\begin{cases} -\frac{\delta}{2} \nabla \cdot W + u = \frac{\delta}{2} \nabla \cdot W_0 + u_0 \\ -\varepsilon^2 \nabla \cdot U + (3\tilde{u}^2 + \rho - 1)u - w = 2\tilde{u}^3 + \rho\tilde{u} \\ \nabla \times W = \nabla \times U = 0 \\ \nabla u - U = \nabla w - W = \mathbf{0}, \end{cases} \quad (3.2)$$

in Ω for each outer time step and each inner linearization step for unknowns $(u, w, U, W) \in \mathcal{V}_1^2 \times \mathcal{V}_2^2$ given approximations $(\tilde{u}, u_0, W_0) \in \mathcal{V}_1^2 \times \mathcal{V}_2$. We define the least squares functional

$$\begin{aligned} G(u, w, U, W; \tilde{u}, u_0, W_0) = & \\ & \left\| \frac{\delta}{2} \nabla \cdot W - u + \frac{\delta}{2} \nabla \cdot W_0 + u_0 \right\|^2 + \left\| \varepsilon^2 \nabla \cdot U - (3\tilde{u}^2 + \rho - 1)u + w + 2\tilde{u}^3 + \rho\tilde{u} \right\|^2 \\ & + \left\| \delta(\nabla \times W) \right\|^2 + \left\| \varepsilon^2(\nabla \times U) \right\|^2 + \left\| \nabla u - U \right\|^2 + \left\| \nabla w - W \right\|^2. \end{aligned}$$

Thus, the discrete solution for $(u^h, w^h, U^h, W^h) \in (\mathcal{V}_1^h)^2 \times (\mathcal{V}_2^h)^2$ at each step is the minimizer of G , where

$$G(u^h, w^h, U^h, W^h; \tilde{u}^h, u_0^h, W_0^h) \leq G(v^h, z^h, V^h, Z^h; \tilde{u}^h, u_0^h, W_0^h)$$

for all $(v^h, z^h, V^h, Z^h) \in (\mathcal{V}_1^h)^2 \times (\mathcal{V}_2^h)^2$. This is equivalent to the solution of the following symmetric variational problem: find $(u^h, w^h, U^h, W^h) \in (\mathcal{V}_1^h)^2 \times (\mathcal{V}_2^h)^2$ such that

$$\mathcal{B}(u^h, w^h, U^h, W^h; v^h, z^h, V^h, Z^h) = \ell(v^h, z^h, V^h, Z^h) \quad (3.3)$$

for all $(v^h, z^h, V^h, Z^h) \in (\mathcal{V}_1^h)^2 \times (\mathcal{V}_2^h)^2$, where the bilinear form $\mathcal{B}$ and the functional ℓ are given by

$$\begin{aligned} \mathcal{B}(u, w, U, W; v, z, V, Z) = & \left\langle -\frac{\delta}{2} \nabla \cdot W + u, -\frac{\delta}{2} \nabla \cdot Z + v \right\rangle \\ & + \left\langle -\varepsilon^2 \nabla \cdot U + (3\tilde{u}^2 + \rho - 1)u - w, -\varepsilon^2 \nabla \cdot V + (3\tilde{u}^2 + \rho - 1)v - z \right\rangle \\ & + \varepsilon^4 \langle \nabla \times U, \nabla \times V \rangle + \delta^2 \langle \nabla \times W, \nabla \times Z \rangle + \langle \nabla u - U, \nabla v - V \rangle + \langle \nabla w - W, \nabla z - Z \rangle \end{aligned}$$

and

$$\ell(v, z, V, Z) = \left\langle \frac{\delta}{2} \nabla \cdot W_0 + u_0, -\frac{\delta}{2} \nabla \cdot Z + v \right\rangle + \langle 2\tilde{u}^3 + \rho\tilde{u}, -\varepsilon^2 \nabla \cdot V + (3\tilde{u}^2 + \rho - 1)v - z \rangle.$$

Now, the overall solution framework can be summarized in Algorithm 1 below. Here, h denotes the meshsize parameter for the domain discretization, T is the maximum simulation time, and $nSteps$ is the number of nonlinear iterations per time step. When using the backward Euler time integration, keeping the previous values of W^h is not needed.

Algorithm 1 Iterative Method Framework

Choose values for: $h, \delta, T, \rho, nSteps$

Set: $t=0$

Initialize: $u_0^h = \tilde{u}^h = f|_{\mathcal{V}_1^h}$ and $W_0^h = \nabla(-\varepsilon^2 \Delta f + f^3 - f)|_{\mathcal{V}_2^h}$.

while $t < T$, **do**

$t = t + \delta$

for $n = 1, 2, \dots, nSteps$, **do**

 Solve problem (3.3) for (u^h, w^h, U^h, W^h) .

$\tilde{u}^h \leftarrow u^h$

end for

 (optional) Adapt the time step δ

 (optional) Adapt the mesh Ω^h

$u_0^h \leftarrow u^h, W_0^h \leftarrow W^h$

end while

4. Theory

In this section, we address theoretical aspects of the iterative method defined above. In this framework, we first analyze the finite element solution of each linearization step and provide error bounds for the spatial discretization. Then, we consider the convergence of the linearization iteration within each time step. Then, convergence of the time discretization is considered. Finally, we examine the evolution of energy and mass conservation, which are of particular interest in this system.

4.1. Finite element convergence in space

We focus on the solution to System (3.2) via the variational problem (3.3), and show optimal finite element convergence rates using standard Lagrangian spaces of equal order for all unknowns. While this paper doesn't focus on the solution of the discrete linear systems, we note that the coupled div-curl-grad structure here produces symmetric, positive definite linear systems that may be efficiently solved by multigrid iterative solvers.

We assume that $\tilde{u}$ and Ω are sufficiently smooth to allow the following H^1 regularity result for the

second order elliptic system: for all $f_1, f_2 \in (H^1(\Omega))^*$, the solution to

$$\begin{cases} -\varepsilon^2 \Delta u + (3\tilde{u}^2 + \rho - 1)u - w = f_1 & \text{in } \Omega \\ -\frac{\delta}{2} \Delta w + u = f_2 & \text{in } \Omega \\ \mathbf{n} \cdot \nabla u = \mathbf{n} \cdot \nabla w = 0 & \text{on } \partial\Omega \end{cases}$$

for $u, w \in \mathcal{V}_1$ satisfies

$$\|u\|_1 + \|w\|_1 \leq C(\|f_1\|_{-1} + \|f_2\|_{-1}). \quad (4.1)$$

We note that this system has principle elliptic operators $-\varepsilon^2 \Delta$ and $-\frac{\delta}{2} \Delta$, coupled via the zero-order terms with the matrix

$$\begin{pmatrix} (3\tilde{u}^2 + \rho - 1) & -1 \\ 1 & 0 \end{pmatrix},$$

which is positive semi-definite when $\rho > 1$.

For brevity, we define the product H^m norm for $m \geq 0$ on all unknowns by the following:

$$\|(u, w, U, W)\|_m := (\|u\|_m^2 + \|w\|_m^2 + \|U\|_m^2 + \|W\|_m^2)^{\frac{1}{2}}. \quad (4.2)$$

Additionally, we denote

$$\begin{aligned} \|(u, w, U, W)\|_G = & (\|\frac{\delta}{2} \nabla \cdot W - u\|^2 + \|\varepsilon^2 \nabla \cdot U - (3\tilde{u}^2 + \rho - 1)u + w\|^2 \\ & + \|\delta(\nabla \times W)\|^2 + \|\varepsilon^2(\nabla \times U)\|^2 + \|\nabla u - U\|^2 + \|\nabla w - W\|^2)^{\frac{1}{2}} \end{aligned} \quad (4.3)$$

as the norm induced by the homogenous least-squares functional. The following theorem establishes equivalence between the H^1 and functional norms and is sufficient to show that the weak problem solved at each step is well posed.

Theorem 1. Assume that Ω is a smooth convex domain, $\rho > 1$, and that $\|\tilde{u}\|_\infty \leq M < \infty$. There are constants $c_0, c_1 > 0$, which depend on ε, δ, M , and Ω , where

$$c_0 \|(u, w, U, W)\|_1 \leq \|(u, w, U, W)\|_G \leq c_1 \|(u, w, U, W)\|_1$$

for all $(u, w, U, W) \in \mathcal{V}_1^2 \times \mathcal{V}_2^2$.

Proof. The upper bound is easily shown by the triangle inequality and the assumption on the smoothness of $\tilde{u}$. We establish the lower bound by bounding each term in (4.2) above by the norm in (4.3).

Define the set $\mathcal{D} = \{(\phi, \psi) \in (H^1(\Omega))^2 : \|\phi\|_1 + \|\psi\|_1 = 1\}$ and use (4.1) to first get that

$$\begin{aligned}
 \|u\|_1 + \|w\|_1 &\leq C(\|-\varepsilon^2 \Delta u + (3\tilde{u}^2 + \rho - 1)u - w\|_{-1} + \|\frac{\delta}{2} \Delta w + u\|_{-1}) \\
 &\leq C \sup_{(\phi, \psi) \in \mathcal{D}} (\langle -\varepsilon^2 \Delta u + (3\tilde{u}^2 + \rho - 1)u - w, \phi \rangle + \langle -\frac{\delta}{2} \Delta w + u, \psi \rangle) \\
 &\leq C \sup_{(\phi, \psi) \in \mathcal{D}} (\langle \varepsilon^2 (\nabla u - U), \nabla \phi \rangle + \langle -\varepsilon^2 \nabla \cdot U + (3\tilde{u}^2 + \rho - 1)u - w, \phi \rangle \\
 &\quad + \langle \frac{\delta}{2} (\nabla w - W), \nabla \psi \rangle + \langle -\frac{\delta}{2} \nabla \cdot W + u, \psi \rangle) \\
 &\leq C(\varepsilon^2 \|\nabla u - U\| \|\nabla \phi\| + \|\varepsilon^2 \nabla \cdot U + (3\tilde{u}^2 + \rho - 1)u - w\| \|\phi\| \\
 &\quad + \frac{\delta}{2} \|\nabla w - W\| \|\nabla \psi\| + \frac{\delta}{2} \|\nabla \cdot W + u\| \|\psi\|) \\
 &\leq C\|(u, w, U, W)\|_G.
 \end{aligned} \tag{4.4}$$

Using (4.4) and the triangle inequality, we have

$$\|U\| + \|W\| \leq \|\nabla u - U\| + \|\nabla u\| + \|\nabla w - W\| + \|\nabla w\| \leq C\|(u, w, U, W)\|_G,$$

$$\|\nabla \cdot U\| \leq C(\|\varepsilon^2 \nabla \cdot U + (3\tilde{u}^2 + \rho - 1)u - w\| + \|u\| + \|w\|) \leq C\|(u, w, U, W)\|_G,$$

and

$$\|\nabla \cdot W\| \leq C(\|\nabla \cdot W + u\| + \|u\|) \leq C\|(u, w, U, W)\|_G.$$

We trivially have $\|\nabla \times U\| + \|\nabla \times W\| \leq \|(u, w, U, W)\|_G$. Moreover, it follows from the assumptions on Ω that

$$\|\nabla U\| \leq C(\|\nabla \cdot U\| + \|\nabla \times U\|),$$

and

$$\|\nabla W\| \leq C(\|\nabla \cdot W\| + \|\nabla \times W\|),$$

which can be shown through a Helmholtz decomposition (see [32, 33], e.g.). Combining each bound above completes the proof.

Because our formulation here has a dominant div-curl structure for the flux variables, the curl terms in the least-squares functional includes scaling by δ and ε^2 to match the magnitude of the scaling coefficients on the corresponding divergence terms in (4.3). While this isn't necessary for the theoretical results shown here, we find that this scaling tends to result in a more uniform level of error across all terms in the functional in numerical tests. Additionally, we note that the formulation highlighted here will be robust for H^1 -conforming finite elements, and we have the freedom to choose spaces based on the desired accuracy or computational availability [29]. We choose to focus on equal order C^0 elements for simplicity, though it is possible to omit the curl constraints on U and W and consider a mixed formulation that uses $H(\text{div})$ -conforming elements for U^h and W^h . There is ample literature on this type of formulation; e.g., see [35–37].

Let I^h be the standard finite element interpolation operator associated with continuous piecewise polynomials of degree k on a triangulation of Ω that admits the approximation property

$$\|v - I^h v\|_1 \leq Ch^{m-1} \|v\|_m \tag{4.5}$$

for $1 \leq m \leq k + 1$ and all $v \in H^m(\Omega)$. For the computational results in this paper, we consider P2 ($k = 2$) and P3 ($k = 3$) elements, but are not limited to those approximation spaces. Now, we are able to prove the convergence bounds.

Theorem 2. Let $(u, w, U, W) \in \mathcal{V}_1^2 \times \mathcal{V}_2^2 \subseteq H^m(\Omega)^6$ represent the exact solution to system (3.2) and take $(u^h, w^h, U^h, W^h) \in (\mathcal{V}_1^h)^2 \times (\mathcal{V}_2^h)^2$ as the solution to (3.3) with degree k polynomial approximations for all unknowns. Thus, the error satisfies

$$\|(u - u^h, w - w^h, U - U^h, W - W^h)\|_1 \leq Ch^{m-1} \|(u, w, U, W)\|_m$$

and

$$\|(u - u^h, w - w^h, U - U^h, W - W^h)\|_G \leq Ch^{m-1} \|(u, w, U, W)\|_m$$

for $1 \leq m \leq k + 1$.

Proof. By using Theorem 1, recognizing that (u^h, w^h, U^h, W^h) is the minimizer of the least squares functional, and applying (4.5) to all components in the solution, we have the following:

$$\begin{aligned} c_0 \|(u - u^h, w - w^h, U - U^h, W - W^h)\|_1 & \\ & \leq \|(u - u^h, w - w^h, U - U^h, W - W^h)\|_G \\ & = G(u^h, w^h, U^h, W^h; \tilde{u}^h, u_0^h, W_0^h)^{1/2} \\ & \leq G(I^h u, I^h w, I^h U, I^h W; \tilde{u}^h, u_0^h, W_0^h)^{1/2} \\ & = \|(u - I^h u, w - I^h w, U - I^h U, W - I^h W)\|_G \\ & \leq c_1 \|(u - I^h u, w - I^h w, U - I^h U, W - I^h W)\|_1 \\ & \leq Ch^{m-1} \|(u, w, U, W)\|_m, \end{aligned}$$

which shows both bounds needed to complete the proof.

This indicates that the finite element approximations should converge in the H^1 and functional norms at $O(h^k)$ when we use spaces of polynomial degree k . Consequentially, we expect that the L^2 error, $\|u - u^h\|$, should converge at $O(h^{k+1})$. We omit a proof of this, but note that arguments for L^2 convergence of least-squares finite element methods can be found in [36] and [37], for example.

4.2. Convergence of the nonlinear iteration

Each timestep in Algorithm 1 involves a regularized Newton iteration to resolve the nonlinearity in the system. In this section, we discuss convergence of this iteration and provide intuition in choosing the number of iterations needed per timestep. First, we note that each timestep can be represented as the solution to the following system:

$$\begin{cases} -\frac{\delta}{2} \nabla \cdot W + W_0 + u - u_0 = 0 \\ -\varepsilon^2 \nabla \cdot U + u^3 - u - w = 0 \\ \nabla \times W = \nabla \times U = 0 \\ \nabla u - U = \nabla w - W = \mathbf{0}, \end{cases} \quad (4.6)$$

where u_0 and W_0 are fixed from the previous timestep. Define $\mathbf{x} = (u, w, U, W)$ and $\mathcal{L} : \mathcal{V}_1^2 \times \mathcal{V}_2^2 \rightarrow \mathbb{R}^6$ such that the exact solution to (4.6) is given by $\mathcal{L}(\mathbf{x}^*) = \mathbf{0}$. We denote $\mathcal{L}'(\phi)[\psi]$ as the Fréchet derivative

of the operator $\mathcal{L}$ at ϕ in the direction of ψ and $\mathcal{L}''(\phi)[\psi, \xi]$ as the second Fréchet derivative of $\mathcal{L}$ at ϕ in the directions of ψ and ξ . Since the nonlinearity in this system is only in terms that involve u , we let $P_1[\mathbf{x}] = (u, \mathbf{0})$ and note that the only nonzero term in $\mathcal{L}''(\phi)[\psi, \xi]$ is $6\phi\psi\xi$ which results from the cubic term in u . Furthermore, let $\mathbf{e}_n = \mathbf{x}_n - \mathbf{x}^*$ and $\mathbf{e}_{n+1} = \mathbf{x}_{n+1} - \mathbf{x}^*$ be the errors in successive steps n and $n + 1$ in the regularized Newton's method. Thus, (3.2) can be represented by the following:

$$(\mathcal{L}'(\mathbf{x}_n) + \rho P_1)[\mathbf{e}_{n+1} - \mathbf{e}_n] + \mathcal{L}(\mathbf{x}_n) = \mathbf{0},$$

which is discretized and solved via (3.3).

To understand the evolution of error in each linearization step, we first consider the truncated Taylor series about $\mathbf{x}_n$,

$$\mathbf{0} = \mathcal{L}(\mathbf{x}^*) = \mathcal{L}(\mathbf{x}_n) + \mathcal{L}'(\mathbf{x}_n)[\mathbf{x}^* - \mathbf{x}_n] + \frac{1}{2}\mathcal{L}''(\zeta)[\mathbf{x}^* - \mathbf{x}_n, \mathbf{x}^* - \mathbf{x}_n],$$

where $\zeta = \theta\mathbf{x}^* + (1 - \theta)\mathbf{x}_n$ for some $\theta \in [0, 1]$. Substituting and rearranging gives

$$\begin{aligned} (\mathcal{L}'(\mathbf{x}_n) + \rho P_1)[\mathbf{e}_{n+1}] &= (\mathcal{L}'(\mathbf{x}_n) + \rho P_1)[\mathbf{e}_n] - \mathcal{L}(\mathbf{x}_n) \\ &= (\mathcal{L}'(\mathbf{x}_n) + \rho P_1)[\mathbf{e}_n] + \mathcal{L}'(\mathbf{x}_n)[\mathbf{x}^* - \mathbf{x}_n] + \frac{1}{2}\mathcal{L}''(\zeta)[\mathbf{x}^* - \mathbf{x}_n, \mathbf{x}^* - \mathbf{x}_n] \\ &= \rho P_1[\mathbf{e}_n] + \frac{1}{2}\mathcal{L}''(\zeta)[\mathbf{e}_n, \mathbf{e}_n] \\ &= \rho(u_n - u^*) + 3\zeta(u_n - u^*)^2. \end{aligned}$$

In the case that $\rho = 0$, this results in the familiar quadratic form of convergence of the pure Newton's method. In the case that $\rho > 0$, the error is dominated by the linear term above, and we can expect linear convergence when the operator

$$\rho(\mathcal{L}'(\mathbf{x}_n) + \rho P_1)^{-1}$$

represents a contraction.

Since the only nonlinearity in System (4.6) is in terms that involve u , we can illustrate the key nature of this mapping with the component $\mathcal{L}_u(u) := u^3 - u$. This leads to $\mathcal{L}'(u_n)[\psi] = 3u_n^2\psi - \psi$, which indicates that the error evolution operator has the form

$$\rho(\mathcal{L}'_u(u_n) + \rho)^{-1} = \frac{\rho}{3u_n^2 - 1 + \rho},$$

which is contractive when $\rho > 1$. This implies that we can expect linear convergence with a rate of approximately $\rho/(2 + \rho)$ toward regions with $u \approx \pm 1$ that minimize the double-well energy potential.

4.3. Convergence in the time discretization

Assuming smooth solutions and using standard arguments based on Taylor series approximations, it is straightforward to show that the backward Euler and Crank-Nicolson time integration schemes have pointwise $O(\delta)$ and $O(\delta^2)$ truncation errors in time, respectively. From this, it is easy to show that the L^2 errors are also $O(\delta)$ and $O(\delta^2)$ in time,

$$\begin{aligned} \text{(BE)} \quad \|(u - u^h)|_{t=T}\| &\leq CT\delta, \\ \text{(CN)} \quad \|(u - u^h)|_{t=T}\| &\leq CT\delta^2, \end{aligned} \tag{4.7}$$

where u is the exact solution to System (1.1).

4.4. Energy dissipation and mass conservation

Define the following mass and energy functionals:

$$\begin{aligned}\mathcal{M}(u) &= \int_{\Omega} u \, d\mathbf{x}, \\ \mathcal{E}(u) &= \int_{\Omega} \left(\frac{1}{2} \varepsilon^2 |\nabla u|^2 + \frac{1}{4} |u^2 - 1|^2 \right) d\mathbf{x}.\end{aligned}$$

Solutions to the Cahn-Hilliard system (1.1) are known to conserve mass and be energy dissipative over time.

Testing (3.3) with $(v^h, z^h, V^h, Z^h) = (1, 2 + \rho, \mathbf{0}, \mathbf{0})$ and applying integration by parts gives the following:

$$\langle u^h - u_0^h, 1 \rangle = \langle \varepsilon^2 \nabla \cdot U^h - (3(\tilde{u}^h)^2 + \rho - 1)u^h + w^h + 2(\tilde{u}^h)^3 + \rho \tilde{u}^h, 3(\tilde{u}^h)^2 - 3 \rangle.$$

Thus, applying the Cauchy-Schwarz inequality and Theorem 1, we have

$$|\langle u^h - u_0^h, 1 \rangle| \leq \| (u^h, w^h, U^h, W^h) \|_G \| 3(\tilde{u}^h)^2 - 3 \|,$$

which, with Theorem 2, implies that

$$|\mathcal{M}(u) - \mathcal{M}(u_0)| \leq Ch^k, \quad (4.8)$$

where k is the polynomial degree of the finite element spaces used. Further, we note that as numerical approximations tend toward $\tilde{u}^h \approx 1$ for much of the domain, we expect $\|(\tilde{u}^h)^2 - 1\|$ to be small. This indicates that the numerical approach here weakly conserves mass, in the least squares sense.

For energy, we note that

$$\frac{d}{dt} \mathcal{E}(u) = \varepsilon^2 \langle \nabla u, \nabla u_t \rangle + \langle u^3 - u, u_t \rangle$$

and assume that u is smooth enough to admit the Taylor expansion

$$\mathcal{E}(u) = \mathcal{E}(u_0) + \delta \frac{d}{dt} \mathcal{E}(u)|_{t=t_0} + O(\delta^2). \quad (4.9)$$

If we further assume that the linearization iteration converges with $\tilde{u}^h \approx u^h$ and apply similar arguments to (3.3) as above, then the backward Euler time discretization can be shown to satisfy the following:

$$\mathcal{E}(u^h) - \mathcal{E}(u_0^h) \leq -\delta \|\nabla w^h\|^2 + c_d \delta^2 + c_e \| (u^h, w^h, U^h, W^h) \|_G, \quad (4.10)$$

where c_d depends on the truncation error in (4.9), and c_e depends on ε , δ , $\|\nabla u^h\|$, $\|\nabla u_0^h\|$, $\|\nabla w^h\|$, and $\|W_0^h\|$. Using Theorem 2 and (4.10), we see that the numerical approach here is energy decreasing when h and δ are chosen to be sufficiently small.

In Section 6, the evolution of mass and energy are shown for several example problems.

5. Adaptivity

As a complement to the main iterative framework above, we introduce the possibility of adaptivity in both the time step size and the mesh discretization. Since we use implicit time stepping methods, we expect to be able to vary the time step according to the timescale of the solution evolution. Similarly, we can expect to gain computational efficiency with adaptive mesh refinement since the developed solutions at each time step tend to have $u \approx \pm 1$ on large subsets of the domain with thin regions of large gradients separating the two phases.

Adaptivity in Time: In Algorithm 1, δ represents the time step parameter, and below we describe how we adapt δ between steps based on the current and previous approximations, u^h and u_0^h , respectively. We define

$$\eta = \|u^h - u_0^h\| / \|u_0^h\|$$

as a relative measure of change between iterates. This approach uses user defined values for the minimum and maximum allowed time steps, δ_{min} and δ_{max} , respectively, and a reference level of allowed relative change in approximation in one step, $\hat{\eta} \in (0, 1)$. We use the geometric mean, $\hat{\delta} = \sqrt{\delta_{max}\delta_{min}}$, as the time step that corresponds to $\hat{\eta}$. For each time step, we compute the adjusted time step parameter as follows:

$$\delta_1 = \delta_{min} + (\delta_{max} - \delta_{min}) \left(\frac{\hat{\delta} - \delta_{min}}{\delta_{max} - \delta_{min}} \right)^{\eta/\hat{\eta}},$$

which is illustrated in Figure 1. Thus, to avoid oscillation between short/long time steps, we choose the next time step parameter by averaging the current time step with δ_1 as follows:

$$\delta \leftarrow \frac{1}{2}(\delta + \delta_1).$$

In practice, we choose the initial time step parameter as $\delta = \delta_{min}$ and the values for δ_{min} , δ_{max} , and $\hat{\eta}$ from the specific problem.

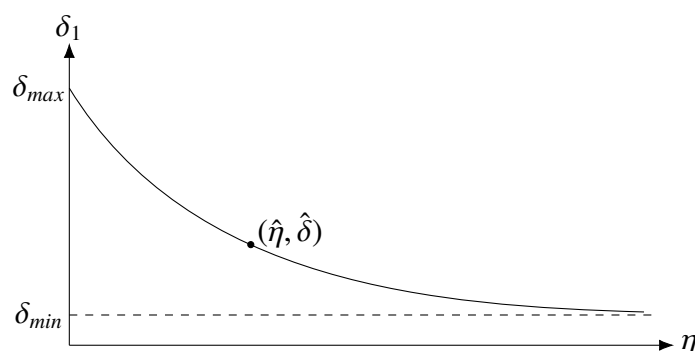


Figure 1. Model for choosing the time step parameter, δ_1 , adjustment from the computed value of the relative measure of change between iterates, η . For each time step, time steps are increased/decreased when the relative change between iterates is small/large. The user-defined value $\hat{\eta}$ corresponds to the geometric mean of the minimum and maximum allowed time steps, $\hat{\delta}$.

Adaptivity in Space: We use an adaptive refinement routine implemented in FreeFEM++, which constructs an estimator from a measure of the Hessian of the current approximation, u^h , and, based on this, creates a new mesh with a set upper bound on the number of elements and the minimum and maximum element size bounded by $h_{max} \leq 10h_{min}$ (see [38] for details). We initially discretize on a uniform or quasiuniform mesh of triangles and adjust the mesh between each time step. All relevant approximations are interpolated to the new mesh for use in the next iteration.

6. Numerical tests

In this section, we provide several tests to demonstrate the efficacy of the proposed method.

Example 1: Accuracy in time and space. For the first computational test, we modify the model by adding a nonhomogenous source function, $g = g(x, y, t)$, to the first equation,

$$\frac{\partial u}{\partial t} = \Delta u + g,$$

chosen to allow for the following exact solution for u :

$$u(x, y, t) = \cos(\pi x) \cos(\pi y) \exp(-t).$$

Using $\Omega = (0, 1)^2$ and discretizing the domain with a uniform mesh of triangles of size h allows the approximate solution to be compared with the exact solution at any point in Algorithm 1.

We begin with an exploration of convergence of the nonlinear iteration for a single time step, which uses $\varepsilon = 0.01$, $\delta = 0.001$, and P3 elements on a uniform mesh with $h^{-1} = 40$. Table 1 below shows the L^2 error after each of 5 iterations of the regularized Newton iteration for the first backward Euler time step for different choices of the regularization parameter ρ .

Table 1. Example 1: Accuracy in Nonlinear Iteration. L^2 Error at regularized Newton step n for $\rho = 0, 0.5, 1.0$, and 1.5 . Each step uses P3 elements on a uniform mesh with $h^{-1} = 40$.

n	L^2 Error			
	$\rho = 0.0$	$\rho = 0.5$	$\rho = 1.0$	$\rho = 1.5$
1	$4.640e-7$	$5.117e-6$	$9.853e-6$	$1.450e-5$
2	$4.553e-7$	$4.592e-7$	$5.527e-7$	$7.520e-7$
3	$4.553e-7$	$4.299e-7$	$4.138e-7$	$4.076e-7$
4	$4.553e-7$	$4.298e-7$	$4.116e-7$	$3.984e-7$
5	$4.553e-7$	$4.301e-7$	$4.117e-7$	$3.982e-7$

This shows that the nonlinear error is resolved in all cases with relatively few steps. The case with $\rho = 0$ corresponds to pure Newton's method and is consistent with fast quadratic convergence. For increasing ρ , the results are also consistent with the expected linear convergence rate. These results also show a slightly different convergence point for different choices of ρ . Since the regularization term, $\rho(u - u_n)$, increases the dependence on u in the least squares functional, it is not surprising to see that a higher value of ρ leads to a smaller L^2 error in the approximation of u . Since the least squares

approach balances the residual across all terms in the functional, different weighting can result in a different distribution of approximation error across the different components.

For the remainder of this example, we use $\rho = 0$ and $nSteps = 2$ nonlinear iterations for each time step and choose $\varepsilon = 0.1$. The following numerical tests independently evaluate convergence in the timestep δ and meshsize h , using fixed values for each.

To demonstrate convergence in the time discretization, we choose an accurate spatial resolution and vary the time step parameter δ . Table 2 shows the L^2 norm of the error as δ is reduced, solving up to $T = 0.1$ using P3 elements for all unknowns with $h^{-1} = 80$. The convergence rate is estimated from the error at the two finest levels, and shows $O(\delta)$ for backward Euler and $O(\delta^2)$ for the Crank-Nicolson discretizations as expected.

Table 2. Example 1: Accuracy in Time. Error vs. timestep δ at final time $T = 0.1$. Each step uses P3 elements on a uniform mesh with $h^{-1} = 80$.

δ^{-1}	L^2 Error	
	BE	CN
20	$1.04e-3$	$8.66e-6$
40	$5.30e-4$	$2.25e-6$
80	$2.68e-4$	$5.65e-7$
160	$1.35e-4$	$1.42e-7$
rate $\approx$	0.99	1.99

Table 3. Example 1: Accuracy in Space. Error vs. meshsize h at final time $T = 10^{-4}$. Each result uses 10 Crank-Nicolson time steps with $\delta = 10^{-5}$ and $nSteps = 2$ nonlinear iterations for each time step.

h^{-1}	L^2 Error		Functional norm	
	P2	P3	P2	P3
10	$4.03e-3$	$6.30e-5$	$1.29e-2$	$2.80e-4$
20	$3.92e-4$	$1.13e-6$	$4.30e-3$	$6.44e-5$
40	$3.06e-5$	$4.86e-8$	$1.22e-3$	$8.52e-6$
80	$2.12e-6$	$3.04e-9$	$3.19e-4$	$1.08e-6$
rate $\approx$	3.85	4.00	1.94	2.98

For convergence in the spatial resolution, we use 10 Crank-Nicolson time steps with $\delta = 10^{-5}$. We show results for both $P2$ and $P3$ elements for a range of mesh resolutions. In addition to the L^2 error, $\|u - u^h\|$, we use the least squares functional norm, defined by

$$\text{Functional Norm} = \left(G(u^h, w^h, U^h, W^h; \tilde{u}^h, u_0^h, W_0^h) \right)_T^{\frac{1}{2}},$$

to demonstrate convergence in all unknowns. Asymptotic optimal convergence rates for the functional norm are $O(h^2)$ and $O(h^3)$ for $P2$ and $P3$ elements, respectively, as anticipated by theorem 2. Likewise, optimal convergence in L^2 is $O(h^3)$ and $O(h^4)$ for $P2$ and $P3$ elements respectively. Table 3 shows that

the computational results are in close agreement with these expected values. The computed L^2 error for $P2$ elements shown on the resolutions here is above the expected rate, but further experiments show that the rates asymptotically approach the expected $O(h^3)$.

From this example, as expected, it is clear that the best accuracy is achieved with the combination of the Crank-Nicolson time integration with $P3$ elements. In the remaining examples, we exclusively use Crank-Nicolson since it has essentially the same cost per step as backward Euler. For the spatial discretization, we use $P3$ rather than $P2$ elements; however, we note that the higher discretization accuracy comes with an increased cost in each linear solve.

Example 2: Adaptivity in Time and Space. In this example, we demonstrate aspects of the adaptive time stepping and adaptive mesh refinement routine described in Section 5. Let $\Omega = (0, 1)^2$, and define the initial condition

$$u(\mathbf{x}, 0) = \begin{cases} 1 & \text{if } (x - 0.35)^2 + (y - 0.5)^2 \leq (0.22)^2 \text{ or } (x - 0.75)^2 + (y - 0.5)^2 \leq (0.15)^2 \\ -1 & \text{otherwise,} \end{cases}$$

as two different sized, nearly adjacent circles of concentration $+1$ in a background of concentration -1 . The projection of $u(\mathbf{x}, 0)$ onto $\mathcal{V}_1^h$ is used for u_0^h and $\tilde{u}^h$. We use $\varepsilon = 0.02$ as the phase separation length and $\text{nSteps} = 2$ nonlinear iterations per time step and discretize with $P3$ elements. For adaptivity, we choose $\delta_{\min} = 10^{-4}$, $\delta_{\max} = 10^{-2}$, and $\hat{\eta} = 0.02$, which allows a 2% relative change between time steps of size $\hat{\delta} = 10^{-3}$.

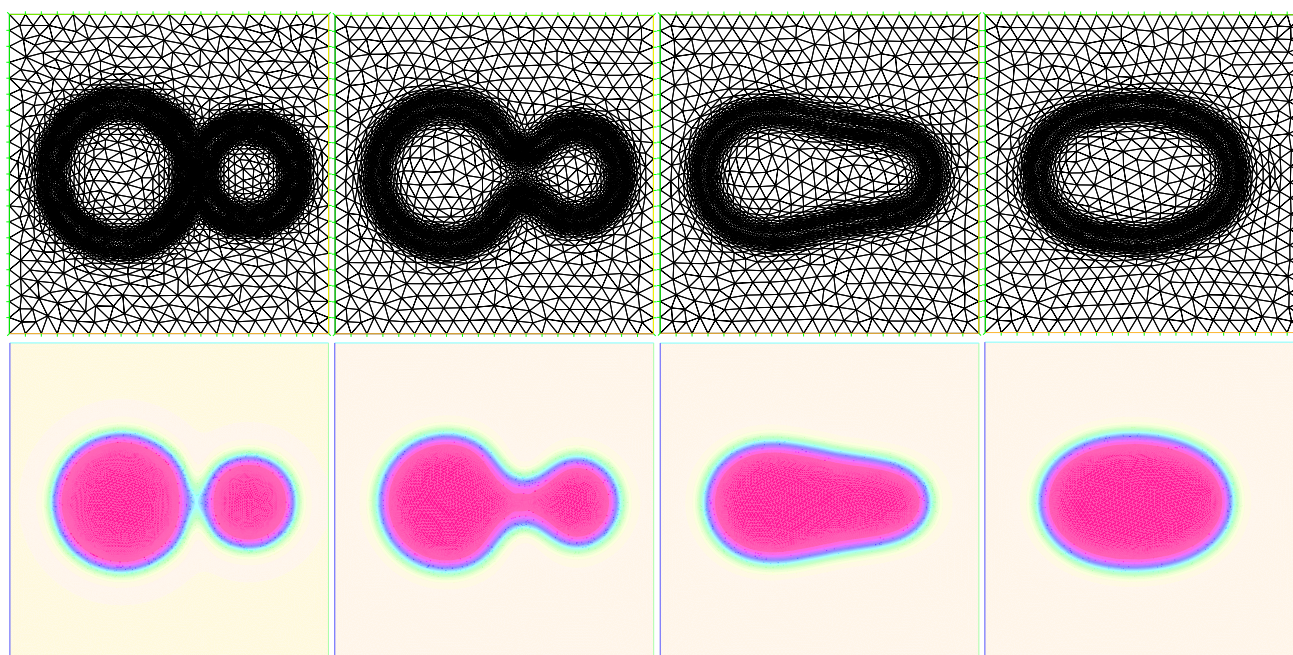


Figure 2. Adapted mesh and solution plots at time steps 3, 10, 50, and 100 (corresp. times $t = 0.000318, 0.00682, 0.120$, and 0.337) for Example 2.

The results for adaptivity are shown in Figure 3, which plots the evolution of the time step size, δ , and the number of elements in the adapted meshes. The solution rapidly changes at the beginning,

and, as the two regions of concentration +1 merge and the solution changes more slowly, the method adjusts the time step and mesh resolution size accordingly.

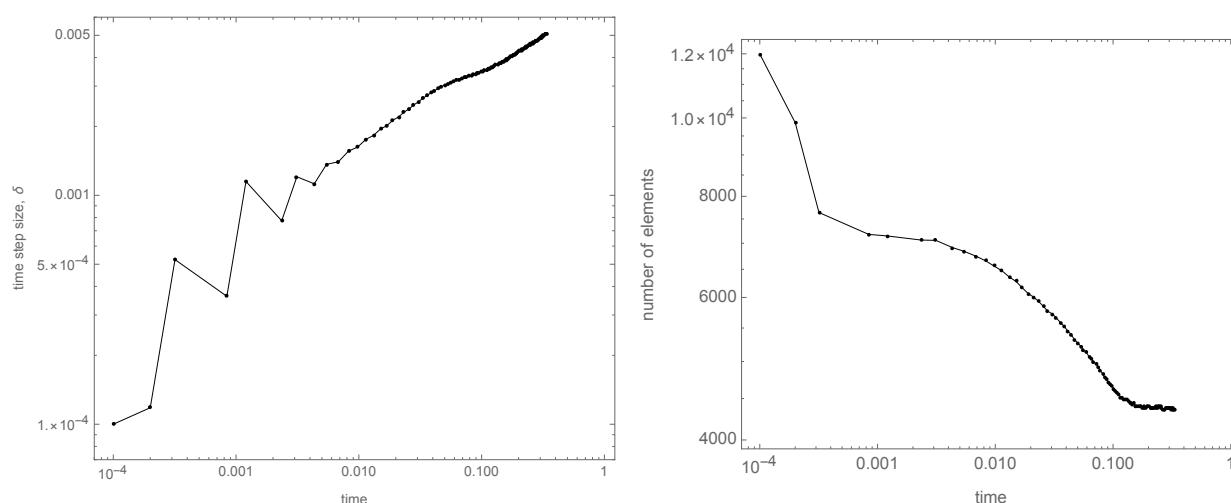


Figure 3. Time step size, δ , vs. time for Example 2.

Figure 4 shows the evolution of the energy and mass over the simulated time period. Consistent with the physics of the problem, the energy is non-increasing and the mass is essentially constant (note: the ratio of observed maximum to minimum absolute mass values is 1.00008).

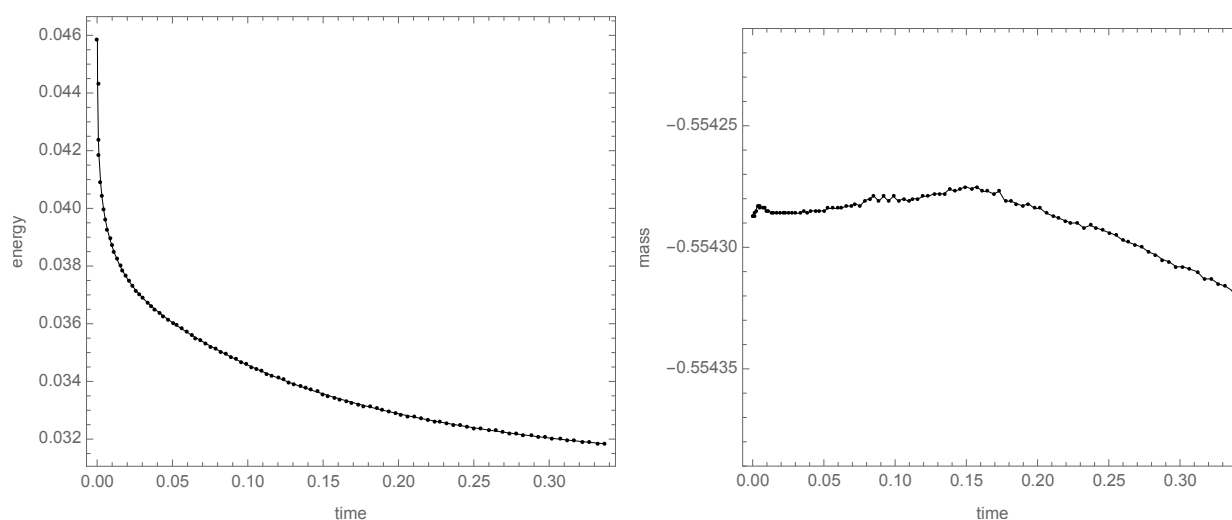


Figure 4. Evolution of $\mathcal{E}(u^h)$ and $\mathcal{M}(u^h)$ for Example 2.

This example closely matches results for similar test problems described in the literature, including [21, 22].

Example 3: Spinodal Decomposition. In this example, we choose $u(\mathbf{x}, 0)$ as (nearly) random values in the range $(-1, 1)$ to demonstrate the rapid coarsening of the solution into distinct regions of different concentrations. As in the previous example, we use $\varepsilon = 0.02$, $nSteps = 2$, $\delta_{min} = 10^{-4}$, $\delta_{max} = 10^{-2}$, and $\hat{\eta} = 0.02$.

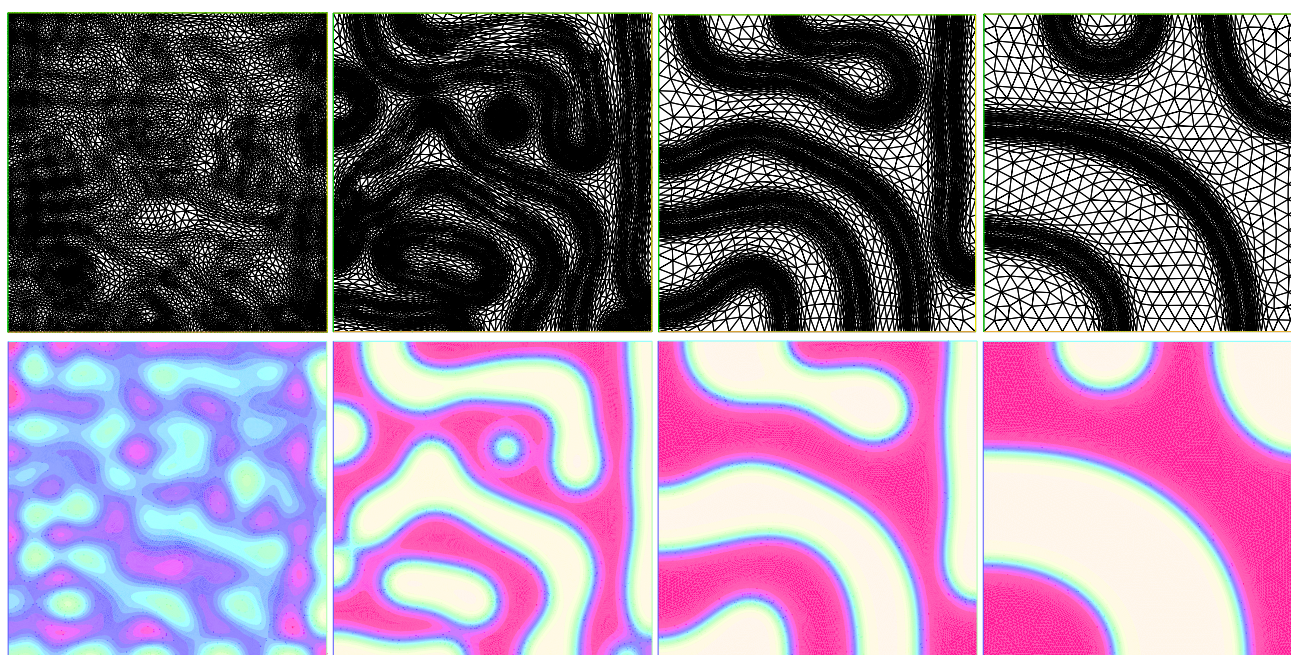


Figure 5. Adapted mesh and solution plots at time steps 12, 115, 200 and 500 (corresp. times $t = 0.00140, 0.0391, 0.135$, and 1.16) for Example 3.

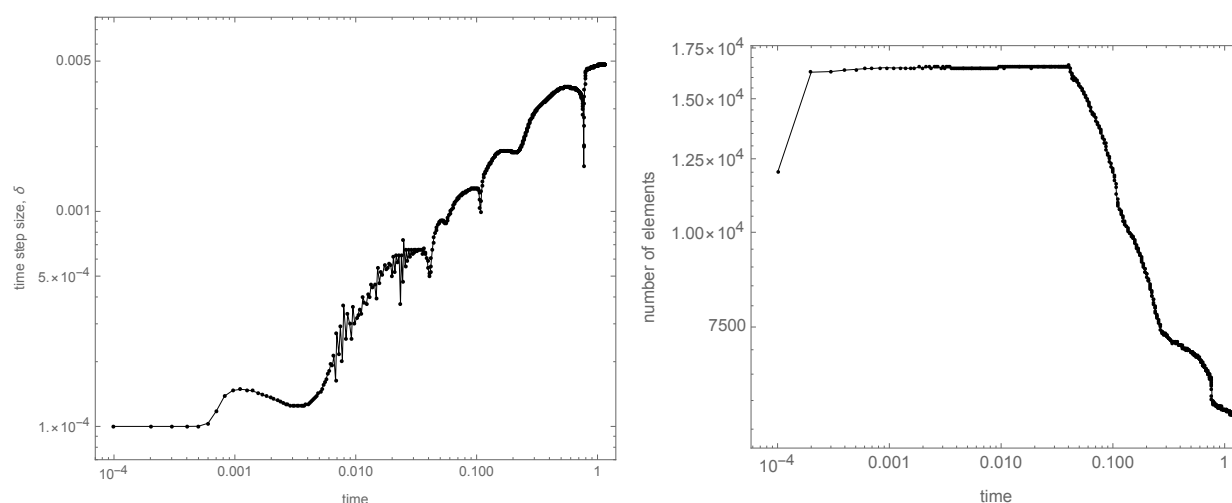


Figure 6. Time step size, δ , vs. time for Example 3.

Figure 5 shows the evolution of the solution in the coarsening process and the computational mesh used. Figure 6 shows the time step size and number of elements used over time. In this case, the initial coarsening process rapidly occurs, and the time steps remain near the minimum until the phases become somewhat distinct. As the process continues, we see the adaptivity in time reflects the so-called *fast-slow-fast* behavior, where the solution slowly evolves except for when separate regions of a phase quickly coalesce. Likewise, during the coarsening, the spatial discretization uses the maximum resolution available until large regions of uniform concentration appear. As the solution evolves, the

approximations generally require fewer total elements to represent the solution at a high resolution.

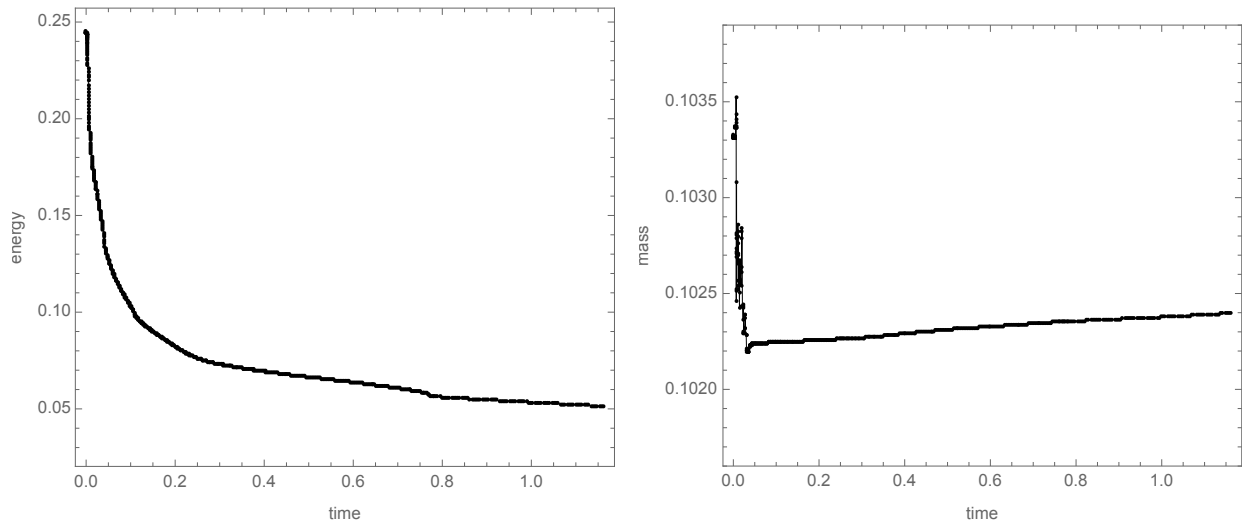


Figure 7. Evolution of $\mathcal{E}(u^h)$ and $\mathcal{M}(u^h)$ for Example 3.

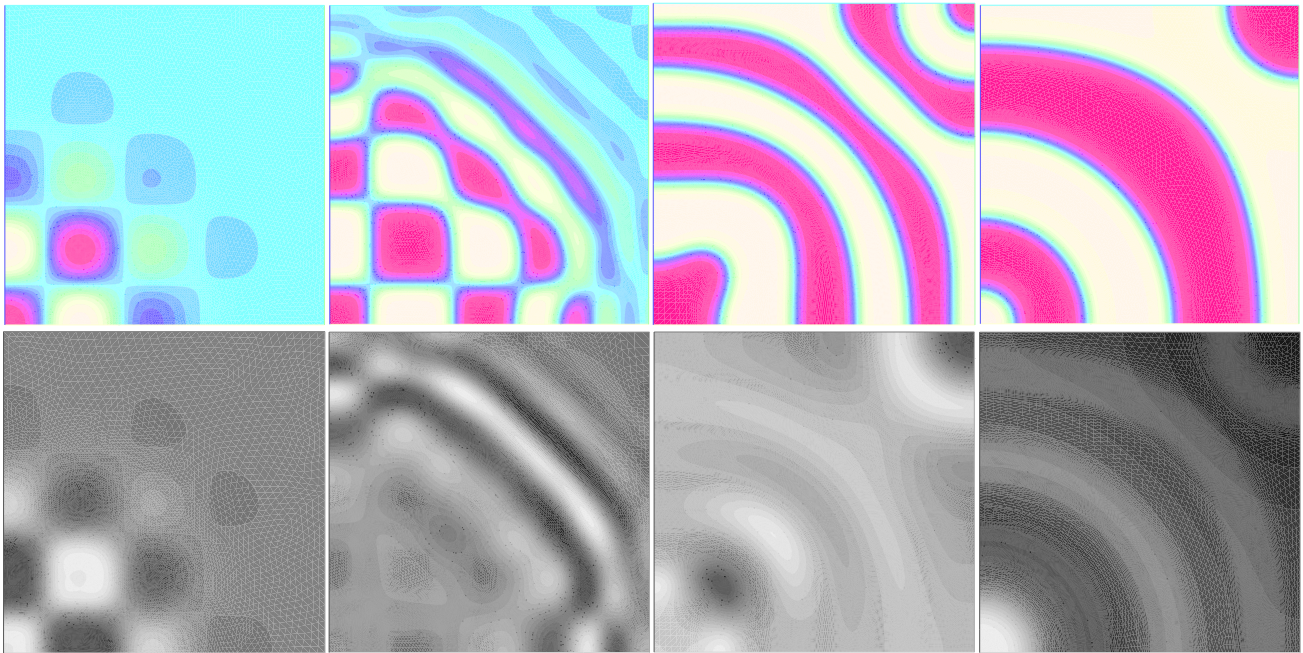


Figure 8. Solution plots for u^h and w^h at time steps 3, 50, 200 and 600 (corresp. times $t = 0.000430, 0.0108, 0.150$, and 1.31) for Example 4.

Figure 7 shows the evolution of the energy and mass of the approximations. As expected, the energy decreases across time. We observe that the mass has the most variation during the short initial coarsening phase, then remains more stable as coherent structures emerge. Additionally, we note that the energy and mass plots are shown in a linear time scale, while the plots in Figure 6 use a log scale for time to better distinguish adaptivity in the coarsening phase.

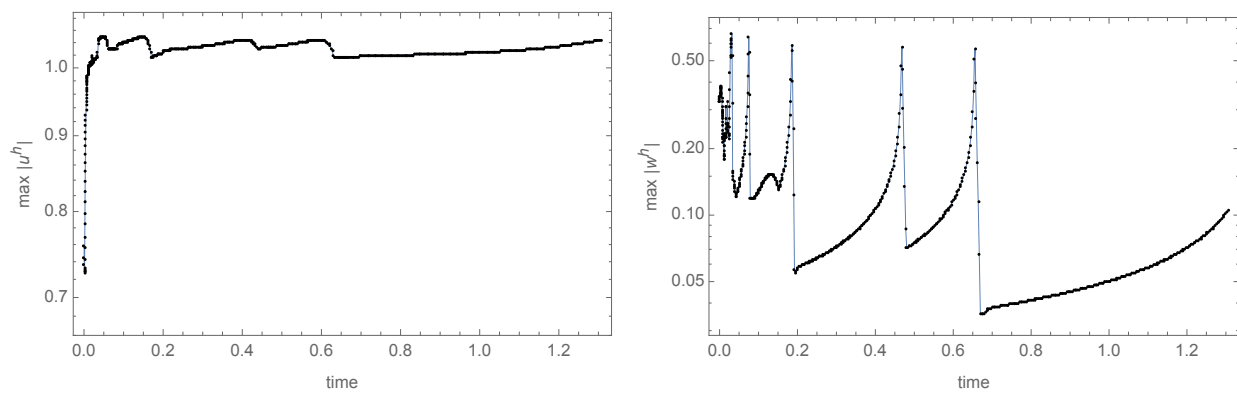


Figure 9. $\|u^h\|_\infty$ and $\|w^h\|_\infty$ vs. time for Example 4.

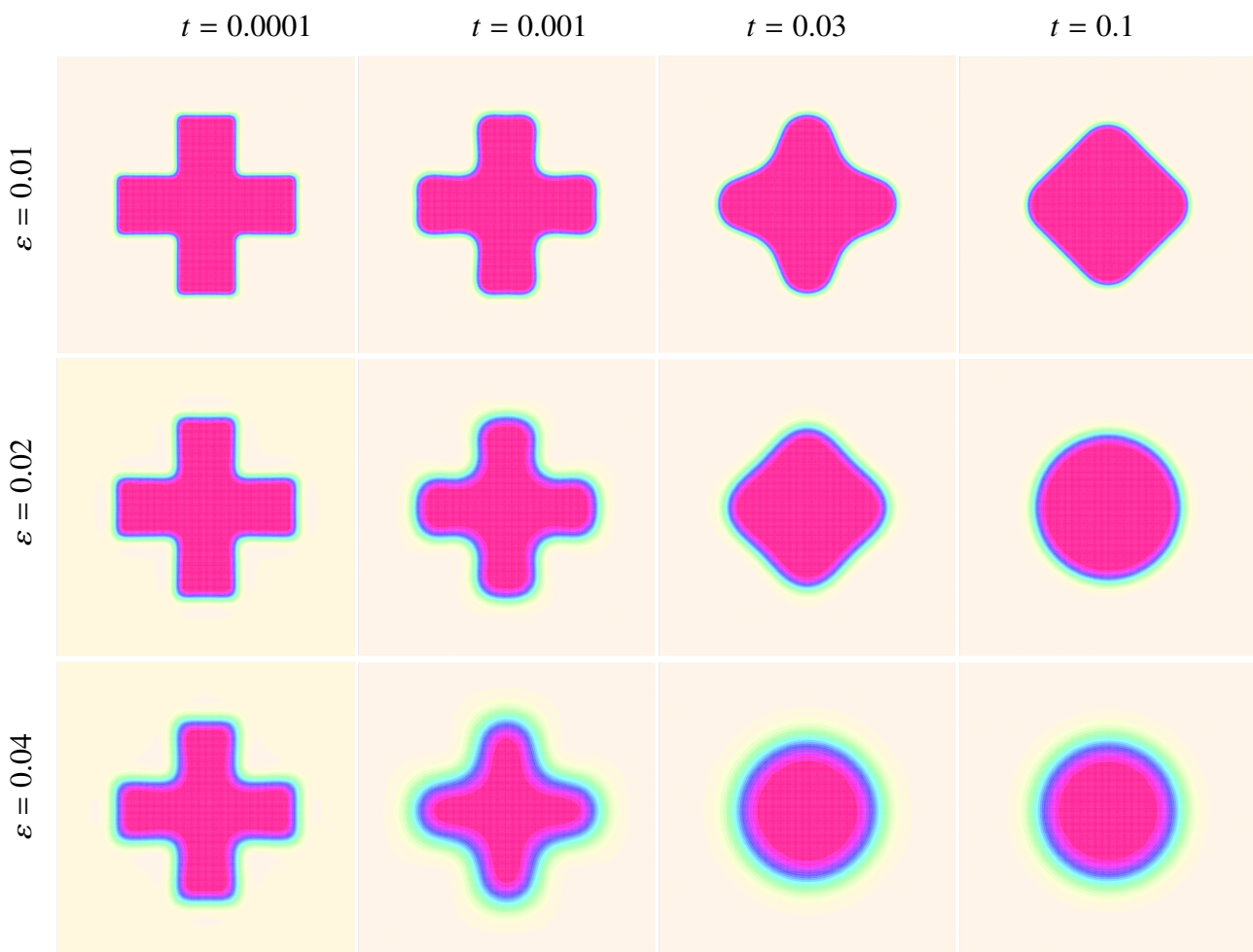


Figure 10. Solution plots for u^h at comparable times with different separation lengths ε for Example 5.

Example 4: Structured Coarsening. In this example, we show the evolution of an initial perturbation from zero and illustrate both the concentration u^h and the chemical potential w^h at corresponding

times. We use the following initial condition:

$$u(\mathbf{x}, 0) = \cos(4\pi x) \cos(4\pi y) \exp\left(-10((x - 1/8)^2 + (y - 1/8)^2)\right).$$

Figure 8 shows that as coherent structures develop, the variation in w^h corresponds to regions where u^h is most rapidly changing. Though not pictured, we also directly approximate solutions for the gradients of u and w , which may be of interest in applications.

In Figure 9, we plot the maximum magnitude of both u^h and w^h for Example 4. We see that $\|u^h\|_\infty$ remains bounded and slightly above 1, which corresponds to the potential component of the energy functional. Additionally, we see that $\|w^h\|_\infty$ significantly varies as the solution develops and structures coalesce.

Example 5: Solution Dynamics and Phase Separation Length. In this final example, we illustrate the solution dynamics of a common test problem (cf. [20, 21, 28]) for different values of the phase separation length parameter, ε . From the form of the Cahn-Hilliard equation (or the energy functional), it is expected that the natural time scale of the system will depend on ε . Figure 10 shows the effect of only changing ε , where all other parameters are the same as in the previous example. We can see the effective width of the interfacial region between phases as well as a much slower evolution for smaller values of ε .

7. Concluding remarks

In this work, we found compelling evidence that a least-squares formulation can provide a robust finite element approach for the Cahn-Hilliard equation. Our approach, based on a first-order system reformulation of the problem, led to a well-posed minimization at each step and allowed for the use of standard H^1 conforming finite element spaces. In this way, we avoided the difficulties of discretizing fourth-order derivatives and the challenges associated with a saddle-point formulation. The computational results confirmed the theory developed for this approach and showed the effectiveness of the iterative method for a range of test problems. Immediate extensions of the approach here include the use of a logarithmic potential function and nonlocal terms [6], and a formulation for multiphase flow problems.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Conflict of interest

The authors declare there is no conflict of interest.

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