Cahn-Hilliard on Surfaces: A Numerical Study

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Abstract
The Cahn-Hilliard system has been used to describe a wide number of phase separation processes, from co-polymer systems to lipid membranes. In this work the convergence properties of a closest-point based scheme is investigated. In place of solving the original fourth-order system directly, two coupled second-order systems are solved. The system is solved using an approximate Schur-decomposition as a preconditioner. The results indicate that with a sufficiently high-order time discretization the method only depends on the underlying spatial resolution.

Keywords: Cahn-Hilliard, Surface PDE, Finite Difference, Closest Point Method

1. Introduction
Phase field models are an important numerical technique for capturing the growth of micro-structures [1] and can be used to model various solidification processes such as that of a binary alloy [2]. Instead of explicitly tracking the solid-liquid interface, an order parameter is introduced that varies continuously over a thin transition layer, which approximates a sharp solid interface with a diffuse one. Using this approach, boundary conditions at the interface can be replaced by localized body-force terms, simplifying the conservation equations that govern the order parameter. Even though the term “phase field” was coined much later, the basic idea has been in existence since the 1800s when van der Waals studied fluid interfaces using a density field [3]. Phase field models have also been used to study many physical applications including defects [4], deformations [5], and the growth of dendrites [6]. A variety of numerical methods have been employed, including finite differences [7], finite elements [8], and spectral methods [9]. One well known conservative method to capture phase dynamics is the Cahn-Hilliard model. The original purpose of this model was to investigate the phase transition of binary alloys [10] and it has been used to model the phase dynamics of polymers and ceramics [11], thermo-capillary flows [12], the Rayleigh-Taylor instability [13], droplet breakup [14], liquid-liquid jets pinching off [15], multicomponent lipid vesicles [16], and for the tracking of tumor growth [17].

Solving the Cahn-Hilliard equation on a curved surface is a difficult task for a number of reasons. It is a fourth order partial differential equation which is numerically stiff, requiring small time steps for stability. In this work, the fourth-order PDE is split into a set of coupled second-order differential equations. The novelty of this work lies in the use of the Closest-Point method [18] and the associated numerical convergence analysis. This particular formulation of the closest point method was originally applied to second-order partial differential equations, while the splitting scheme here allows for the solution of fourth-order differential equations. Additionally, a qualitative spatial analysis is also shown to demonstrate that sufficient spatial resolution is required to capture all aspects of the dynamics.

$^\star$This work has been supported by the National Science Foundation through the Division of Chemical, Bioengineering, Environmental, and Transport Systems Grant #1253739.

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2. Governing Equations

Consider the boundary of a region, Γ, with an outward facing normal \( n \). The non-dimensional surface Cahn-Hilliard equations describe the temporal evolution of an order parameter \( f(x,t) \) on the surface Γ, where the evolution is driven by the gradient of the chemical potential,

\[
\frac{\partial f}{\partial t} = \frac{1}{\text{Pe}} \nabla_s \cdot (\nu \nabla_s \mu),
\]

(1)

where \( \nabla_s \) is the surface gradient operator, \( \nu \) is the mobility, and \( \text{Pe} \) is the surface Peclet number which relates the strength of any surface advection to diffusion. The chemical potential, \( \mu \), is the variational derivative of the surface free energy,

\[
E_s = \int_{\Gamma} \left( g(f) + \frac{C_n}{2} \| \nabla_s f \|^2 \right) \, dA,
\]

(2)

where \( g \) is often taken as a double well potential and \( C_n \) is the Cahn number, which indicates the strength of the energy penalty associated with surface boundaries. This results in the following expression for the chemical potential,

\[
\mu = \frac{dg}{df} - C_n \Delta_s f,
\]

(3)

where \( \Delta_s \) is the surface Laplacian operator. Using the chemical potential expression in Eq. (1) results in a fourth-order evolution equation for the phase field.

3. Numerical Methods

Assume that the mobility is constant and equal to 1 and that the equations are discretized on a standard Cartesian grid using finite difference approximations. Let the interface be described by a level set Jet scheme [19]. The Cahn-Hilliard system can be written as a pair of coupled, second-order differential equations [20, 21],

\[
\frac{\partial f}{\partial t} - \frac{1}{\text{Pe}} \Delta_s \mu = 0 \quad \text{and} \quad \mu + C_n^2 \Delta_s f = g'(f).
\]

(4)

Discretizing this in time the system can be written as

\[
\begin{bmatrix}
I & C_n^2 L_s \\
-\frac{\Delta t}{\text{Pe} \rho_0} L_s & I
\end{bmatrix}
\begin{bmatrix}
\mu^{n+1} \\
f^{n+1}
\end{bmatrix}
= \begin{bmatrix}
g'(\hat{f}) \\
-\frac{\gamma_0}{\beta_0} f^n - \frac{\gamma_2}{\beta_2} f^{n-1}
\end{bmatrix},
\]

(5)

where \( f^n \) and \( f^{n-1} \) are the solutions at times \( t^n \) and \( t^{n-1} \), respectively, with \( \Delta t = t^n - t^{n-1} \) a constant time step, and \( L_s \) is the discrete approximation to the surface Laplacian, \( \Delta_s \). The approximation to the solution at time \( t^{n+1} \) is given by \( \hat{f} \) and \( I \) is the identity matrix. A first-order backward-finite-difference (BDF1) scheme is given by \( \beta_0 = 1, \beta_1 = -1, \) and \( \beta_2 = 0 \) with \( \hat{f} = f^n \). A second-order backward-finite-difference (BDF2) scheme is given by \( \beta_0 = 3/2, \beta_1 = -2, \) and \( \beta_2 = 1/2 \) with \( \hat{f} = 2f^n - f^{n-1} \) [22].

The discretization of the surface Laplacian is performed using a version of the Closest-Point Method introduced by Chen and Macdonald [18]. The basic idea is to extend the solution away from the interface such that it is constant in the normal direction. With this extension, it is possible to write a surface differential equation as a standard differential equation in the embedding space. In this scheme points far from the interface do not need to be considered. Note that in situations where a grid point might be near multiple interfaces extension errors may be introduced, but for time-evolving interfaces, such as those undergoing pinch-off, this error will be temporary.

Let \( E_1 \) be a linear polynomial interpolation operator and \( E_3 \) be a cubic polynomial interpolation operator. For any point \( x \) not on the interface these operators return the value of a function at the interface point
closest to x. For example, the operation $E_3 f$ returns the value of $f$ at the point on the interface closest to $x$ using the cubic interpolation function. Using this notation, Eq. (5) is re-written as

$$
\begin{bmatrix}
  I \\
  -\frac{\Delta t}{\rho c_h^2} [E_1 L + \alpha(E_3 - I)]
\end{bmatrix}
\begin{bmatrix}
  \mu^{n+1} \\
  I
\end{bmatrix}
= 
\begin{bmatrix}
  g'(\hat{f}) \\
  -\frac{\beta_1}{\beta_2} f^n - \frac{\beta_2}{\beta_1} f^{n-1}
\end{bmatrix},
$$

(6)

with $\alpha = 6/h^2$ where $h$ is the uniform grid spacing and $L$ represents the Cartesian finite difference approximation to the standard Laplacian, $\Delta$. The addition of $\alpha$ term ensures that the solutions are constant in the normal direction. If this extension holds then surface operators can be replaced with standard Cartesian operators. See Chen and Macdonald for complete details [18].

The block system shown in Eq. (6) is solved using the preconditioned Flexible GMRES algorithm available in PETSc [23, 24, 25], where the preconditioner is an approximate Schur inverse. Let $L_E = E_1 L + \alpha (E_3 - I)$. The preconditioner is then

$$
P = 
\begin{bmatrix}
  I & -Cn^2 L_E \\
  0 & I
\end{bmatrix}
\begin{bmatrix}
  I & 0 \\
  0 & \hat{S}^{-1}
\end{bmatrix}
\begin{bmatrix}
  I & 0 \\
  0 & \frac{\Delta t}{\rho c_h^2} L_E
\end{bmatrix},
$$

(7)

with a Schur complement of $\hat{S} = I + Cn^2 \Delta t_{max} L_E L_E$, where $\Delta t_{max} = 10^{-2}$ is the maximum time-step considered here. The inverse of the Schur complement is calculated using an explicit LU-decomposition using MUMPS [26, 27]. Note that for a time step of $\Delta t = 10^{-2}$, this results in an exact method and the GMRES algorithm converges within one iteration. For smaller time steps the Schur complement is no longer exact and GMRES algorithm converges after two or three iterations. Additionally, for small Cahn numbers, say $Cn \sim 3h$, where $h$ is the grid spacing, the numerical stiffness of the system is greatly reduced, which might remove the need for such a preconditioner.

4. Results

First consider the quantitative convergence of the method by comparing to a higher-order scheme. Results here are presented on a unit sphere in a domain spanning $[-1.25, 1.25]^3$ with uniform grid spacing $h$ and fixed time step $\Delta t$. The initial condition is taken to be $\cos (\cosh (5xz) - 10y)$, where $(x, y, z)$ is a point on the sphere. The mixing energy is a simple double-well potential, $g(f) = (f^4)/4 - (f^2)/2$, while the parameters are set to $Cn = 0.1$ and $Pe = 1.0$. The reference solution is calculated via the spectral spherical operators in the Chebfun Matlab package using a uniform 2562 mesh [28] and LIRK4, which is a fourth-order accurate scheme, using a time step of $10^{-4}$ [29]. All $l_\infty$-errors are computed at a time of $t = 0.5$.

The errors for both the BDF1 and BDF2 schemes as a function of time step for various grid spacings are shown in Fig. 1. Several items become apparent from this figure. First, at large time steps both the
Figure 1: Time convergence results are presented for first and second order time schemes for different grid spacing. At lower time steps, error is independent of the time scheme used and is dominated by the grid size.

Figure 2: Evolution of the Cahn-Hilliard equation on a torus using a time step of $10^{-4}$ and varying grid sizes. The results do not qualitatively change when using a mesh size of $161^3$ or higher.
first-order and second-order schemes converge at the expected rate. Second, it is observed that for a given grid size at sufficiently small time steps the error becomes constant. In fact, both the first- and second-order in time schemes have the same error at small time steps.

This behavior can be explained by considering the expected error. Due to the interpolation operators this solver is similar to those used for semi-Lagrangian methods. In semi-Lagrangian methods the error obeys \( \epsilon \approx O(\Delta t^k) + O(h^l) + O(h^p/\Delta t) \), where \( k \) is the order of time discretization, \( l \) is the truncation error of the derivative approximations, and \( p \) is the truncation error of the interpolant [30]. As the time-discretization errors decrease for a fixed grid spacing the overall error should be dominated by the interpolation error, \( O(h^p/\Delta t) \). It is interesting to note that the error for this particular solution does not increase with decreasing time step, but remains constant. One possible explanation is that the closest point location does not change over the course of the current simulation, which could mean that the \( O(h^p/\Delta t) \) term is not present in the current error. Another possible explanation is that the time step simply has not become small enough for the effect to become evident.

The errors using \( \Delta t = 2.5 \times 10^{-6} \) with the BDF2 scheme are shown in Table 1. At this time step the error is dominated by the grid spacing. It is unknown why the convergence rate between the 129\(^3\) and 161\(^3\) grids is much lower than the other rates. Despite this, the spatial convergence is approximately second-order for both the phase field and chemical potential.

Next consider the qualitative convergence of the Cahn-Hilliard system. The Cahn-Hilliard system is solved on a torus with an inner radius of 0.5 and an outer radius of 1.5 on a grid which spans \([-1.75, 1.75]^3\]. The mixing energy in this case is \( g(f) = (f^4)/40 - (f^2)/20 \). To ensure that the initial condition is the same across all grid sizes, a random initial concentration which spans \([-0.41, -0.39]\) is created on the 97\(^3\) grid and is then interpolated using a spline interpolant to the finer meshes. In this case the time step is fixed at \( 10^{-4} \) and the BDF2 scheme is used. The other parameters in this study are \( Cn = 0.05 \) and \( Pe = 1.0 \). To ensure the conservation of the phase field over long simulation times the correction of Xu, Li, Lowengrub, and Zhao has been implemented [31].

The results for various times can be seen in Fig. 2. The initial homogeneous phase quickly segregates, as seen at \( t=0.2 \), into many separate circular domains. After segregation the domains start to slowly coarsen in time. The large domains grow larger in size at the expense of the smaller domains. From Fig. 2, it can be seen that the solution on the grid size of 97\(^3\) differs from the others. For example, at a time of \( t = 2 \), a domain which exists in the larger grids (in the lower-right corner of the figure) does not exist in the 97\(^3\) case. Additionally, only five visible domains exist at a time of \( t = 5 \) for the 97\(^3\) case, while six are seen in the other mesh sizes. From these results it appears that qualitative convergence is obtained for meshes larger than 161\(^3\). This indicates that sufficient spatial resolution is required to capture all aspects of the dynamics.

5. Conclusions

In this work the surface Cahn-Hilliard system is solved via a set of coupled second-order differential equations. The surface operators are discretized using the Closest-Point Method. To aid in the solution of the resulting linear systems, a Schur decomposition is used as a preconditioning matrix. For large time steps the method converges at a rate dependent on the time discretization method. At small time steps the error of the scheme becomes dominated by the spatial errors. Based on this result the second-order scheme was used to demonstrate qualitative convergence of the Cahn-Hilliard system on a torus with a random initial condition.

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