A VARIATIONAL CONSTRUCTION OF ANISOTROPIC MOBILITY IN PHASE-FIELD SIMULATION

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Abstract. In the phase-field modeling of the mesoscopic morphology and microstructure evolution in many material processes, an anisotropic mobility is often needed that depends on the interfacial normal direction. It is a challenge to define the anisotropic mobility function on the whole simulation domain while the interfacial normal can only be meaningfully determined on the interface. We propose a variational approach for the construction of a smoothed mobility function that mimics the prescribed anisotropic mobility on the interface and extends smoothly to the whole simulation domain. Some theoretical analysis of the proposed method are made to ensure its validity and to provide hints on the effects and the choices of various parameters. An iterative scheme for the numerical solution of the variational problem is also described. Several numerical tests are presented to illustrate the effect of a smoother anisotropic mobility on the interfacial dynamics, and the advantage over using a cutoff mobility.

1. Introduction. The Allen-Cahn equation \[ \frac{\partial \eta}{\partial t} = M(f(\eta) + \sigma^2 \Delta \eta) \] (1) is a key component in the diffuse interface theory used in the concurrent phase-field modeling of mesoscopic morphological and microstructure evolution. The phase-field method has been applied to a wide variety of important materials processes including solidification microstructures, solid state phase transformations, grain growth, surface growth, dislocation dynamics, crack propagation in amorphous solids and domain evolution in thin films, etc (see for example, [3, 4, 6, 8, 14, 15, 16, 18, 19, 25, 24]). Here, \( \eta \) is a long-range order parameter describing the phase of the material, \( M = M(x, t, \eta) > 0 \) is the mobility function, \( f = f(\eta) \) is the bulk free energy gradient, and the Laplacian term comes from the variation of the interface energy where \( \sigma^2 \) is a gradient energy coefficient. In the original Allen-Cahn equation, the mobility function is taken to be a constant. However, in many applications such as precipitate growth, dendritic solidification and grain growth [9, 12, 17, 20, 23], an anisotropic mobility function needs to be introduced that accounts for the dramatically different speeds at which the interfaces with different...
orientations migrate. The purpose of this paper is to develop a variational method for the construction of an anisotropic mobility that leads to more stable and faithful numerical simulation of such anisotropic interfacial dynamics.

While motivated by more complicated phase-field models for precipitate growth, for simplicity, we here only consider equation (1) with a double-well free energy density function $F = F(\eta)$ having two equilibrium phases given by $\eta = \pm 1$ so that $f(\eta) = -F'(\eta) = -\eta(\eta - 1)(\eta + 1)$. We focus on the stage of microstructure evolution where the system’s kinetics is dominated by interface motion. In other words, the order parameter $\eta$ is nearly at its equilibrium values $-1$ and $1$ almost everywhere except in thin interfacial regions (called the antiphase boundary) where $\eta$ takes intermediate values.

In [2], Allen and Cahn have analyzed the equilibrium profile and the motion of the antiphase boundary defined by the equation (1) with an isotropic constant mobility $M(x, t, \eta) \equiv M$. For example, they have shown that the interfacial thickness over which the normal derivative $\frac{\partial \eta}{\partial n}$ differs appreciably from zero is proportional to $\sigma$, and it can be easily inferred from their analysis that the equilibrium profile of a planar antiphase boundary is given by a tanh function of the signed distance normal to the interface. As for the dynamics of the interface, they have shown that in the limit of thin interface, i.e. when the principle radius of curvature is much greater than the interfacial thickness, all iso-$\eta$ contours move with the same normal speed given by

$$V = M \sigma^2 \kappa$$

where $\kappa$ is the interfacial curvature. The direction of the interface motion is such that the total interfacial energy is reduced.

While limited to an isotropic constant mobility, the results of Allen and Cahn nevertheless provide intuitive guidelines for devising anisotropic mobility functions on the whole computational domain. To facilitate a concrete discussion, we consider the $m$-fold anisotropic mobility function $M_0 = a + b \cos(m\Theta)$, which is related to crystallographic symmetry of the underlying materials and is often used in modeling microstructure evolution to test the effects of mobility anisotropy (for example [17]). Here, $\Theta$ is the angle of the normal vector to the interface, i.e. $(\cos \Theta, \sin \Theta) = \nabla \eta / |\nabla \eta|$. Due to the degeneracy of $\nabla \eta$ away from the antiphase boundary, the function $M_0$ is only meaningfully defined on the interface where $|\nabla \eta|$ differs appreciably from zero. However, the setup of the Allen-Cahn equation (1) requires mobility throughout the simulation domain. Note that the physical mobility far away from the interface is not well defined, since in the bulk, the free energy is assumed to be constant, and there is therefore no driving force. Consequently, whatever mobility we apply away from the interface will not affect the physics of the underlying problem but it does affect the numerical solution of the phase field models. The challenge of how to extend the anisotropic mobility away from the interface in the phase field simulation is a major issue we are trying to address in this paper.

For convenience of the following discussion, in the rest of the paper, we reserve the symbol $M$ for the smoothened mobility generated by a variational principle to be proposed later. The function $M_0$ is called the raw mobility function. Since in practical computation, the raw mobility function often exhibit spurious noise away from the interface, a natural alternative often used in practice is the cutoff mobility
For $M_0 = a + b \cos(m\Theta)$, the associated cutoff mobility can be defined as

$$M_c = \begin{cases} a + b \cos(m\Theta) & \text{wherever } |\eta| < 1 - \delta_c, \\ a & \text{otherwise} \end{cases}$$

where $\delta_c > 0$ is a user-defined parameter.

What are the desirable features of the mobility function $M$? Firstly, it is clear that we would like it to be close to the prescribed mobility function $M_0$ on the interface. However, since the order parameter $\eta$ is nearly at equilibrium away from the interface, intuitively, we have quite large freedom to assign values to $M$ there to satisfy certain smoothness properties, and to ensure that at the same time the interfacial dynamics is essentially unchanged. To take advantage of this liberty is a distinct feature of our variational method as opposed to assigning a rather arbitrary constant in the cutoff mobility method. Secondly, we would like $M$ to vary only slightly across the interface in the normal direction. This feature is entailed by the asymptotic result in (2), and ensures that the interfacial profile is maintained as all the iso-$\eta$ contours migrate with the normal speed proportional to the mobility $M$.

We point out that a similar issue arises in modeling sharp interface motion using the level-set method [21, 22]. In the level-set formulation, the velocity is required on the whole simulation domain (or at least on a narrow band around the interface), whereas in many applications only the normal velocity of the interface is available. To maintain the signed distance function, it is desirable to extrapolate the velocity function to make it nearly a constant across the normal direction (see for example [21] for the techniques to achieve this). This is feasible in the level-set formulation largely due to the nature of the level-set function, namely, the level-set function is usually kept close to a signed distance function, which renders the determination of the normal directions even away from the interface a trivial task. Unfortunately, the normal directions away from the interface cannot be conveniently evaluated in the phase-field simulation, which motivates the next desirable feature of the mobility function. Thirdly, we would like $\nabla M$ (the full gradient instead of the normal derivative) to be relatively small away from the interface, in a sense that will become clear in our variational formulation. In contrast to the cutoff mobility, the second and third features incorporate the idea of a smoothly varying mobility function throughout the computational domain. And theoretically speaking, the higher regularity of the mobility function facilitates more accurate numerical approximation to the Allen-Cahn equation by, for example, the Fourier-spectral method.

Taking the above considerations into account, we propose in section 2 a variational principle whose minimizer is used as the smoothened mobility function. The well-posedness of the variational formulation, and the regularity and maximum principle of the solution to the Euler-Lagrange equation are then established. Without loss of generality, much of our discussion is limited to the equation (1) defined on a 2D square $\Omega = [0,1] \times [0,1]$ with the periodic boundary condition, as we are primarily interested in modeling the interfacial dynamics in the bulk of the material. The extension to the three dimensional case is readily available. To understand further the behavior of the smoothened mobility function, the solution to the Euler-Lagrange equation is analyzed for a circular interface in section 3. In particular, the questions of interest are whether the variational principle generates an undesirable sharp boundary or interior transition layer for the mobility function, and how the coefficients of the variational principle affect the potential damping of the mobility anisotropy. An algorithmic description of the proposed construction
along with the semi-implicit Fourier-spectral approximation of the equation (1) is presented in section 4, including the discussion on an iterative scheme to numerically solve the Euler-Lagrange equation. Finally in section 5, we present several numerical tests in order to illustrate the effect of the smoothened mobility on numerical simulation of the interfacial dynamics and the advantage of the smoothened mobility over cutoff mobility.

2. Variational Principle Formulation. Motivated by the above, we propose to construct a smoothened mobility function $M$ from a variational problem at any time $t > 0$:

$$
\min_{\Omega} \int_{\Omega} \alpha(x)|M - M_0|^2 + \beta(x)(\nabla M \cdot \frac{\nabla \eta}{|\nabla \eta|})^2 + \gamma(x)|\nabla M|^2 dx
$$

(4)

where $M_0$ is a prescribed raw mobility function. Here and also in the next section, for notational convenience, we drop the explicit dependence on the time variable, and simply use $M = M(x)$ to denote the constructed mobility function at time $t$. Similar convention is used for other functions $M_0, \alpha, \beta, \gamma$ and $\eta$ as well unless specified otherwise.

The first term in the energy functional (4) accounts for the requirement that the smoothened mobility stays close to the raw mobility on the interface, the second term is aimed at damping the variation of the mobility in the normal direction of the interface, and the purpose of the third term is to damp the overall oscillation away from the interface. The nonnegative user-defined parameters $\alpha = \alpha(x)$ and $\beta = \beta(x)$ are taken to be concentrated on the interface, while $\gamma = \gamma(x)$ on the contrary is taken to be concentrated away from the interface. In particular, as $\eta$ varies in $[-1, 1]$, we use the following forms for $\alpha(x), \beta(x),$ and $\gamma(x)$ in this paper,

$$
\alpha = c(x)(1 - \eta^2),
$$

(5)

$$
\beta = \mu(1 - \eta^2),
$$

(6)

$$
\gamma = \mu \eta^2.
$$

(7)

Here, $c = c(x)$ may be taken as a constant or a spatially varying function depending on the local curvature of the interface (more details are given later). The smoothing constant $\mu$ is an important parameter that controls the relative strength of the smoothing effect as compared with the intention for $M$ to faithfully reproduce the raw mobility $M_0$ on the interface. We will study its effect in conjunction with other parameters of the interface extensively in later sections.

In the sequel, for each Sobolev space $H(\Omega)$, we denote by $\bar{H}(\Omega)$ the subspace of $H(\Omega)$ whose components satisfy the periodic boundary condition which may be defined either as the closure of smooth periodic functions in the corresponding spaces or as the set of functions with their periodic extensions on a larger domain, say $(0, 2)^2$, belonging to $H((0, 2)^2)$. We let $H(\Omega)$ be equipped with the same norm as $H(\Omega)$. The well-posedness of a regularized variational problem is established in the following simple lemma.

**Lemma 1.** Given constants $\epsilon_1, \epsilon_2 \geq 0$, and $\eta \in H^1(\Omega)$, $\alpha, \beta, \gamma, M_0 \in L^\infty(\Omega)$ with $\alpha, \beta, \gamma \geq 0$. Assume further that the set $\{x : \alpha(x) \neq 0\}$ has a nonzero measure, then the following regularized version of the variational problem (4):

$$
\min_{\bar{H}(\Omega)} E_\epsilon(M) := \int_{\Omega} \alpha(x)|M - M_0|^2 + \beta(x)(\nabla M \cdot \frac{\nabla \eta}{|\nabla \eta| + \epsilon_1})^2 + (\gamma(x) + \epsilon_2)|\nabla M|^2 dx
$$

(8)

where the minimization is over all functions in $H^1(\Omega)$, has a unique minimizer.
The continuity of $E_e$ in $\tilde{H}^1(\Omega)$ is obvious, under the assumptions on the parameters. The key to the existence proof is to establish the coercivity condition on $E_e$, and the rest of the proof is a trivial exercise of the variational calculus.

Note that the set $\{x : \alpha(x) \neq 0\}$ has a nonzero measure, there exists a constant $\delta > 0$, such that the measure of $\{x : \alpha(x) \geq \delta\}$ is strictly positive. Let $\Omega_0 = \{x : \alpha(x) \geq \delta\}$. It follows that

$$E_e(M) \geq \delta \int_{\Omega_0} M^2 dx + \epsilon_2 \int_{\Omega} |\nabla M|^2 dx - C_0$$

with some constant $C_0$, independent of $M$ and $\epsilon$. It is easy to establish the inequality

$$\delta \int_{\Omega_0} M^2 dx + \epsilon_2 \int_{\Omega} |\nabla M|^2 dx \geq C \int_{\Omega} M^2 dx \quad \forall M \in \tilde{H}^1(\Omega).$$

The coercivity of $E_e$ then follows. The proof of uniqueness is a consequence of the convexity of the energy functional $E_e(M)$.

To determine the unique minimizer of the convex functional $E_e$ is equivalent to solving its corresponding Euler-Lagrange equation,

$$\nabla \cdot [(A + \epsilon_2 I) \nabla M] = \alpha(x)(M - M_0)$$

where $I$ is the identity matrix, and the $2 \times 2$ matrix $A$ is given by

$$A = \beta(x) \frac{\nabla \eta}{|\nabla \eta| + \epsilon_1} \otimes \frac{\nabla \eta}{|\nabla \eta| + \epsilon_1} + \gamma(x).$$

An iterative scheme to numerically solve this equation based on the Fourier-spectral method will be described in section 3. Here we make a comment that in practice, $\epsilon_1$ can be taken to be the smallest number allowed by machine precision, and we take $\epsilon_2$ to be one tenth of the smoothing constant $\mu$ as used in (6) and (7).

Utilizing the Euler-Lagrange equation (11), one may further improve the regularity of the minimizer from $\tilde{H}^1$ to $\tilde{H}^2$ with reasonable assumptions on the data. More specifically, invoking standard elliptic regularity argument, we may verify the following result:

**Lemma 2.** Assume that the entries of the matrix $A$ in (12) are Lipschitz continuous on $\Omega$ satisfying the periodic boundary condition, and that $M_0, \alpha \in L^\infty(\Omega)$. Then, the solution $M = M(x)$ to (11) is in $\tilde{H}^2(\Omega)$.

We next show that the smoothened mobility $M = M(x)$ is bounded by the lower and upper bounds of the raw mobility function $M_0(x)$. Since the coefficient $\alpha = \alpha(x)$ may be degenerate and the straightforward maximum principle argument gives no control over the extrema of $M(x)$ where $\alpha(x) = 0$, we present, instead, an argument based on regularizing the coefficient $\alpha$. This, as expected, allows us to take advantage of the assumption that the set $\{x : \alpha(x) \neq 0\}$ has nonzero measure. Here, we pursue the maximum principle for the classical solution of (11). The maximum principle for the weak solution may be established via mollifying the coefficients $A$, $\alpha(x)$ and $M_0(x)$.

**Lemma 3.** In addition to the hypotheses in Lemma 1 and Lemma 2, we further assume that the data of the Euler-Lagrange equation (11) are such that the solution $M(x)$ is in $C^2(\Omega)$ satisfying the periodic boundary condition. We have

$$\min_{x \in \Omega} M_0(x) \leq M(x) \leq \max_{x \in \Omega} M_0(x), \quad \forall x \in \Omega.$$  

(13)
We consider the regularized equation,
\[
\nabla \cdot [(A + \varepsilon_2 I)\nabla M_\xi] = (\alpha(x) + \xi)(M - M_0)
\]
(14)
for a positive constant \(\xi\). By the assumptions, (14) has a solution \(M_\xi \in C^2(\bar{\Omega})\) satisfying the periodic boundary condition. Suppose \(M_\xi\) attains its absolute maximum at \(x_0\). Thanks to the positive definiteness of \((A + \varepsilon_2 I)\), we have
\[
\nabla \cdot [(A + \varepsilon_2 I)\nabla M]_{x_0} \leq 0.
\]
Hence, the right-hand side of (14) is non-positive, which implies that \(M_\xi(x_0) \leq \max_{x \in \Omega} M_0(x)\). The lower bound \(M_\xi(x_0) \geq \min_{x \in \Omega} M_0(x)\) can be derived analogously.

Next, we seek to pass to the limit as \(\xi \to 0\). Denote by \(\mathcal{E}_{e,\xi} = \mathcal{E}_{e,\xi}(M)\) the modified energy functional by adding \(\xi\) to \(\alpha(x)\) in (8). Since \(M_\xi\)'s are minimizers of \(\mathcal{E}_{e,\xi}\), it is obvious that \(\mathcal{E}_{e,\xi}(M_\xi)\) and thus \(\mathcal{E}_{\xi}(M_\xi)\) are uniformly bounded as \(\xi \to 0\).

By the coercivity of \(\mathcal{E}_{e}\) (which relies on the hypothesis that \(\{x : \alpha(x) > 0\}\) has a nonzero measure), the sequence \(M_\xi\) is uniformly bounded in \(H^2(\Omega)\) as \(\xi \to 0\). Applying the standard elliptic regularity result, we have that \(M_\xi\)'s are uniformly bounded in \(H^2(\Omega)\). Hence, there exists a subsequence of \(M_\xi\), still denoted by \(M_\xi\), that converges weakly in \(H^2(\Omega)\) to \(M = M(x)\), the solution to (11). Finally, by compact embedding of \(H^2\) into \(C^0\) in 2D, and the pointwise bound on \(M_\xi\), we get \(\min_{x \in \Omega} M_0(x) \leq M(x) \leq \max_{x \in \Omega} M_0(x)\) in \(\Omega\).

With the upper and lower bounds on the constructed mobility function and a smooth initial data, one can apply a boot-strapping argument to verify the well-posedness of the Allen–Cahn equation (11) corresponding to the anisotropic mobility function. Further regularity results on the solution of equation (11) can also be obtained. The detailed are not pursued here, but it can be expected that the time dependent solution remains smooth, thus, the Fourier-spectral spatial discretization becomes readily applicable. The algorithmic descriptions are given in section 4.

3. Analysis for a Circular Interface. We now analyze the solution \(M = M(x)\) to the Euler-Lagrange equation when the order parameter \(\eta = \eta(x)\) defines a circular interface. This simple case enables us to gain some insight on the profile of the smoothened mobility, and also to discover a damping effect that may potentially weaken the prescribed mobility anisotropy.

3.1. Precluding boundary layers. Denote the polar coordinates by \((r, \theta)\). Suppose the order parameter is given by a \(\tanh\) function of \(r\),
\[
\eta = \tanh\left(\frac{r - r_0}{\varepsilon}\right)
\]
(15)
where \(r_0\) indicates the location of the zero-contour of the order parameter \(\eta\). And the constant \(\varepsilon\), with a different meaning from the previous section, is a positive parameter proportional to the thickness of the diffuse interface. In relation to the Allen-Cahn equation (1), \(\varepsilon\) is normally on the order of \(\sigma\).

Since the order parameter is assumed to be only a function of \(r\), we get the normal vector \(\nabla \eta / |\nabla \eta| = (\cos \theta, \sin \theta)\). We are interested in solving the Euler-Lagrange equation (11) on a ring with inner radius \(r_1 < r_0\) and the outer radius \(r_2 > r_0\). The radii are chosen so that the domain boundaries are far away from the interface. Notice that if the raw mobility function \(M_0\) is a constant, then the Euler-Lagrange equation has a trivial constant solution. Therefore, we only need to analyze the anisotropic part the mobility functions, which we denote by \(\tilde{M}_0\),

Proof. We consider the regularized equation,
and $\tilde{M}$. We may assume that $\tilde{M}$ is nearly zero far from the interface, and thus we impose the convenient Dirichlet boundary condition, $\tilde{M}(r_1, \theta) = M(r_2, \theta) = 0$ (instead of adopting the periodic boundary condition as in the earlier sections). For the moment, we ignore the regularization factors $\epsilon_1$ and $\epsilon_2$ in (11). We analyze the Euler-Lagrange equation when the coefficients $\alpha$, $\beta$ and $\gamma$ take the forms (5), (6) and (7), and set $c(x) \equiv 1$ in (5).

In the polar coordinates, it is straightforward to check that

$$\nabla \cdot \left[ \beta \frac{\nabla \eta}{|\nabla \eta|} \otimes \frac{\nabla \eta}{|\nabla \eta|} \right] \nabla \tilde{M} = \frac{\partial}{\partial r} \left( \beta \frac{\partial \tilde{M}}{\partial r} \right) + \frac{\beta}{r} \frac{\partial \tilde{M}}{\partial r}$$

(16)

and

$$\nabla \cdot (\gamma \nabla \tilde{M}) = \frac{\partial}{\partial r} \left( \gamma \frac{\partial \tilde{M}}{\partial r} \right) + \frac{\gamma}{r} \frac{\partial \tilde{M}}{\partial r} + \frac{\gamma}{r^2} \frac{\partial^2 \tilde{M}}{\partial \theta^2}$$

(17)

Adding these up and using (5), (6) and (7), the Euler-Lagrange equation (11) has the following special form on a ring domain:

$$\mu \frac{d^2 \tilde{M}}{dr^2} + \mu \frac{d \tilde{M}}{dr} + \frac{\mu \eta^2}{r^2} \frac{\partial^2 \tilde{M}}{\partial \theta^2} = (1 - \eta^2)(\tilde{M} - \tilde{M}_0).$$

(18)

Let us now consider the $m$-fold anisotropic mobility $\tilde{M}_0 = \cos(m \theta)$ mentioned in the Introduction. The equation (18) can then be reduced to an ordinary differential equation by taking the ansatz $\tilde{M}(r, \theta) = \tilde{M}(r) \cos(m \theta)$:

$$\mu \frac{d^2 \tilde{M}}{dr^2} + \mu \frac{d \tilde{M}}{dr} - (1 - \eta^2 + \frac{\mu \eta^2 m^2}{r^2})\tilde{M} = -(1 - \eta^2)$$

(19)

with the boundary conditions $\tilde{M}(r_1) = \tilde{M}(r_2) = 0$. The ansatz implies that the anisotropy is damped uniformly in all directions.

To explore whether $\tilde{M}(r)$ possesses an undesirable sharp transition layer, we first investigate an idealized case that $\eta$ takes a special form of a step function:

$$\eta(r) = \begin{cases} 
-1 & \text{for } r_1 < r < r_0 - 2\epsilon, \\
0 & \text{for } r_0 - 2\epsilon < r < r_0 + 2\epsilon, \\
1 & \text{for } r_0 + 2\epsilon < r < r_2.
\end{cases}$$

We can then find a piecewise smooth solution $\tilde{M}(r)$ in $C^0(r_1, r_2)$ that satisfies (19) in the distribution sense,

$$\tilde{M}(r) = \begin{cases} 
a_1 r^m + b_1 r^{-m} & \text{for } r_1 < r < r_0 - 2\epsilon \\
1 & \text{for } r_0 - 2\epsilon < r < r_0 + 2\epsilon \\
a_2 r^m + b_2 r^{-m} & \text{for } r_0 + 2\epsilon < r < r_2
\end{cases}$$

(20)

where the constants $a_1$, $a_2$, $a_3$ and $a_4$ can be easily determined from the boundary condition and the continuity of $\tilde{M}(r)$. It is remarkable that the powers in this function are independent of the thickness of the interface, and for moderate values of $m$, there exist no boundary or interior layers over which the values of $\tilde{M}(r)$ experience a sharp transition.

3.2. The problem of damping. Next, we consider the solution to (19) with a more realistic order parameter $\eta$ given by (15). Our major goal is to investigate the interplay of the smoothing parameter and the other physical parameters of the interface such as its width and radius, and their combined effects on the solution to (19).

Since the equation is no longer explicitly solvable in this case, we present a numerical solution obtained by the MATLAB ODE solver, with the following parameters
\( m = 2, r_1 = 0.2, r_2 = 3, r_0 = 1.65, \epsilon = 0.025, \) and \( \mu = 0.0005. \) Figure 1 shows the numerical solution (the smooth curve) in comparison with our analytic expression given in (20). We see that idealizing \( \eta \) as a step function does capture the shape of \( \bar{M}(r) \) away from the interface especially in light of \( \tilde{M}(r) \) showing no sign of sharp boundary or interior layers.

![Figure 1. Solution to (19) with \( \eta \) in (15) versus formula (20).](image)

Meanwhile, notice that the maximum of the smooth solution is slightly less than 1, indicating that the anisotropic mobility on the interface is slightly less than the desired level. In fact, this damping effect becomes more severe as a larger \( \mu \) is chosen, and will sometimes affect the dynamics of the phase-field simulation dramatically. So, this raises another interesting and practically important question on how small \( \mu \) should be chosen relative to the other physical parameters of the interface in order to minimize the damping effect. We next present a rough asymptotic analysis to illuminate the origin of damping and the proper choice of \( \mu. \)

In (19), we take \( r = r_0 \) so that \( \eta \) vanishes, and we assume the maximum of \( \tilde{M}(r) \) occurs at \( r_0 \) so that its first derivative vanishes. The equation (19) then becomes

\[ \tilde{M}(r_0) = 1 + \mu \tilde{M}''(r_0). \]

Assuming \( r_1 \) is close to 0, we now estimate asymptotically the amount of damping \( -\mu \tilde{M}''(r_0) \) (since \( \tilde{M}''(r_0) \) is positive) as \( r_0 \) and \( \epsilon \) become small. The second order derivative can be approximated as \( -(\tilde{M}'(r_0 - 2\epsilon) - \tilde{M}'(r_0 + 2\epsilon))/(4\epsilon) \). Moreover, as the radius of the interface \( r_0 \) becomes smaller, \( \tilde{M}'(r_0 - 2\epsilon) \) can be estimated, with the aid of (20), to be proportional to \( 1/r_0 \). Since \( \tilde{M}'(r_0 + 2\epsilon) \) stays bounded as \( r_0 \) becomes small, we have that the amount of damping \( -\mu \tilde{M}''(r_0) \) is asymptotic to \( \mu/(r_0\epsilon) \). Hence, to keep the damping effect small, the following choice is recommended:

\[ \mu = o(\kappa/\epsilon) \tag{21} \]

where \( \kappa = 1/r_0 \) is the curvature of the interface and \( \epsilon \), as stated before, measures the thickness of the interface.

In actual phase-field simulation, the local curvature and the width of the interface may be inhomogeneous in space, and therefore it is sometimes a disadvantage to
use a spatially uniform-valued \( \mu \). Although it is much more involved to devise a spatially varying \( \mu \) based only on the local information of the interface, the same goal can be achieved via a modification of the coefficient \( c \) in (5) which only needs to be defined on the interface. After all, it is the ratio of \( \alpha \) and \( \mu \) that determines the strength of the smoothing terms in the variational principle. We will present later a numerical test for which using a spatially uniform \( c = 1 \) leads to a serious damping problem, while using a spatially varying and local curvature dependent \( c \) of the form:

\[
c = 1 + |\n \cdot (\frac{\n \cdot \eta}{|\n \cdot \eta|})|
\]

will largely alleviate the problem of damping. The second term on the right-hand side of (22) measures the interfacial curvature. Due to the possible degeneracy of \( \n \cdot \eta \) away from the interface, (22) is only applied where \( \eta \) differs appreciably from \( \pm 1 \), and elsewhere \( c(x) \) is still taken to be 1.

4. Description of Algorithms. We first give a brief description of the semi-implicit Fourier-spectral method in [5, 26] used to numerically solve the Allen-Cahn equation, and then propose the coupling with an iterative scheme to solve the Euler-Lagrange equation (11).

The advantage of the semi-implicit Fourier-spectral method lies in its high accuracy in space than conventional finite-difference methods for smooth solutions, and its better stability for time integration in allowing larger time steps than fully explicit time stepping procedures. Let us first describe the method for the Allen-Cahn equation with an isotropic mobility \( M \equiv \text{const.} \) Let \( \tau \) denote the time step size and \( \eta^0 \) be the approximation of the initial condition. In the semi-implicit Fourier-spectral method, the Laplacian term on the right-hand side of (1) is treated implicitly, whereas the remaining non-linear term is treated explicitly. For \( n \geq 0 \), the resulting discrete-in-time equation at time \( (n+1)\tau \)

\[
\eta^{n+1} = \eta^n + \tau [M(f(\eta^n) + \sigma^2 \Delta \eta^{n+1})]
\]

(23)
can be solved in the Fourier space via FFT without the need for solving linear systems. Denoting the (discrete) Fourier transform of \( \eta^n(x) \) by \( \tilde{\eta}^n(\xi) \), and the Fourier transform of \( f(\eta^n) \) by \( \{f(\eta^n)\}_{\xi} \), the above equation in the Fourier space reads

\[
(1 + \tau M\sigma^2 \xi^2)\tilde{\eta}^{n+1}(\xi) = \tilde{\eta}^n(\xi) + \tau \{Mf(\eta^n)\}_{\xi}
\]

(24)

One may determine \( \tilde{\eta}^{n+1} \) based on the previous value \( \tilde{\eta}^n(\xi) \). And the actual values of the order parameter \( \eta^{n+1} \) can then be recovered from \( \tilde{\eta}^{n+1} \) via the inverse Fourier transform.

In case of an anisotropic mobility function \( M = M(x, t, \eta) \), the treatment of the Laplacian term in the above description needs to be slightly modified to deal with the variable coefficient \( M \) of the Laplacian term. A standard approach is to split a major constant component from \( M(x, t, \eta) \) and treat only this constant multiple of \( \Delta \eta \) implicitly. In case of a two-fold mobility function \( M = a + b \cos(2\Theta) \) where \( a > b > 0 \), which we use in all our numerical tests, the splitting strategy amounts to solving

\[
(1 + \tau a \sigma^2 \xi^2)\tilde{\eta}^{n+1}(\xi) = \tilde{\eta}^n(\xi) + \tau \{M^n f(\eta^n)\}_{\xi} + \tau \{(M^n - a) \Delta \eta^n\}_{\xi}
\]

(25)

We note that it is possible to introduce a splitting of the nonlinear term so that the time integration can be more stable in case that the coefficient \( \sigma \) is small.
In [10, 11], some higher order integration schemes with similar advantages of the semi-implicit scheme have also been presented for the equation (1) with a constant isotropic mobility, their generalizations to the case corresponding to anisotropic mobility can also be made. We leave them to our future work.

Given a time discretization of the equation (1), it is obviously important that the time-dependent mobility can be efficiently updated. We next propose an iterative scheme to numerically solve the Euler-Lagrange equation (11), similar to the above splitting strategy. More specifically, we wish to control the differential operator on the left-hand side of (11) by $(\mu + \epsilon_2)\Delta$ (recall that $\beta + \gamma = 1$), and we use $\bar{\alpha}M$, where $\bar{\alpha} = \bar{\alpha}_{n+1}$ is an upper bound of $\alpha_{n+1}(x)$, to control the term $\alpha M$ on the right-hand side.

At a particular time $(n + 1)\tau$, let $M^{0} = M^n$ be the mobility at the previous time step, and $M_0$ be the raw mobility at the given time. Thus, with the mobility function at the $m$th iteration be given by $M^{(m)}$, the iterative scheme computes $M^{(m+1)}$ via

$$[(\mu + \epsilon_2) \Delta - \bar{\alpha}]M^{(m+1)} = -\nabla \cdot [(A - \mu I)\nabla M^{(m)}]$$

$$+ \alpha(M^{(m)} - M_0) - \bar{\alpha}M^{(m)}$$

where $A$ is defined in (12). Since the differential operator on the left-hand side of the above equation is of constant coefficient, the equation can be readily solved using FFT as in the semi-implicit Fourier-spectral method. For analysis of a similar iterative technique for treating inhomogeneous elasticity in the phase field models, we refer to a recent work [25].

In addition to exploiting Fourier-spectral method, another advantage of the proposed scheme lies in its iterative structure. When the order parameter $\eta$ evolves in time in a phase-field simulation, the coefficients of the Euler-Lagrange equation change in time as well. As the evolution gradually takes place, we expect the solution to the Euler-Lagrange equation at a new time step to only differ slightly from its value in the previous time step. The iterative scheme is well suited to this situation, in that the final iterate from the previous time step can be taken as the initial iterate for (26) at the current time. We note that the iterative scheme may also be viewed as a discrete version of the gradient flow to the energy (8).

Adopting this strategy, we now summarize the numerical algorithm of simulating the Allen-Cahn equation with the smoothened mobility obtained from solving the Euler-Lagrange equation by the proposed iterative scheme. Given the order parameter $\eta^n$ and the smoothened mobility $M^n$ at time $n\tau$, we follow the steps,

1. Update $\eta^{n+1}$ using the semi-implicit Fourier-spectral scheme (24). The mobility used in this equation is taken to be $M^n$.
2. Taking $M^n$ as the initial iterate of the scheme (26). Obtain $M^{n+1}$ by a total of $N$ iterations, where $N$ is a user-defined parameter.

In all the numerical tests presented, we choose $N = 5$. For the initial time step, there is no smoothened mobility function available from previous time steps. In this case, the initial iterate is simply taken to be constant (for example, we take constant $a$ if the raw mobility is $M_0 = a + b \cos(2\Theta)$), and a large number of iterations are performed to ensure the convergence of (26) for the initial time step.

5. Numerical Results. In this section, we present several test problems of the phase-field simulation using the smoothened mobility function in comparison with results by using the cutoff mobility.
The purpose of the first test problem is to illustrate the smooth profile of the mobility function generated from the variational principle and its evolution during an actual phase-field simulation. The point of the second test problem is to illustrate the problem of damping and its remedy by using a spatially varying $c(x)$ in (5). The final test problem gives an example in which using the cutoff mobility results in non-physical interfacial profiles due to the lack of spatial resolution, while no such problem is encountered when using the smoothened mobility.

5.1. A Weakly Anisotropic Case. We consider the evolution of an initially circular interface under a smoothened anisotropic mobility corresponding to the raw mobility $M_0(x) = a + b\cos(2\Theta)$, where $a = 1$ and $b = 0.5$. For this weakly anisotropic case, we will see that it suffices to use a constant $c(x) = 1$ in (5), and the smoothing constant $\mu$ is taken to be $10^{-4}$. The simulation is performed on the domain $[0, 1] \times [0, 1]$ with periodic boundary condition, and with the gradient energy constant $\sigma = 0.02$ in the Allen-Cahn equation. A $100 \times 100$ spatial grid (i.e., 100 Fourier modes for each spatial variable) is used and a time step $\tau$ is set to be 0.1. Such a step size is well within the stability regime of the semi-implicit discretization. Moreover, our numerical experiments indicate that the further refinement of the spatial grid or the time step does not change the results presented.

For comparison purposes, we also perform the same simulation but with the cutoff mobility defined in (3), where the cutoff constant $\delta_c = 0.01$. Numerical experiences indicate that with the current level of high resolution (about 10 grid points across the interface), using a cutoff mobility does not result in any numerical instability. The cutoff mobility is used here rather as a benchmark to evaluate the effect of the smoothened mobility on the interfacial dynamics.

Figure 2 shows the evolutions of the interface by using the cutoff mobility and the smoothened mobility respectively. The diffuse interface is represented by three contour lines corresponding to $\eta = -0.8, 0$ and 0.8. Due to the anisotropy of the mobility function favoring the motion in the horizontal direction, the initially circular interface develops into an elliptic shape. It can be seen that the dynamics of the interface is essentially unchanged by switching to the smoothened mobility function.

Figure 3 displays the profiles of the cutoff and smoothened mobility functions during the simulation. It can be seen that the smoothened mobility function mimics the cutoff mobility on the interface. However, away from the interface, the cutoff mobility exhibits an apparent sharp transition while the profiles of the smoothened mobility function remain rather smooth in the course of the simulation. It is also interesting to observe that the smoothened mobility function evolves together with the interface.

5.2. A Strongly Anisotropic Case. Next, we consider the mobility function $M_0(x) = a + b\cos(2\Theta)$ where $a = 1$ and $b = 0.995$. The ratio of the maximum mobility and the minimum mobility in this case is more than 100 times bigger than the previous case. In contrast to the previous example, the strong anisotropy in the mobility results in a sharp corner at the top and the bottom of the interface where the normal has an angle approximately equal to $\pi/2$. This can be seen in figure 4, which shows the interface at $t = 100$ in the phase-field simulation using the cutoff mobility.

As the previous analysis on the circular interface implies, the problem of damping will manifest its severe effect in regions of high curvature if a spatially uniform
Figure 2. Evolution of an initially circular interface under anisotropic mobility functions at time $t = 40, 80$ and $100$: the top row is with the cutoff mobility while the bottom row is with the smoothened mobility. The dynamics of the interface is unchanged by switching to the smoothened mobility.

Figure 3. The cutoff mobility function versus the smoothed mobility function at time $t = 40, 80$ and $100$: the top row is with the cutoff mobility while the bottom row is with the smoothened mobility. The smoothing effect is obvious.

c = c(x) = 1 is used in (5). The artificial weakening of the anisotropy in mobility is indeed observed in our phase-field simulation using the smoothened mobility with $c = 1$. To minimize the damping effect, we have chosen the smoothing constant $\mu$ to be $8 \times 10^{-7}$, so small that the noisy pattern of the raw mobility function has started to emerge in the “smoothened” mobility function. The resulting interface at $t = 100$
Figure 4. The $\eta = -0.8, 0$ and $0.8$ contour plots of the interface under the influence of the strongly anisotropic mobility. The cutoff mobility is used in the phase-field simulation.

is plotted in figure 5. Clearly, the top and bottom corners do not lag behind as much as in the simulation using the cutoff mobility, creating a less skewed particle shape. This indicates that the smoothened mobility in these high-curvature regions is bigger than their prescribed value $a - b = 0.005$. To confirm this, we plot in the figure 5 the smoothened mobility function along the vertical axis of the particle $x = 0.5$. The minimum of the mobility function at the corners is obviously higher than 0.005.

Figure 5. Simulation using smoothened mobility generated from the variational principle with a spatially uniform $c(x)$. Left: interface. Right: Mobility along $x = 0.5$.

An improvement to the above method is to use a spatially varying coefficient $c = c(x)$, as proposed in section 3.2. Using the curvature-dependent $c(x)$ in (22) and $\mu = 10^{-5}$, the dynamics of the interface in the simulation using the cutoff mobility can be mostly recovered, as can be seen in figure 6. The plot of mobility along $x = 0.5$ also confirms that the mobility at the top and bottom corners is much closer to its expected value 0.005 than the previous attempt. Although the plot of the full mobility function on the 2D domain is omitted here, it shows no apparent sign of the noisy pattern of the raw mobility function.

5.3. A Dumbbell with Inhomogeneous Interfacial Thickness. Finally, we present a test problem to illustrate the advantage of using the smoothened mobility over the cutoff mobility. In theory, the higher regularity of the smoothened mobility enables the Fourier-spectral method to achieve very high accuracy in an asymptotic
sense. Thus in practice, one expects that the advantage of adopting a smoothened
mobility will manifest itself more clearly in situations where the spatial resolution
is lacking due to the limited computing resources. We now consider the evolution
of a dumbbell-shaped interface on $[0, 1] \times [0, 1]$ discretized on a regular 50 $\times$ 50
grid. To further strengthen the topological inhomogeneity, anisotropic gradient
energy coefficient of the form $\sigma^2 (c + d \cos(2\Theta))$ is introduced in addition to the
anisotropic mobility $M(x) = a + b \cos(2\Theta)$. The anisotropic energy can be naturally
incorporated into the Allen-Cahn equation by changing the Laplacian term $\Delta \eta$
into $(c + d) \frac{\partial^2 \eta}{\partial x^2} + (c - d) \frac{\partial^2 \eta}{\partial y^2}$, and the “skewed” Laplacian gives rise to inhomogeneous
interfacial thickness. The parameters we use are $\sigma = 0.02$, $a = 1$, $b = 0.99$, $c = 1$,
$d = -0.99$. The smoothened mobility is obtained with the spatially uniform$c = 1$, and $\mu = 10^{-4}$.

Given an initial dumbbell shown in figure 7 at time $t = 10$, the diffuse interfaces
obtained with the cutoff mobility and the smoothened mobility are plotted in the
figure 8. The interface contours produced by using the cutoff mobility exhibit non-
physical oscillations, while those produced with the smoothened mobility remain
smooth. We have checked that refining the time step $\tau = 0.1$ does not alter the
oscillation in the cutoff mobility case. Thus, this numerical artifact is purely due
to the lack of resolution in the spatial discretization. It is a remarkable fact that
the regularization effect coming from the smoothened mobility prevents such non-
physical phenomena from happening, even though there are only about 2 to 5 grid
points across the thinner or thicker parts of the interface.

6. Conclusion. An important issue in prescribing the anisotropic mobility depen-
dent upon the interfacial normal direction in phase-field simulation is the lack of
meaning of the “normal direction” away from the interface. We have proposed a
variational approach to constructing a smoothened mobility function that is close
to the prescribed mobility on the interface and extends to the whole computational
domain with certain smoothness properties. A simple analysis on a circular in-
terface and several numerical tests have helped us understand the profile of the
smoothened mobility, its effect on the interfacial dynamics, and its advantage over
the cutoff mobility in simulations with only low spatial resolution. Future work will
involve applying the proposed method to more realistic phase-field simulation of

Figure 6. Simulation using smoothened mobility generated from
the variational principle with a spatially varying $\alpha$. Left: interface.
Right: Mobility along $x = 0.5$. The minimum value of the mobility
is about 0.01.
such problems as precipitate growth as well as a more rigorous numerical analysis of the convergence of the Fourier-spectral approximations.

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