Multiphase Allen-Cahn and Cahn-Hilliard Models and Their Discretizations with the Effect of Pairwise Surface Tensions

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Abstract

In this paper, the mathematical properties and numerical discretizations of multiphase models that simulate the phase separation of an \(N\)-component mixture are studied. For the general choice of phase variables, the unisolvent property of the coefficient matrix involved in the \(N\)-phase models based on the pairwise surface tensions is established. Moreover, the symmetric positive-definite property of the coefficient matrix on an \((N - 1)\)-dimensional hyperplane — which is of fundamental importance to the well-posedness of the models — can be proved equivalent to some physical condition for pairwise surface tensions. The \(N\)-phase Allen-Cahn and \(N\)-phase Cahn-Hilliard equations can then be derived from the free-energy functional. A natural property is that the resulting dynamics of concentrations are independent of phase variables chosen. Finite element discretizations for \(N\)-phase models can be obtained as a natural extension of the existing discretizations for the two-phase model. The discrete energy law of the numerical schemes can be proved and numerically observed under some restrictions pertaining to time step size. Numerical experiments including the spinodal decomposition and the evolution of triple junctions are described in order to investigate the effect of pairwise surface tensions.

Keywords: Multiphase, Allen-Cahn, Cahn-Hilliard, pairwise surface tensions

1. Introduction

Multiphase flows are frequently encountered in biomedical, chemical, and engineering applications. The dynamics of multiphase flows associate with a wide range of fundamental physical properties such as pairwise surface tensions, wetting spreading, and forming contact angles among multiple materials [1]. On the other hand, multiphase flows are challenging from the points of view of both mathematical modeling and numerical methods due to the complexity of the moving interface.

There are two main approaches to moving interface problems: the direct approach and the indirect approach. The direct approach obtains information pertaining to the interface by tracking quantities associated with it. Therefore, the direct approach relies on the parameterization method [2], the immersed boundary method [3], the volume-of-fluid method [4], and/or the front tracking...
method \[5\]. It is known that the direct approach commonly encounters difficulty handling topological changes, such as pinches, splits, and merging — all of which can be handled easily by the indirect approach. The level set method \[6\] and the phase field method \[7\] are both examples of popular indirect methods. In this paper, however, we focus on the phase field method for modeling the effect of pairwise surface tensions for \(N\)-phase flows \((N \geq 2)\).

With the phase field method, the thickness of the sharp interface between the two phases is supposed to be very small but positive. The state of the system is then represented by a set of smooth functions called phase variables or order parameters. The evolution of the system is driven by the gradient of a total free-energy, which is the sum of two terms: a bulk free-energy term, whose effect tends to separate the flows, and a capillary term, whose effect tends to mix the flows. The capillary term depends on the gradient of the order parameters, which accounts for the energy of the interfacial tensions between flows.

Drawing on the large body of research on two-phase flows \[8, 9, 10, 11, 12, 13\], researchers have produced many theoretical and numerical studies on three-phase flows involving the effect of pairwise surface tensions \[14, 15, 16, 17, 18\]. In these models, the given pairwise surface tensions \(\sigma_{ij}\) are decomposed into three positive phase-specific surface-tension coefficients as

\[
\sigma_{12} = \sigma_1 + \sigma_2, \quad \sigma_{13} = \sigma_1 + \sigma_3, \quad \sigma_{23} = \sigma_2 + \sigma_3,
\]

whose existence is equivalent to the triangle inequality of the pairwise surface tensions. However, this decomposition encounters difficulties for cases in which \(N \geq 4\), as the number of pairwise tensions would be greater than the number of phase-specific surface-tension coefficients, which leads to an overdetermined system \[19, 20\]. In \[17\], a phenomenological continuum surface tension force was introduced by coupling Navier-Stokes equations through the mean curvature of the interface. Further, the generalization of this approach to an arbitrary number of phases with the purpose of avoiding the solvability issue was discussed in \[19\].

Generalizations of diffuse models to an arbitrary number of phases have recently been introduced and studied. In most of the existing models for multiphase flows, the phase variables are chosen specifically as concentrations of mixture \(c_i\), whose sum is equal to 1. Examples of such models include \(N\)-phase Allen-Cahn equations \[21, 22\] and \(N\)-phase Cahn-Hilliard equations \[23, 24, 25, 26, 27, 28\]. An benefit of these models is that their consistency with the two-phase model can be easily proven. However, the pairwise surface tensions are not involved in the energy-density function so that the homogeneous surface tensions are implied in most of the existing models intrinsically. As the physical concentrations must belong to the \((N-1)\)-dimensional Gibbs simplex \[29\], a variable Lagrangian multiplier should be introduced in the dynamic equations.

In order to incorporate the pairwise surface tensions into the phase field model, several generalized models have been proposed based on the generalized total free-energy functional. In \[30\], Elliott and Luckhaus set the total free-energy functional as

\[
\mathcal{E}(\tilde{c}) := \int_{\Omega} \left[ \Psi(\tilde{c}) + \frac{1}{2} (\Gamma \nabla \tilde{c}) : \nabla \tilde{c} \right],
\]

where \(\Gamma\) is the \(N \times N\) symmetric-positive semi-definite matrix, i.e. a symmetric coefficient matrix is introduced in the capillary-energy term. They also gave a global existence result under constant mobility when \(\Gamma = \gamma I\). Eyre \[31\] then studied this system and determined its equilibrium and dynamic behavior. Recently, Boyer and Minjeaud \[32\] proposed a generalization of the well-known two-phase Cahn-Hilliard model for the modeling of \(N\)-phase mixtures using the concentrations as
the phase variables. Dong \cite{33} established an algebraic relationship between the coefficient matrix and the pairwise surface tensions under a special choice of phase variables and gave the coupled system between the phase field and Navier-Stokes equations in the thermodynamics framework \cite{34}. One main feature of these works is that, thanks to a relevant choice of free-energy, the model coincides exactly with the two-phase model. Dong then derived a formulation for the general phase variables in \cite{35} by eliminating one variable in order to relax the algebraic relationship.

In this paper, we begin by applying the general phase variables without eliminating any of the variables, and we rebuild the relationship between the coefficient matrix and the pairwise surface tensions in a compact form. By drawing on a recent work on the close connection between the symmetric matrix space and simplex \cite{36}, we obtain the unisolvent property of the coefficient matrix on the tangent space of the solution manifold. Furthermore, the symmetric positive-definite (SPD) property on the tangent space proposed as an open problem in \cite{32, 33, 35}, is answered by two equivalent conditions from both the algebraic and the geometric point of view, see Theorem 2.3. We note that this property is fundamentally important to the well-posedness of the dynamic system. This is the first major contribution of the present study to the field.

The second principle contribution of the present study is the derivation of the $N$-phase Allen-Cahn and Cahn-Hilliard equations under the generalized total free-energy functional. As the gradient flow on the solution manifold, the Allen-Cahn equations make sense only under the given inner product on the tangent space in energy-variation framework. Here, we apply the inner product on the tangent space induced from the choice of generalized phase variables, so that the dynamics of the concentrations are independent of the choice of phase variables. A similar technique can be applied to $N$-phase Cahn-Hilliard equations to obtain the same property. When $N$-phase Allen-Cahn and Cahn-Hilliard equations are written in a strong formulation, the orthogonal projection to the tangent space will naturally translate into the variable Lagrangian multiplier as shown in models reported in \cite{21, 22, 23, 24, 25, 26, 27}. This implies that our models can be viewed as a natural extension of the existing models while accounting for and including effect of pairwise surface tensions on the multiphase flows.

Based on the above properties, we propose finite element discretizations for $N$-phase models. The semi-implicit, fully-implicit, and modified Crank-Nicolson scheme, are considered for $N$-phase Allen-Cahn equations, and the semi-implicit, fully-implicit, and modified Crank-Nicolson scheme, are considered for $N$-phase Cahn-Hilliard equations. Each of these schemes can be viewed as a natural extension of the existing numerical schemes for two-phase flows \cite{37, 13}. The discrete energy law of the numerical schemes is also discussed.

The rest of this paper is organized as follows. In Section 2, we consider the generalized phase variables and the free-energy functional with a coefficient matrix in the capillary term. The solvability and SPD property of the coefficient matrix are discussed. We also derive $N$-phase Allen-Cahn and Cahn-Hilliard equations so that the corresponding dynamics of concentrations are independent of the choice of phase variables. In Section 3, the finite element discretizations of the $N$-phase models are described and energy stability of each is considered. Numerical experiments showing the effect of the pairwise tensions on the multiphase flows and the accuracy of the schemes are presented in Section 4. Some closing remarks are given in Section 5.

2. $N$-phase Models

First, we introduce some notation that will be used throughout this paper. Let $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) be the bounded domain, and $\partial \Omega$ the domain boundary. The unit outer normal vector of $\partial \Omega$ is
denoted by \( \nu \). For integer \( m \geq 0, n \geq 1 \), let \( H^m(\Omega; \mathbb{R}^n) \) be the standard Sobolev space with a norm \( \| \cdot \|_m \) given by

\[
\| \vec{v} \|^2_m := \sum_{i=1}^{n} \sum_{|\alpha| \leq m} \| D^\alpha v_i \|^2_{L^2(\Omega)}, \quad \forall \vec{v} \in H^m(\Omega; \mathbb{R}^n).
\]

In particular, the norm and inner product of \( L^2(\Omega; \mathbb{R}^n) = H^0(\Omega; \mathbb{R}^n) \) are denoted by \( \| \cdot \|_0 \) and \( (\cdot, \cdot) \), respectively. For any vector field \( \vec{v} \in H^1(\Omega; \mathbb{R}^n) \), we define

\[
\nabla \vec{v} = \begin{pmatrix} \nabla v_1 \\ \vdots \\ \nabla v_n \end{pmatrix} = \begin{pmatrix} \partial_{x_1} v_1 & \cdots & \partial_{x_d} v_1 \\ \vdots & \ddots & \vdots \\ \partial_{x_1} v_n & \cdots & \partial_{x_d} v_n \end{pmatrix} \in \mathbb{R}^{n \times d}.
\]

The inner product of the vector is defined as \( \vec{v} \cdot \vec{w} = \sum_{i=1}^{n} v_i w_i \), for all \( \vec{v}, \vec{w} \in \mathbb{R}^n \). Moreover, the Frobenious inner product of the matrix is defined as

\[
\langle A, B \rangle = A : B = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} b_{ij}, \quad A, B \in \mathbb{R}^{n \times m}.
\]

In this section, we will give a derivation of the models describing the \( N \)-phase flows with the effect of pairwise surface tensions. To this end, we state three assumptions:

**Assumption 1** The \( i \)-th phase is characterized by \( c_i \), which satisfies \( \sum c_i = 1 \) and \( 0 \leq c_i \leq 1 \). Specifically, \( c_i \) corresponds to the volume (or mole) fraction of the \( i \)-th fluid.

**Assumption 2** The free-energy density of the \( N \)-phase model will reduce to the corresponding free-energy density of the \( L \)-phase model if only \( L \) (\( 2 \leq L \leq N - 1 \)) phases are present.

**Assumption 3** If \( N - K \) (\( 2 \leq K \leq N - 1 \)) phases are not present at the initial time, they will not appear artificially during the evolution of the system.

Let \( \vec{c} = (c_1, c_2, \cdots, c_N)^T \in \mathbb{R}^N \). Given an invertible \( A \in \mathbb{R}^{N \times N} \) and \( \vec{b} \in \mathbb{R}^N \), we define the phase variables \( \vec{\phi} \) as

\[
\vec{\phi} = A \vec{c} + \vec{b}. \tag{2.1}
\]

Let \( \sigma_{ij}(1 \leq i, j \leq N) \) denote the pairwise surface tension between phase \( i \) and phase \( j \) (\( \sigma_{ij} = \sigma_{ji} \)), and \( \sigma_{ii} = 0 \) for \( 1 \leq i \leq N \). In light of \( [32, 33, 34] \), we introduce the free-energy density of the \( N \)-phase system as

\[
W(\vec{\phi}, \nabla \vec{\phi}) := \sum_{i,j=1}^{N} \frac{\eta}{2} \lambda_{ij} \nabla \phi_i \cdot \nabla \phi_j + \frac{1}{\eta} F(\vec{c}) = \frac{\eta}{2} (\Lambda \nabla \vec{\phi}) : \nabla \vec{\phi} + \frac{1}{\eta} F(\vec{c}), \tag{2.2}
\]

where the form of nonlinear potential \( F(\cdot) \) satisfies the **Assumption 2** \([32, 33, 34]\), especially when \( L = 2 \):

\[
F(\vec{c}) = 2 \sigma_{ij} [f(c_i) + f(c_j)], \quad \text{if } c_i + c_j = 1, c_k = 0 \ (k \neq i, j). \tag{2.3}
\]

Here, \( f(\cdot) = \alpha^2 (1 - \epsilon^2) \), and the symmetric coefficient matrix \( \Lambda = (\lambda_{ij}) \in \mathbb{R}^{N \times N} \) is assumed to be constant. We note that the introduction of \( \Lambda \) constitutes the major difference between \( \text{(2.2)} \) and the \( N \)-phase models presented in the literature \([16, 18, 19, 20, 25, 22, 27, 28]\). The constant

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$\eta > 0$ denotes a characteristic scale of the interfacial thickness. With the free-energy density, the corresponding Liapunov free-energy functional is

$$E(\phi) = \int_{\Omega} W(\phi, \nabla \phi) dx = \int_{\Omega} \frac{\eta}{2} (\mathbf{A} \nabla \phi : \nabla \phi) + \frac{1}{\eta} F(\phi). \quad (2.4)$$

Now, we will use Assumption 2 to build the relationship between $\Lambda$, $A$, and the pairwise surface tensions. For the two-phase case, the phase variable $\phi$ satisfies

$$c_1 = \frac{1 + \phi}{2}, \quad c_2 = \frac{1 - \phi}{2},$$

and the free-energy density in [12] can be written as

$$W(\phi, \nabla \phi) = \frac{\bar{\lambda}}{2} \nabla \phi \cdot \nabla \phi + \frac{\bar{\lambda}}{4\epsilon^2} (1 - \phi^2)^2$$

$$= \frac{\bar{\lambda}}{2} \nabla (c_1 - c_2) \cdot \nabla (c_1 - c_2) + \frac{2\sigma_{12}}{\eta} [c_1^2 (1 - c_1)^2 + c_2^2 (1 - c_2)^2] \quad (2.5)$$

where $\epsilon = \sqrt{\eta\bar{\lambda}/\sigma_{12}}$. Moreover, based on the equilibrium 1D surface energy [12], the relationship between $\bar{\lambda}$ and the interfacial surface tension $\sigma_{12}$ can be derived as

$$\sigma_{12} = \frac{2\sqrt{2}}{3} \frac{\epsilon}{\eta} = \frac{2\sqrt{2} \epsilon}{3 \eta\sigma_{12}},$$

which yields

$$\epsilon = \frac{3}{2\sqrt{2} \eta}, \quad \text{and} \quad \bar{\lambda} = \frac{9}{8} \eta \sigma_{12}. \quad (2.6)$$

It can be proved in [12] that (2.6) gives the interfacial tension in the sharp-interface limit. Notice that $\sigma = O(1)$ such that we have $\bar{\lambda} = O(\eta)$ and $\epsilon = O(\eta)$, which is consistent with the physical model in the two-phase case. We also note that different phase interfaces have the same interface thickness in this model.

Now we assume that only two phases, i.e. $k$ and $l$, are present in the $N$-phase model,

$$c_k + c_l = 1, \quad \text{and} \quad c_i = 0 \text{ for } i \neq k, l.$$

Then, the free-energy density (2.2) is shown to be

$$W(\phi, \nabla \phi) = \sum_{i,j=1}^{N} \frac{\eta \lambda_{ij}}{2} (a_{ik} \nabla c_k + a_{il} \nabla c_l) \cdot (a_{jk} \nabla c_k + a_{jl} \nabla c_l) + \frac{2}{\eta} [c_k^2 (1 - c_k)^2 + c_l^2 (1 - c_l)^2]$$

$$= \left( \sum_{i,j=1}^{N} \frac{\eta \lambda_{ij}}{2} (a_{ik} - a_{il})(a_{jk} - a_{jl}) \right) \nabla c_k \cdot \nabla c_k + \frac{2}{\eta} [c_k^2 (1 - c_k)^2 + c_l^2 (1 - c_l)^2].$$

By comparing the above equation with (2.5), we immediately have

$$\sum_{i,j=1}^{N} \lambda_{ij} (a_{ik} - a_{il})(a_{jk} - a_{jl}) = \frac{4\bar{\lambda}}{\eta} = \frac{9}{2} \sigma_{kl}, \quad 1 \leq k < l \leq N, \quad (2.7)$$
where $\sigma_{kl}$ is the interfacial surface tension between phases $k$ and $l$. Denote $\vec{a}_k = (a_{1k}, a_{2k}, \cdots, a_{Nk})^T \in \mathbb{R}^N$. Then, (2.7) is shown to be the following matrix equation for $\Lambda$:

$$(\vec{a}_k - \vec{a}_l)^T \Lambda (\vec{a}_k - \vec{a}_l) = \frac{9}{2} \sigma_{kl}, \quad 1 \leq k < l \leq N.$$  

(2.8)

Define $\vec{L}_{kl} = \vec{a}_k - \vec{a}_l$. Then, (2.8) can be recast as

$$(\vec{L}_{kl} \vec{L}_{kl}^T) : \vec{a} = \frac{9}{2} \sigma_{kl}, \quad 1 \leq k < l \leq N.$$  

(2.9)

**Remark 2.1.** In most of the well-studied $N$-phase models [21, 22, 23, 26, 27, 28], the original concentrations $\vec{c}$ are used as the phase variables and $\Lambda$ is set as $\sigma I$, which means that the models describe the homogeneous pairwise surface tensions such that $\sigma_{ij} = \frac{4}{9} \sigma$.

### 2.1. Solvability and properties of the coefficient matrix

Given the phase variables (2.1) and the free-energy density (2.2), one basic problem is the solvability of mixing energy density coefficient matrix $\Lambda = (\lambda_{ij})$. We note that the number of equations in (2.8) is $N(N-1)/2$, whereas the number of unknowns is $(N+1)N/2$. Therefore, we can show only that $\Lambda$ is unisolvent on the $(N-1)$-dimensional hyperplane.

Notice that $\sum_{i=1}^{N} c_i = 1$ from Assumption 1. Then,

$$1 = \vec{1}^T \vec{c} = \vec{1}^T \Lambda^{-1} (\vec{\phi} - \vec{b}) = \vec{d}^T (\vec{\phi} - \vec{b}),$$

where $\vec{1} = (1, 1, \cdots, 1)^T \in \mathbb{R}^N$ and $\vec{d} = \Lambda^{-T} \vec{1}$. It is easy to check that $\vec{d} \neq 0$, as $\Lambda$ is invertible. Then, $\vec{\phi}$ lies in the following $(N-1)$-dimensional manifold (hyperplane):

$$\Sigma = \{ \vec{\phi} \in \mathbb{R}^N \mid \vec{d}^T \vec{\phi} - \vec{d}^T \vec{b} = 1 \},$$

the tangent space of which is denoted by

$$T\Sigma = \{ \vec{v} \in \mathbb{R}^N \mid \vec{d}^T \vec{v} = 0 \}.$$  

(2.10)

Furthermore, we have

$$\vec{d}^T \vec{a}_k = \vec{1}^T \Lambda^{-1} \vec{a}_k = 1, \quad \vec{d}^T \vec{L}_{kl} = 0,$$

which means that $\vec{d} \perp \vec{L}_{kl}$, therefore, $\vec{L}_{kl} \in T\Sigma$. Let $\vec{P} = \vec{I} - \frac{\vec{d}\vec{d}^T}{\vec{d}^T \vec{d}}$ be the orthogonal projection to $T\Sigma$ such that $\vec{P}^T = \vec{P}$ and

$$\vec{P} \vec{L}_{kl} = \vec{L}_{kl}, \quad \vec{P} \vec{L}_{kl} \vec{L}_{kl}^T \vec{P} = \vec{L}_{kl} \vec{L}_{kl}^T.$$

Then, (2.9) is shown to be

$$(\vec{L}_{kl} \vec{L}_{kl}^T) : \tilde{\vec{\Lambda}} = \frac{9}{2} \sigma_{kl}, \quad 1 \leq k < l \leq N,$$

(2.12)

where $\tilde{\vec{\Lambda}} = \vec{P} \vec{\Lambda} \vec{P}$. Based on the property of the symmetric matrix space, we will establish the unique solvability of $\tilde{\vec{\Lambda}}$ next.
Definition 2.1. For a given $n$-dimensional vector space $U \subset \mathbb{R}^N$, $P : \mathbb{R}^N \mapsto U$ is the orthogonal projection. Define the symmetric matrix space on $U$ as

$$S(U) = \{PMP \mid M \in \mathbb{R}^{N \times N}, M^T = M\}.$$ 

As the dimension of $\ker(P)$ is $N - n$, then $\dim(S(U)) = \frac{n(n+1)}{2}$. Let inner product $\langle \cdot, \cdot \rangle$ be the Frobenious inner product, then it is easy to determine that $(S(U), \langle \cdot, \cdot \rangle)$ is a Hilbert space.

In Lemma 2.2 of [36], Hu determined a crucial relationship between the $n$-dimensional simplex and the $n$-dimensional symmetric matrix space. We extend this lemma to a hyperplane to obtain the following lemma.

Lemma 2.1. $\{\vec{L}_{kl}\vec{L}_{kl}^T, 1 \leq k < l \leq N\}$ forms a basis of $S(T\Sigma)$.

Proof. It is easy to see that $\vec{L}_{kl}\vec{L}_{kl}^T$ constitutes a symmetric matrix of rank one in $S(T\Sigma)$ and that

$$\dim \left( \{\vec{L}_{kl}\vec{L}_{kl}^T, 1 \leq k < l \leq N\} \right) \leq \frac{N(N-1)}{2} = \dim(S(T\Sigma)).$$

On the other hand, notice that $A$ is invertible. Then, $[\vec{a}_1, \cdots, \vec{a}_{N-1}]$ comprise an $(N-1)$-dimensional simplex on the hyperplane

$$\mathcal{M} = \{\vec{v} \in \mathbb{R}^N \mid \vec{d}^T \vec{v} = 1\}.$$ 

If $\sum_{kl} \alpha_{kl} \vec{L}_{kl}\vec{L}_{kl}^T = 0$, then by testing the normal vector $\vec{n}_N \in \mathcal{M}$ of the $(N-2)$-dimensional hyperplane $[\vec{a}_1, \cdots, \vec{a}_{N-1}]$ on both sides (see Figure 2.1a), we obtain

$$\sum_{k=1}^{N-1} \alpha_{kN} \vec{L}_{kN}\vec{L}_{kN}^T \vec{n}_N = 0,$$

as

$$\vec{L}_{kl}^T \vec{n}_N = 0, \quad 1 \leq k < l \leq N - 1.$$ 

Notice that $\vec{L}_{kN}^T \vec{n}_N \neq 0$ and $\{\vec{L}_{kN}, 1 \leq k \leq N - 1\}$ are linear independent. Then, we immediately have

$$\alpha_{kN} = 0, \quad 1 \leq k \leq N - 1.$$ 

By a similar argument, we can prove that $\alpha_{kl} = 0$, which means that $\{\vec{L}_{kl}\vec{L}_{kl}^T, 1 \leq k < l \leq N\}$ forms a basis of $S(T\Sigma)$.

Theorem 2.2. Assume that $\Lambda$ satisfies the linear algebraic system (2.8). Then, $\tilde{\Lambda} = P\Lambda P$ is uniquely determined by the interfacial surface tension $\sigma_{kl}$.

Proof. This theorem can be directly proved by Lemma 2.1 and the Riesz representation theorem in Hilbert space.

In Theorem 2.2, we build a bridge between the $N$-phase models and the vertices of the $(N - 1)$-dimensional simplex. Based on this idea, we will present a sufficient and necessary condition for $\tilde{\Lambda}$ to be symmetric positive-definite (SPD) on the tangent space $T\Sigma$.

Theorem 2.3. The following statements are equivalent:
1. $\hat{\Lambda}$ is SPD on the tangent space $T\Sigma$.
2. For any (or there exists) $1 \leq m \leq N$, the matrix $\hat{\sigma}^m = (\hat{\sigma}_{ij}^m) \in \mathbb{R}^{(N-1) \times (N-1)}$ is SPD, where $\hat{\sigma}^m$ is obtained from $\hat{\sigma}$ by removing the $m$-th row and column:
\[
(\hat{\sigma})_{ij} = \frac{\sigma_{im} + \sigma_{jm} - \sigma_{ij}}{2}, \quad 1 \leq i, j \leq N.
\] (2.13)
3. The surface tensions can compose a non-degenerate $(N-1)$-dimensional simplex $K = [\vec{p}_1, \ldots, \vec{p}_N]$ with $|\vec{p}_i - \vec{p}_j| = \sqrt{\sigma_{ij}}$.

Proof. $1 \Leftrightarrow 2$: It is easy to check that \{\(\vec{L}_{km}, 1 \leq k \leq N, k \neq m\)\} forms a basis of $T\Sigma$. Then, any $\vec{v} \in T\Sigma$ can be written as
\[
\vec{v} = \sum_{k \neq m} \alpha_k \vec{L}_{km} = [\vec{L}_{1m}, \ldots, \vec{L}_{(k-1)m}, \vec{L}_{(k+1)m}, \ldots, \vec{L}_{Nm}] \overrightarrow{\alpha}^m := \mathbf{L}^m \overrightarrow{\alpha}^m,
\]
where $\overrightarrow{\alpha}^m = (\alpha_1, \ldots, \alpha_{m-1}, \alpha_{m+1}, \ldots, \alpha_N)^T$ and $\mathbf{L}^m \in \mathbb{R}^{N \times (N-1)}$. It can easily be seen from (2.12) that
\[
\frac{9}{2} \sigma_{ij} = \vec{L}_{ij}^T \hat{\Lambda} \vec{L}_{ij} = (\vec{L}_{im} - \vec{L}_{jm})^T \hat{\Lambda} (\vec{L}_{im} - \vec{L}_{jm}) = \frac{9}{2} \sigma_{im} + \frac{9}{2} \sigma_{jm} - 2 \vec{L}_{im}^T \hat{\Lambda} \vec{L}_{jm}.
\]
Then, we have
\[
\vec{v}^T \hat{\Lambda} \vec{v} = (\overrightarrow{\alpha}^m)^T (\mathbf{L}^m)^T \hat{\Lambda} \mathbf{L}^m \overrightarrow{\alpha}^m = \frac{9}{2} (\overrightarrow{\alpha}^m)^T \hat{\sigma}^m \overrightarrow{\alpha}^m,
\]
which means that the SPD of $\hat{\Lambda}$ on $T\Sigma$ is equivalent to the SPD of $\hat{\sigma}^m$ defined in (2.13).

$2 \Rightarrow 3$: We choose $m = N$ for simplicity. For the SPD matrix $\hat{\sigma}^N \in \mathbb{R}^{(N-1) \times (N-1)}$, there exists an invertible matrix $\mathbf{T}$ such that $\hat{\sigma}^N = \mathbf{T}^T \hat{\sigma} \mathbf{T}$. Define $\vec{p}_N = 0$ and
\[
\vec{p}_i = (t_{1i}, t_{2i}, \ldots, t_{(N-1)i})^T \in \mathbb{R}^{N-1}, \quad i = 1, \ldots, N - 1.
\]
Then, we immediately know that $\vec{p}_1, \ldots, \vec{p}_N$ form a non-degenerate simplex. By checking the diagonal terms of $T^T T$, we have $|\vec{p}_i| = \sqrt{\sigma_{iN}}$. Furthermore, the off-diagonal terms of $T^T T$ imply that
\[
\frac{\sigma_{iN} + \sigma_{jN} - \sigma_{ij}}{2} = \frac{|\vec{p}_i|^2 + |\vec{p}_j|^2 - |\vec{p}_i - \vec{p}_j|^2}{2} = \frac{\sigma_{iN} + \sigma_{jN} - |\vec{p}_i - \vec{p}_j|^2}{2},
\]
which yields $|\vec{p}_i - \vec{p}_j| = \sqrt{\sigma_{ij}}$.

3 $\Rightarrow$ 2: If 3 holds, then there exists an affine mapping from unit simplex $\hat{K} = [\vec{e}_1, \ldots, \vec{e}_{N-1}, 0]$ to $K = [\vec{p}_1, \ldots, \vec{p}_N]$: $\hat{y} = G(\hat{y}) = T\hat{y} + \vec{p}_N, \forall \hat{y} \in \hat{K}$.

Then, it is easy to check that
\[
T = (\vec{p}_1 - \vec{p}_N, \vec{p}_2 - \vec{p}_N, \ldots, \vec{p}_{N-1} - \vec{p}_N),
\]
which implies that
\[
\hat{\sigma}^N = T^T T.
\]
The non-degenerate property of $K$ means that $\det(T) \neq 0$, which leads to the SPD of $\hat{\sigma}^N$.

**Remark 2.2.** Statement 3 in Theorem 2.3 is the geometric condition (we call it simplicial condition) for the pairwise surface tensions, see Figure 2.1b for the case in which $N = 4$. We can easily find that a necessary condition for the SPD property of $\hat{\Lambda}$ on the tangent space is
\[
|\sqrt{\sigma_{ij}} - \sqrt{\sigma_{jk}}| < \sqrt{\sigma_{ik}} < \sqrt{\sigma_{ij}} + \sqrt{\sigma_{jk}}, \quad \text{for different } i, j, k. \tag{2.14}
\]
For the case in which $N = 3$, condition (2.14) is obviously the sufficient condition from Theorem 2.3. However, for the case in which $N \geq 4$, (2.14) is not sufficient, which makes it difficult to extend the existing three-phase models [14, 15, 16, 17, 18] to an arbitrary number of phases.

2.2. $N$-phase Allen-Cahn equations

It is well known that $N$-phase Allen-Cahn equations can be derived as the gradient flow, which implies that
\[
\gamma \frac{\partial \phi}{\partial t} = -\text{grad} W(\phi, \nabla \phi). \tag{2.15}
\]
Here, parameter $\gamma$ is set as $O(\eta)$ consistent with the mean curvature flow for the two-phase case [38]. In light of (2.17) below, we know that grad $W$ belongs to the dual space of $T\Sigma$. Therefore, the left-hand side of the gradient flow (2.15) should also be interpreted as the dual space of $T\Sigma$, which means that the metric on $T\Sigma$ must be considered. First, we define the Sobolev spaces on manifold $\Sigma$ and tangent space $T\Sigma$ as
\[
H^1(\Sigma) := H^1(\Omega; \mathbb{R}^n) \cap \Sigma = \{ \vec{\phi} \in H^1(\Omega; \mathbb{R}^n) \mid d^T \vec{\phi} - d^T \vec{b} = 1 \},
\]
\[
H^1(T\Sigma) := H^1(\Omega; \mathbb{R}^n) \cap T\Sigma = \{ \vec{v} \in H^1(\Omega; \mathbb{R}^n) \mid d^T \vec{v} = 0 \}. \tag{2.16}
\]
It can be seen that $H^1(\Sigma) = H^1(T\Sigma) + \vec{b} + \frac{d}{|d|^2}$. 

Let $\vec{\phi} \in H^1(\Sigma)$ and $(\nabla \vec{\phi})\nu = 0$ on $\partial \Omega$. For any $\vec{v} \in H^1(T\Sigma)$, we obtain the gradient of $E(\vec{\phi}, \nabla \vec{\phi})$ on the manifold $\Sigma$ as
\[
\langle \text{grad} E, \vec{v} \rangle = \int_\Omega \frac{d}{d\theta} W(\vec{\phi} + \theta \vec{v}, \nabla \vec{\phi} + \theta \nabla \vec{v}) \bigg|_{\theta = 0} \, dx
\]
\[
= \int_\Omega \eta (A \nabla \vec{\phi}) : \nabla \vec{v} + \frac{1}{\eta} (A^{-T} \frac{\partial F}{\partial \vec{c}}) \cdot \vec{v} \, dx
\]
(2.17)

Denote the manifold (hyperplane) of the concentration as $\Sigma_c = \{ \vec{c} \in \mathbb{R}^N | \vec{1}^T \vec{c} = 1 \}$.

Then, we have $\Sigma_c \xrightarrow{\mathcal{A}_c \vec{c} + \mathcal{B}_c} \Sigma$, $T\Sigma_c \xrightarrow{\mathcal{A}_c} T\Sigma$.

If a given inner product $(\cdot, \cdot)_{X_c}$ is used for $T\Sigma_c$, then the induced inner product for $T\Sigma$ will be $(\cdot, \cdot)_{X} := (\mathcal{A}_c X_c^{-1} \cdot, \mathcal{A}_c^{-1} \cdot)_{\Omega}$, (2.18)

where $X = A^{-T} X_c A^{-1}$. When choosing $X_c = M_{AC}$, the weak formulation of the $N$-phase Allen-Cahn equations can be written as
\[
\gamma \int_\Omega (M_{AC} A^{-1} \frac{\partial \vec{c}}{\partial t}) \cdot (A^{-1} \vec{v}) \, dx + \int_\Omega \eta (\mathcal{A}_c \nabla \vec{c}) : \nabla \vec{v} + \frac{1}{\eta} (\mathcal{A}_c^{-1} \frac{\partial F}{\partial \vec{c}}) \cdot \vec{v} \, dx = 0, \quad \forall \vec{v} \in H^1(T\Sigma),
\]
(2.19)

whereas the strong form can be written as
\[
\begin{cases}
\gamma \mathcal{A}_c M_{AC} A^{-1} \frac{\partial \vec{c}}{\partial t} - \nabla \cdot (\eta A \nabla \vec{c}) + \frac{1}{\eta} (\mathcal{A}_c^{-1} \frac{\partial F}{\partial \vec{c}}) \cdot \vec{v} = 0, \quad \text{in } \Omega \times (0, T],
\vspace{1em}
(\nabla \vec{c})\nu = 0, \quad \text{on } \partial \Omega \times (0, T].
\end{cases}
\]
(2.20)

We will prove that the $N$-phase Allen-Cahn equations (2.19) are independent of the choice of $\mathcal{A}$ in the following theorem.

**Theorem 2.4.** Let $\mathcal{P}_c = I - \frac{\mathcal{A}_c}{\mathcal{A}_c^T} \mathcal{A}_c$, $\mathcal{A}_c = \mathcal{P}_c \mathcal{A}_c \mathcal{P}_c$, and $\vec{v}_c = A^{-1} \vec{v}$. Then, (2.19) is equivalent to
\[
\gamma \int_\Omega (M_{AC} \frac{\partial \vec{c}}{\partial t}) \cdot \vec{v}_c \, dx = \int_\Omega \eta (\mathcal{A}_c \nabla \vec{c}) : \nabla \vec{v}_c + \frac{1}{\eta} (\mathcal{P}_c \frac{\partial F}{\partial \vec{c}}) \cdot \vec{v}_c \, dx, \quad \forall \vec{v}_c \in H^1(T\Sigma_c),
\]
(2.21)

or to the strong form
\[
\begin{cases}
\gamma \mathcal{P}_c M_{AC} \frac{\partial \vec{c}}{\partial t} - \nabla \cdot (\eta \mathcal{A}_c \nabla \vec{c}) + \frac{1}{\eta} \mathcal{P}_c \frac{\partial F}{\partial \vec{c}} = 0, \quad \text{in } \Omega \times (0, T],
\vspace{1em}
(\nabla \vec{c})\nu = 0, \quad \text{on } \partial \Omega \times (0, T].
\end{cases}
\]
(2.22)
Proof. It is easy to check that $\tilde{v}_c \in H^1(T\Sigma_c)$. Then, (2.19) is shown to be

\[
\gamma \int_\Omega (M^A_c A^{-1} \frac{\partial \tilde{\phi}}{\partial t}) \cdot \tilde{v}_c \, dx = \int_\Omega \eta (\tilde{\Lambda} \tilde{\phi}) : \tilde{v}_c + \frac{1}{\eta} \tilde{\phi} (\tilde{\Lambda} (P_c P A^{-T} \frac{\partial F}{\partial \tilde{c}})) \cdot \tilde{v}_c \, dx \\
= \int_\Omega \eta (P_c A^{T} \tilde{\Lambda} \tilde{\phi}) : \tilde{v}_c + \frac{1}{\eta} (P_c A^{T} P A^{-T} \frac{\partial F}{\partial \tilde{c}}) \cdot \tilde{v}_c \, dx \\
= \int_\Omega \eta (P c A^{T} \tilde{\Lambda} (A P c)) : \tilde{v}_c + \frac{1}{\eta} (P c A^{T} P A^{-T} \frac{\partial F}{\partial \tilde{c}}) \cdot \tilde{v}_c \, dx.
\]

For the right-hand side of (2.23), it is easy to determine that

\[
P c A^{T} P A^{-T} = P c (I - \tilde{L}^{T} \tilde{L}) = P c.
\]

On the other hand, we have

\[
AP c (\tilde{e}_k - \tilde{e}_l) = A (\tilde{e}_k - \tilde{e}_l) = \tilde{L}_{kl}.
\]

Thus, when

\[
[(\tilde{e}_k - \tilde{e}_l)(\tilde{e}_k - \tilde{e}_l)^{T}] : [(A P c)^{T} \tilde{\Lambda} (A P c)] = (L_{kl} L_{kl}^{T}) : \tilde{\Lambda} = \frac{9}{2} \sigma_{kl},
\]

is taken together with the unisolvent property in Theorem 2.2, we obtain

\[
(A P c)^{T} \tilde{\Lambda} (A P c) = \tilde{\Lambda} c.
\]

Take (2.24) and (2.25) into (2.23) to obtain the desired results.

Since $M^A_c$ is SPD on $T\Sigma_c$, by taking $\bar{v} = \dot{\bar{\phi}}$ in (2.19), we immediately find the following energy law for $N$-phase Allen-Cahn equations:

\[
\frac{dE(\bar{\phi})}{dt} = -\gamma \int_\Omega (M^A_c A^{-1} \bar{\phi}) \cdot \bar{\phi} \, dx = -\gamma \int_\Omega (M^A_c \bar{\phi}_t) \cdot \bar{\phi}_t \, dx \leq 0,
\]

which depends only on the dynamics of concentrations, as expected.

Remark 2.3. If $\frac{\partial F}{\partial \tilde{c}} = (f'(c_1), f'(c_2), \ldots, f'(c_N))^{T}$, then (2.22) implies that

\[
P c \frac{\partial F}{\partial \tilde{c}} = (I - \frac{1}{N} \tilde{L}) \frac{\partial F}{\partial \tilde{c}} = \frac{\partial F}{\partial \tilde{c}} - \frac{1}{N} \sum_{i=1}^{N} f'(c_i) = \frac{\partial F}{\partial \tilde{c}} + \beta(\tilde{c}),
\]

where $\beta(\tilde{c}) = -\frac{1}{N} \sum_{i=1}^{N} f'(c_i)$ is exactly the variable Lagrangian multiplier used in the existing works [21, 22, 26, 27, 28].
2.3. N-phase Cahn-Hilliard equations

For Cahn-Hilliard equations, it is well known that the Hele-Shaw flow constitutes limiting dynamics in the two-phase case \([39, 40]\). Let \(M_c^{\text{CH}}\) be the mobilities associated with \(c\) that is SPD on \(T\Sigma_c\). Similar to the argument for the N-phase Allen-Cahn equations, by choosing \((\cdot, \cdot)_c = (\cdot, \cdot)_{r_c}\) as the inner product on \(T\Sigma_c\), the N-phase Cahn-Hilliard equations under the induced inner product \([2.18]\) are

\[
\begin{align*}
\int_{\Omega} (A^{-1} \frac{\partial \phi}{\partial t}) \cdot \langle A^{-1} \tilde{q} \rangle \, dx & = - \int_{\Omega} (M_c^{\text{CH}} A^{-1} \nabla \tilde{w}) : (A^{-1} \nabla \overline{q}) \, dx, \quad \forall \overline{q} \in H^1(T\Sigma), \\
\int_{\Omega} (A^{-1} \tilde{w}) \cdot (A^{-1} \tilde{v}) \, dx & = \int_{\Omega} \eta (\Lambda \nabla \phi) : \nabla \tilde{v} + \frac{1}{\eta} (P A^{-T} \frac{\partial F}{\partial c}) : \tilde{v} \, dx, \quad \forall \tilde{v} \in H^1(T\Sigma),
\end{align*}
\]

where \(\tilde{w}\) denotes the chemical potentials. In light of the weak formulation \([2.27]\), the strong form of N-phase Cahn-Hilliard equations can be written as

\[
\begin{align*}
P A^{-T} A^{-1} \frac{\partial \tilde{\phi}}{\partial t} & = \nabla \cdot [(A^{-1} P)^T M_c^{\text{CH}} A^{-1} P \nabla \tilde{w}], \quad \text{in } \Omega \times (0, T], \\
P A^{-T} A^{-1} \tilde{w} & = - \nabla \cdot (\eta \tilde{\Lambda} \nabla \tilde{\phi}) + \frac{1}{\eta} P A^{-1} \frac{\partial F}{\partial c}, \quad \text{in } \Omega \times (0, T], \\
(\nabla \tilde{\phi})_\nu & = (\nabla \tilde{w})_\nu = 0, \quad \text{on } \partial \Omega \times (0, T].
\end{align*}
\]

Similar to Theorem 2.5, we have the following theorem for the invariant dynamics of concentrations for N-phase Cahn-Hilliard equations.

**Theorem 2.5.** Let \(\tilde{\nu}_c = A^{-1} \tilde{v}\) and \(\tilde{\nu}_c = A^{-1} \tilde{w}\). Then, \([2.27]\) is equivalent to

\[
\begin{align*}
\int_{\Omega} \frac{\partial \tilde{c}}{\partial t} \cdot \tilde{\nu}_c \, dx & = - \int_{\Omega} (M_c^{\text{CH}} \nabla \tilde{\nu}_c) : \nabla \tilde{\nu}_c \, dx, \quad \forall \tilde{\nu}_c \in H^1(T\Sigma_c), \\
\int_{\Omega} \tilde{\nu}_c \cdot \tilde{\nu}_c \, dx & = \int_{\Omega} (\eta \tilde{\Lambda}_c \nabla \tilde{\nu}_c) : \nabla \tilde{\nu}_c + \frac{1}{\eta} (P_c \frac{\partial F}{\partial \tilde{c}}) : \tilde{\nu}_c \, dx, \quad \forall \tilde{\nu}_c \in H^1(T\Sigma_c),
\end{align*}
\]

or to the strong form

\[
\begin{align*}
P_c \frac{\partial \tilde{c}}{\partial t} & = \nabla \cdot (P_c M_c^{\text{CH}} P_c \nabla \tilde{\nu}_c), \quad \text{in } \Omega \times (0, T], \\
P_c \tilde{\nu}_c & = - \nabla \cdot (\eta \tilde{\Lambda}_c \nabla \tilde{\nu}_c) + \frac{1}{\eta} P_c \frac{\partial F}{\partial \tilde{c}}, \quad \text{in } \Omega \times (0, T],
\end{align*}
\]

\[(\nabla \tilde{\nu}_c)_\nu = (\nabla \tilde{\nu}_c)_\nu = 0, \quad \text{on } \partial \Omega \times (0, T].\]

It is easy to verify the global mass conservation and energy law of the N-phase Cahn-Hilliard model. First, by the first equation of \([2.29]\), we have

\[
\frac{d}{dt} \int_{\Omega} P_c \tilde{c} \, dx = 0.
\]

Note that \(\Gamma^T \tilde{c} = 0\). Then, we have \(\frac{d}{dt} \int_{\Omega} \tilde{c} \, dx = 0\). Further, by taking \(\tilde{v} = \tilde{\phi}_c\) and \(\tilde{q} = \tilde{w}\) in \([2.27]\),
we obtain
\[
\frac{dE(\tilde{\phi})}{dt} = \int_\Omega (A^{-1}\tilde{w}) \cdot (A^{-1}\tilde{\phi}_t) \, dx = -\int_\Omega (M_{\text{CH}}A^{-1}\nabla \tilde{w}) \cdot (A^{-1}\nabla \tilde{w}_t) \, dx \leq 0.
\] (2.32)

From (2.32), we see that the \(N\)-phase Cahn-Hilliard equations describe the energy law in a conservation system, as for the two-phase case.

2.4. Determine of \(M_{AC}^c\) and \(M_{\text{CH}}^c\), and choices of \(F(\cdot)\)

Now, we will use the Assumption 3, to determine the \(M_{AC}^c\) and \(M_{\text{CH}}^c\) appearing in (2.22) and (2.30), respectively. First, since SPD operator is invertible, we know that for any \(W_c\) SPD on \(T\Sigma_c\), there uniquely exists a \(W_c^\dagger\), such that \(W_c W_c^\dagger = W_c^\dagger W_c = I_c\). Clearly, \(W_c\) is also SPD. By direct calculation,

\[
[\nabla \cdot (\hat{A}_c \nabla \tilde{c})]_i = \sum_{k=1}^N \sum_{j=1}^d \partial x_j (\hat{A}_c)_{ik} \partial x_k c_j = \sum_{k=1}^N (\hat{A}_c)_{ik} \Delta c_k = (\hat{A}_c \Delta \tilde{c})_i.
\]

Then, (2.22) can be recast as

\[
\gamma \frac{\partial \tilde{c}}{\partial t} - \eta (M_{AC}^c \hat{A}_c) \Delta \tilde{c} + \frac{1}{\eta} (M_{AC}^c P_c) \frac{\partial F}{\partial \tilde{c}} = 0.
\]

Therefore, the Assumption 3 is equivalent to the following property:

If \(c_i = 0\), then
\[
-\eta \sum_{j=1}^N (M_{AC}^c \hat{A}_c)_{ij} \Delta c_j + \frac{1}{\eta} (M_{AC}^c P_c) \frac{\partial F}{\partial \tilde{c}}_i = 0,
\]

which requires that both the nonlinear potential term and the second-order differential term should vanish identically. Therefore, it is in particular needed that

If \(c_i = 0\), then
\[
\sum_{j=1}^N (M_{AC}^c \hat{A}_c)_{ij} \Delta c_j = 0.
\] (2.33)

Lemma 2.6. For any \(N \geq 2\), (2.33) holds if and only if there exists a constant \(C\) such that

\[
M_{AC}^c \hat{A}_c = CI_c.
\] (2.34)

Proof. It is straightforward that \(M_{AC}^c \hat{A}_c\) is a linear operator from \(T\Sigma_c\) to \(T\Sigma_c\). When \(N = 2\), clearly (2.34) is true as \(\dim(T\Sigma_c) = 1\). When \(N \geq 3\), consider the following set of basis of \(T\Sigma_c\):

\[
\{\tilde{e}_1 - \tilde{e}_N, \tilde{e}_2 - \tilde{e}_N, \ldots, \tilde{e}_{N-1} - \tilde{e}_N\}.
\]

From the property (2.33), each basis forms an invariant 1-dimensional subspace under \(M_{AC}^c \hat{A}_c\), namely

\[
M_{AC}^c \hat{A}_c(\tilde{e}_i - \tilde{e}_N) = \beta_i (\tilde{e}_i - \tilde{e}_N), \quad i = 1, \ldots, N-1.
\]

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Note that for any \(1 \leq i < j \leq N-1\), \(\{\vec{e}_i - \vec{e}_j\}\) is also an invariant 1-dimensional subspace under \(M_{AC}^{\Lambda_c, \dagger}\). Hence,

\[
M_{c}^{AC, \dagger} \Lambda_c(\vec{e}_i - \vec{e}_j) = M_{c}^{AC, \dagger} [(\vec{e}_i - \vec{e}_N) - (\vec{e}_i - \vec{e}_N)] = \beta_i (\vec{e}_i - \vec{e}_N) - \beta_j (\vec{e}_j - \vec{e}_N) \in \{\vec{e}_i - \vec{e}_j\},
\]

which implies that \(\beta_i = \beta_j\). Therefore, there exists a constant \(C\) such that \(\beta_i = C\) for all \(1 \leq i \leq N-1\), which gives rise to (2.34).

For conciseness, the constant \(C\) can be absorbed into the parameter \(\gamma\) in the \(N\)-phase Allen-Cahn equation. Therefore, we choose \(M_{AC}^{\Lambda_c} = \Lambda_c\).

In the similar manner, the Assumption 3 implies the following choice of \(M_{c}^{CH}\) for the \(N\)-phase Cahn-Hilliard equations

\[
M_{c}^{CH} \Lambda_c = M_0 I_c, \quad \text{or} \quad M_{c}^{CH} = M_0 \Lambda_c^{\dagger},
\]

where the positive constant \(M_0\) is called the mobility.

The construction of the nonlinear potential \(F(\cdot)\) satisfying the Assumption 3 is very challenging. This problem is entirely answered for the simplest case in which the pairwise surface tensions are homogeneous, namely \(\sigma_{ij} = \sigma\),

\[
F^{\sigma}(\vec{c}) := F_0^{\sigma}(\vec{c}) + F_1^{\sigma}(\vec{c}),
\]

where

\[
F_0^{\sigma}(\vec{c}) = 2\sigma \sum_{i=1}^{N} f(c_i), \quad F_1^{\sigma}(\vec{c}) = \begin{cases} 0, & N = 2, 3, \\ 8\sigma \sum_{i_1 < i_2 < i_3 < i_4} c_{i_1} c_{i_2} c_{i_3} c_{i_4}, & N \geq 4. \end{cases}
\]

We refer to the Proposition 3.3 in [32]. For the inhomogeneous case, we consider the following nonlinear potential in this paper,

\[
F^{\sigma_{ij}}(\vec{c}) := F_0^{\sigma_{ij}}(\vec{c}) + sF_1^{\sigma_{ij}}(\vec{c})
\]

where

\[
F_0^{\sigma_{ij}}(\vec{c}) = \sum_{i,j=1}^{N} \sigma_{ij} [f(c_i) + f(c_j) - f(c_i + c_j)], \quad F_1^{\sigma_{ij}}(\vec{c}) = \sum_{i,j=1}^{N} \sigma_{ij} c_i^2 c_j^2 (\sum_{k \neq i,j} c_k^2),
\]

and \(s\) is a stabilization parameter in the nonlinear potential. We note that such a choice meets the Assumption 3 when \(K = 2\) [32], namely if only a pair of two fluid phases is present in the system, the \(N\)-phase Allen-Cahn and Cahn-Hilliard equations will fully reduce to those for the corresponding two-phase system. In Section 3.2.2 of [32], the authors successfully constructed the nonlinear potential that meets the Assumption 3 when \(K \leq 3\). However, the construction of the consistent \(N\)-phase nonlinear potential is still an open problem.
2.5. Phase variables with special choice of $A$

Basically, the choice of $A$ in our $N$-phase model does not affect the dynamics of concentrations. In practice, $A$ can be chosen such that the tangent space $T\Sigma$ can easily be represented. To this end, a convenient choice is

$$A = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & \cdots & 1 \end{pmatrix}, \quad A^{-1} = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ -1 & \cdots & -1 \end{pmatrix}, \quad \vec{b} = \vec{0}. \quad (2.39)$$

In this case, the phase variables are

$$\vec{\phi} = \begin{pmatrix} 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N-1} \end{pmatrix} = \begin{pmatrix} c_1 \\ \vdots \\ c_{N-1} \end{pmatrix}. \quad (2.40)$$

We also have $\vec{d} = A^{-1}\vec{1} = (0, \cdots, 0, 1)^T = \vec{e}_N$ and

$$T\Sigma = \{ \vec{v} \mid v_N = 0 \}, \quad P = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 0 \end{pmatrix}. \quad (2.41)$$

Furthermore, in Theorem 2.3 we have $\vec{L}_{kN} = \vec{a}_k - \vec{a}_N = \vec{e}_k$. Thus,

$$\tilde{\Lambda} = \begin{pmatrix} \frac{9}{2} \bar{\sigma}_N & 0 \\ 0 & 0 \end{pmatrix}. \quad (2.42)$$

By combining (2.39) and (2.40), we obtain the $N$-phase Allen-Cahn equations (2.20) under the special choice as

$$\frac{9\gamma}{2} \bar{\sigma}_N \frac{\partial}{\partial t} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N-1} \end{pmatrix} - \nabla \cdot \left( \frac{9\eta}{2} \bar{\sigma}_N \begin{pmatrix} \nabla c_1 \\ \nabla c_2 \\ \vdots \\ \nabla c_{N-1} \end{pmatrix} \right) + \frac{1}{\eta} \begin{pmatrix} \frac{\partial F}{\partial c_1} - \frac{\partial F}{\partial c_N} \\ \frac{\partial F}{\partial c_2} - \frac{\partial F}{\partial c_N} \\ \vdots \\ \frac{\partial F}{\partial c_{N-1}} - \frac{\partial F}{\partial c_N} \end{pmatrix} = 0. \quad (2.41)$$
Similarly, we obtain the $N$-phase Cahn-Hilliard equations (2.28) under the special choice as

\[
\begin{aligned}
\tilde{A} \frac{\partial}{\partial t} \left( \begin{array}{c}
c_1 \\
c_2 \\
\vdots \\
c_{N-1}
\end{array} \right) &= \nabla \cdot \left( \frac{2M_0}{9} \tilde{A} (\tilde{\sigma}^N)^{-1} \tilde{A} \right) \left( \begin{array}{c}
\nabla w_1 \\
\nabla w_2 \\
\vdots \\
\nabla w_{N-1}
\end{array} \right), \\
\tilde{A} \left( \begin{array}{c}
w_1 \\
w_2 \\
\vdots \\
w_{N-1}
\end{array} \right) &= -\nabla \cdot \left( \frac{9\eta}{2} \tilde{\sigma}^N \right) \left( \begin{array}{c}
\nabla c_1 \\
\nabla c_2 \\
\vdots \\
\nabla c_{N-1}
\end{array} \right) + \frac{1}{\eta} \left( \begin{array}{cccc}
\frac{\partial F}{\partial c_1} - \frac{\partial F}{\partial c_N} \\
\frac{\partial F}{\partial c_2} - \frac{\partial F}{\partial c_N} \\
\vdots \\
\frac{\partial F}{\partial c_{N-1}} - \frac{\partial F}{\partial c_N}
\end{array} \right),
\end{aligned}
\]

(2.42)

where

\[
\tilde{A} := \left( \begin{array}{cccc}
2 & 1 & \cdots & 1 \\
1 & 2 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & \cdots & 1 & 2
\end{array} \right) \in \mathbb{R}^{(N-1) \times (N-1)}.
\]

We note that in [33, 35], where the pairwise surface tensions are also considered, the dynamics of concentrations are dependent on the choice of $A$. On the other hand, our model can be viewed as extending the literature by adding the effect of the pairwise surface tensions. For the two-phase case, the $N$-phase Allen-Cahn equations (2.41) are shown to be

\[
\begin{aligned}
\frac{9\gamma}{2} \frac{\partial c_1}{\partial t} - \nabla \cdot \left( \frac{9\eta}{2} \nabla c_1 \right) + \frac{8}{\eta} c_1 (1 - c_1) (1 - 2c_1) = 0.
\end{aligned}
\]

Let $\gamma = \eta$ and take the transformation $c_1 = \frac{1 + \phi}{2}$. Therefore, we have

\[
\frac{\partial \phi}{\partial t} - \Delta \phi + \frac{8}{9\eta^2} (\phi^3 - \phi) = 0,
\]

which yields the standard two-phase Allen-Cahn equation when $\epsilon = \frac{3}{2}\sqrt{2}\eta$, see (2.6).

Similarly, when $N = 2$, the $N$-phase Cahn-Hilliard equations (2.42) are shown to be

\[
\begin{aligned}
2 \frac{\partial c_1}{\partial t} &= \nabla \cdot \left( \frac{8M_0}{9\sigma} \nabla w_1 \right), \\
2w_1 &= -\nabla \cdot \left( \frac{9\eta\sigma}{2} \nabla c_1 \right) + \frac{8\sigma}{\eta} c_1 (1 - c_1) (1 - 2c_1),
\end{aligned}
\]

or

\[
\phi_t + \nabla \cdot \left( \frac{4M_0}{9} \nabla \left( \frac{9\eta}{4} \Delta \phi - \frac{2}{\eta} (\phi^3 - \phi) \right) \right) = 0,
\]

which yields the standard two-phase Cahn-Hilliard equation

\[
\frac{\partial \phi}{\partial t} + \Delta \left( \epsilon \Delta \phi - \frac{1}{\epsilon} (\phi^3 - \phi) \right) = 0,
\]

when $\epsilon = \frac{3}{2}\sqrt{2}\eta$ and $M_0 = \frac{3}{2\sqrt{2}}$. 

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3. Discretization for the $N$-phase Models

In this section, we present some numerical schemes for both $N$-phase Allen-Cahn and $N$-phase Cahn-Hilliard equations. Because of the fundamental role that energy law plays in the phase field model, we will focus on the energy-stable property of the numerical schemes in the discrete level.

The time step size is denoted by $k$. Denote the Hessian matrix of $F(\vec{c})$ as

$$H(\cdot) = \frac{\partial^2 F(\cdot)}{\partial \vec{c}^2}. \quad (3.1)$$

In the two-phase case, it is well-known that the Allen-Cahn equation satisfies the maximum principle, which is also satisfied for the Cahn-Hilliard equations for truncated potentials [41]. The admissible states (3.2) can be regarded as the generalization of the maximum principle in the two-phase case:

$$\mathcal{A}_c = \{ \vec{c} \in \mathbb{R}^N \mid 0 \leq c_i \leq 1, \sum_{i=1}^{N} c_i = 1 \}. \quad (3.2)$$

We note that the SPD property of the coefficient matrix is the critical point for the maximum principle in the two-phase Allen-Cahn equation. For the $N$-phase Allen-Cahn and $N$-phase Cahn-Hilliard equations, we recall that the physical conditions $\vec{c} \in \mathcal{A}_c$ cannot be guaranteed in our models.

From the numerical aspect, let $\mathcal{A}_{c,h}$ be the numerical admissible states of the concentrations. That is, the numerical concentrations are allowed to lie only in $\mathcal{A}_{c,h}$. Then, we define two constants:

$$L_1 := \max_{\xi \in \mathcal{A}_{c,h}} \left| \lambda_{\max} \left( H(\xi) \right) \right|, \quad L_2 := \max_{\xi \in \mathcal{A}_{c,h}} \left| \lambda_{\min} \left( H(\xi) \right) \right|. \quad (3.3)$$

We note that both $L_1$ and $L_2$ depend on the pairwise surface tensions and the stabilization parameter seen in (2.38).

3.1. Numerical schemes for $N$-phase Allen-Cahn equations

In this subsection, we will extend some existing schemes for two-phase Allen-Cahn equations to the $N$-phase versions. Let $V_h$ denote the finite element subspace of $H^1(\Sigma)$. We note again that $\gamma = O(\eta)$ in the $N$-phase Allen-Cahn model is used to render the model consistent with mean curvature flow for the two-phase model. Moreover, by virtue of (2.35) and (2.25), we have

$$A^{-T}M^{AC}A^{-1} = \tilde{\Lambda}.$$ 

Therefore, the strong form of the $N$-phase Allen-Cahn equations (2.20) turn out to be

$$\begin{align*}
\gamma P A \frac{\partial \phi}{\partial t} - \nabla \cdot (\eta \tilde{\Lambda} \nabla \phi) + \frac{1}{\eta} PA^{-T} \frac{\partial F}{\partial \vec{c}} &= 0, \quad \text{in } \Omega \times (0, T], \\
(\nabla \phi) \nu &= 0, \quad \text{on } \partial \Omega \times (0, T].
\end{align*} \quad (3.4)$$
3.1.1. First-order semi-implicit scheme

The first-order semi-implicit scheme for N-phase Allen-Cahn equations (3.4) can be written as

\[
\left( \frac{\gamma}{k} \tilde{A}(\tilde{\phi}_n^h - \tilde{\phi}_n^{n-1}), \tilde{v}_h \right) + (\eta \tilde{\Lambda} \tilde{\phi}_n^h, \nabla \tilde{v}_h) + \left( \frac{1}{\eta} A^{-T} \frac{\partial F}{\partial \tilde{c}}(\tilde{\phi}_n^{n-1}), \tilde{v}_h \right) = 0, \quad \forall \tilde{v}_h \in V_h. \tag{3.5}
\]

Define

\[
G(\tilde{\phi}) := \int_{\Omega} \left( \frac{\eta}{2} \tilde{A} \nabla \tilde{\phi} : \nabla \tilde{\phi} \right)
\]

which can be easily verified to be convex on \( T\Sigma \) thanks to the SPD property of \( \tilde{A} \).

**Theorem 3.1.** For (3.5), under the condition that

\[
k \leq \frac{2 \lambda_{c, \min}}{L_1} \gamma \eta,
\]

the following discrete energy-stability holds:

\[
E(\tilde{\phi}_h^n) + \left( \frac{\gamma \lambda_{c, \min}}{k} \frac{L_1}{2\eta} \right) \| c_h^n - c_h^{n-1} \|_0^2 \leq E(\tilde{\phi}_h^{n-1}),
\]

where \( \lambda_{c, \min} \) is the minimal eigenvalue of \( \tilde{A}_c \) on \( T\Sigma_c \).

**Proof.** In light of the convexity of \( G(\cdot) \), we have

\[
G(\tilde{\phi}_h^n) - G(\tilde{\phi}_h^{n-1}) \leq G'(\tilde{\phi}_h^n)(\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}) = \left( \eta \tilde{\Lambda} \nabla \tilde{\phi}_h^n, \nabla (\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}) \right)
\]

\[
= -\left( \frac{1}{\eta} \tilde{A}^{-T} \frac{\partial F}{\partial \tilde{c}}(\tilde{\phi}_h^{n-1}), \tilde{\phi}_h^n - \tilde{\phi}_h^{n-1} \right) - \left( \frac{\gamma}{k} \tilde{A}(\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}), \tilde{\phi}_h^n - \tilde{\phi}_h^{n-1} \right)
\]

\[
= -\left( \frac{1}{\eta} \frac{\partial F}{\partial \tilde{c}}(\tilde{\phi}_h^{n-1}), \tilde{c}_h^n - \tilde{c}_h^{n-1} \right) - \left( \frac{\gamma}{k} \tilde{A}_c(\tilde{c}_h^n - \tilde{c}_h^{n-1}), \tilde{c}_h^n - \tilde{c}_h^{n-1} \right)
\]

\[
= -\left( \frac{1}{\eta} F(\tilde{\phi}_h^n), 1 \right) + \left( \frac{1}{\eta} F(\tilde{\phi}_h^{n-1}), 1 \right)
\]

\[
- \left( \frac{\gamma}{k} \tilde{A}_c - \frac{1}{2\eta} H(\tilde{c}) \right) (\tilde{c}_h^n - \tilde{c}_h^{n-1}, \tilde{c}_h^n - \tilde{c}_h^{n-1}).
\]

The last equality is derived by the Taylor expansion of \( F(\cdot) \) around \( \tilde{\phi}_h^{n-1} \):

\[
F(\tilde{\phi}_h^n) - F(\tilde{\phi}_h^{n-1}) = \frac{\partial F(\tilde{\phi}_h^{n-1})}{\partial \tilde{c}} \cdot (\tilde{c}_h^n - \tilde{c}_h^{n-1}) + \frac{1}{2}(\tilde{c}_h^n - \tilde{c}_h^{n-1})^T H(\xi)(\tilde{c}_h^n - \tilde{c}_h^{n-1}).
\]

Then, we have

\[
E(\tilde{\phi}_h^n) - E(\tilde{\phi}_h^{n-1}) \leq -\left( \frac{\gamma \lambda_{c, \min}}{k} \frac{L_1}{2\eta} \right) \| c_h^n - c_h^{n-1} \|_0^2.
\]

This completes the proof. \(\square\)
3.1.2. First-order fully-implicit scheme

The first-order fully-implicit scheme for N-phase Allen-Cahn equations (2.19) is:

\[
\left( \frac{\gamma}{k} \bar{A}(\bar{\phi}_h^n - \bar{\phi}_h^{n-1}), \bar{v}_h \right) + (\eta \bar{A} \nabla \bar{\phi}_h^n, \nabla \bar{v}_h) + \left( \frac{1}{\eta} A^{-T} \frac{\partial F}{\partial \bar{c}}(\bar{\phi}_h^n), \bar{v}_h \right) = 0, \quad \forall \bar{v}_h \in V_h. \tag{3.6}
\]

Similar to Theorem 3.1, we have the following theorem for the discrete energy-stability and convexity of the fully-implicit scheme.

**Theorem 3.2.** For (3.6), under the condition that

\[
k \leq \frac{2c_{\text{min}}}{L_2} \gamma \eta,
\]

the following discrete energy-stability holds:

\[
E(\bar{\phi}_h^n) + \left( \frac{\gamma c_{\text{min}}}{k} \frac{L_2}{2 \eta} \right) \| \bar{c}_h^n - \bar{c}_h^{n-1} \|_0^2 \leq E(\bar{\phi}_h^{n-1}).
\]

Furthermore, let

\[
E_1(\bar{\phi}) = \left( \frac{\gamma}{2k} \bar{A}(\bar{\phi} - \bar{\phi}_h^{n-1}), \bar{\phi} - \bar{\phi}_h^{n-1} \right) + \int_{\Omega} \frac{1}{\eta} F(\bar{\phi}) \, dx,
\]

such that (3.6) can be written as \( E_1'(\bar{\phi}_h^n)(\bar{v}_h) + G'(\bar{\phi}_h^n)(\bar{v}_h) = 0 \). Then, \( E_1(\cdot) + G(\cdot) \) is convex when

\[
k \leq \frac{c_{\text{min}}}{L_2} \gamma \eta.
\]

**Proof.** We take the Taylor expansion around \( \bar{\phi}_h^n \) instead to obtain

\[
F(\bar{\phi}_h^n) - F(\bar{\phi}_h^{n-1}) = \frac{\partial F(\bar{\phi}_h^n)}{\partial \bar{c}} \cdot (\bar{c}_h^n - \bar{c}_h^{n-1}) - \frac{1}{2} (\bar{c}_h^n - \bar{c}_h^{n-1})^T \bar{H}(\bar{c}_h^n)(\bar{c}_h^n - \bar{c}_h^{n-1}).
\]

In light of the convexity of \( G(\cdot) \) again, we have

\[
G(\bar{\phi}_h^n) - G(\bar{\phi}_h^{n-1}) \leq G'(\bar{\phi}_h^n)(\bar{\phi}_h^n - \bar{\phi}_h^{n-1})
\]

\[
= -\left( \frac{1}{\eta} F(\bar{\phi}_h^n), 1 \right) + \left( \frac{1}{\eta} F(\bar{\phi}_h^{n-1}), 1 \right)
\]

\[
- \left( \frac{\gamma}{k} \bar{A}_c \left[ \frac{1}{2} H(\bar{\xi}) \right] (\bar{c}_h^n - \bar{c}_h^{n-1}), (\bar{c}_h^n - \bar{c}_h^{n-1}) \right).
\]

Thus,

\[
E(\bar{\phi}_h^n) - E(\bar{\phi}_h^{n-1}) \leq -\left( \frac{\gamma c_{\text{min}}}{k} \frac{L_2}{2 \eta} \right) \| \bar{c}_h^n - \bar{c}_h^{n-1} \|_0^2.
\]

When \( k \leq \frac{c_{\text{min}}}{L_2} \gamma \eta \) and the Taylor expansion is applied again, we have

\[
E_1(\bar{\phi}) - E_1(\bar{\phi}_h^{n-1}) - E_1'(\bar{\phi})(\bar{\phi} - \bar{\phi}_h^{n-1}) - \left[ \frac{\gamma}{2k} \bar{A}_c \left[ \frac{1}{2} H(\bar{\xi}) \right] A^{-1}(\bar{\phi} - \bar{\phi}_h^{n-1}), A^{-1}(\bar{\phi} - \bar{\phi}_h^{n-1}) \right] \leq 0,
\]

which means that \( E_1(\cdot) \) is convex. Hence, \( \bar{\phi}_h^n \) in (3.6) is the local minimizer of the convex functional \( E_1(\cdot) + G(\cdot) \) on \( V_h \). □
3.1.3. Modified Crank-Nicolson scheme

Now we will try to extend the modified Crank-Nicolson scheme \cite{37, 42} to the \(N\)-phase Allen-Cahn equations. Define the finite difference of \(f\) as

\[
 f[c, c^\ast] := \begin{cases} \frac{f(c) - f(c^\ast)}{c - c^\ast}, & c \neq c^\ast, \\ \frac{f'(c)}{c^\ast}, & c = c^\ast. \end{cases} \tag{3.7}
\]

For any set \(i = \{i_1, i_2, \cdots, i_k\}\) and monomial \(q_i(\vec{c}) = c_{i_1}c_{i_2} \cdots c_{i_k}\), we define the finite difference of \(q_i\) as

\[
 q_i[\vec{c}, \vec{c}^\ast] = \frac{1}{k!} \sum_{l=1}^{k} \left[ \sum_{j \subset i - \{i_l\}} |j|!(k - |j| - 1)!q_j(\vec{c})q_{i - j - \{i_l\}}(\vec{c}^\ast) \right] \vec{e}_{i_l}, \tag{3.8}
\]

where we denote \(q_{\emptyset} = 1\). Then, we have the following crucial lemma.

**Lemma 3.3.** It holds that

\[
 q_i(\vec{c}) - q_i(\vec{c}^\ast) = q_i[\vec{c}, \vec{c}^\ast] \cdot (\vec{c} - \vec{c}^\ast). \tag{3.9}
\]

**Proof.** We will prove it by induction. It is straightforward that \(q_i[\vec{c}, \vec{c}^\ast] = \vec{e}_{i_l}\) when \(k = 1\). Assume \eqref{3.9} holds for \(|i| = k - 1\). From the fact that for any \(i = \{i_1, i_2, \cdots, i_k\}\),

\[
 q_i(\vec{c}) - q_i(\vec{c}^\ast) = q_{i - \{i_s\}}(\vec{c})(c_{i_s} - c_{i_s}^\ast) + c_{i_s}^\ast \left[ q_{i - \{i_s\}}(\vec{c}) - q_{i - \{i_s\}}(\vec{c}^\ast) \right], \quad \forall 1 \leq s \leq k,
\]

we have

\[
 q_i(\vec{c}) - q_i(\vec{c}^\ast) = \frac{1}{k} \left\{ \sum_{s=1}^{k} q_{i - \{i_s\}}(\vec{c})(c_{i_s} - c_{i_s}^\ast) + c_{i_s}^\ast \left[ q_{i - \{i_s\}}(\vec{c}) - q_{i - \{i_s\}}(\vec{c}^\ast) \right] \right\}
\]

\[
 = \frac{1}{k} \left[ \sum_{s=1}^{k} q_{i - \{i_s\}}(\vec{c}) \vec{e}_{i_s} \right] \cdot (\vec{c} - \vec{c}^\ast)
\]

\[
 + \frac{1}{k!} \sum_{s=1}^{k} \sum_{l=1, l \neq s}^{k} c_{i_s}^\ast \left[ \sum_{j \subset i - \{i_s, i_s\}} |j|!(k - |j| - 2)!q_j(\vec{c})q_{i - j - \{i_s, i_s\}}(\vec{c}^\ast) \right] \vec{e}_{i_l} \cdot (\vec{c} - \vec{c}^\ast)
\]

Notice that

\[
 \frac{1}{k!} \sum_{s=1}^{k} \sum_{l=1, l \neq s}^{k} c_{i_s}^\ast \left[ \sum_{j \subset i - \{i_s, i_s\}} |j|!(k - |j| - 2)!q_j(\vec{c})q_{i - j - \{i_s, i_s\}}(\vec{c}^\ast) \right] \vec{e}_{i_l}
\]

\[
 = \frac{1}{k!} \sum_{l=1}^{k} \sum_{s=1, s \neq l}^{k} \left[ \sum_{j \subset i - \{i_s\}} |j|!(k - |j| - 2)!q_j(\vec{c})q_{i - j - \{i_l\}}(\vec{c}^\ast) \right] \vec{e}_{i_l}
\]

\[
 = \frac{1}{k!} \sum_{l=1}^{k} \left[ \sum_{j \subset i - \{i_l\}, j \neq i - \{i_l\}} |j|!(k - |j| - 1)!q_j(\vec{c})q_{i - j - \{i_l\}}(\vec{c}^\ast) \right] \vec{e}_{i_l}.
\]

Therefore, we have \eqref{3.9} when \(|i| = k\). This completes the proof. \qed

\textit{20}
In light of the above lemma, we define the finite difference of the nonlinear potential \( F \) as follows. For the homogeneous case (2.37),

\[
F^\sigma [\tilde{c}, \tilde{c}^*] := 2\sigma \begin{pmatrix} f[c_1, c_1^*] \\ f[c_2, c_2^*] \\ \vdots \\ f[c_N, c_N^*] \end{pmatrix} + 8\sigma \sum_{i_1 < i_2 < i_3 < i_4} q(i_1, i_2, i_3, i_4) [\tilde{c}, \tilde{c}^*].
\]  

(3.10)

For the inhomogeneous case (2.38),

\[
F^{\sigma ij} [\tilde{c}, \tilde{c}^*] := \left( \sum_{j=1}^{N} \sigma_N \left( f[c_1, c_1^*] - f[c_1 + c_j, c_1^* + c_j^*] \right) \right) + 8\sum_{i,j=1, k \neq i,j}^{N} \sigma_N \left( f[c_1, c_1^*] - f[c_1 + c_j, c_1^* + c_j^*] \right) q(i,j,k) [\tilde{c}, \tilde{c}^*].
\]  

(3.11)

Let \( F = F^\sigma \) or \( F^{\sigma ij} \). Then, a routine calculation shows that

\[
F(c) - F(c^*) = F[\tilde{c}, \tilde{c}^*] \cdot (\tilde{c} - \tilde{c}^*).
\]

We, therefore, obtain the following modified Crank-Nicolson scheme:

\[
\left( \frac{\gamma}{k} \tilde{A} (\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}), \tilde{v}_h \right) + (\eta \tilde{A} \nabla \tilde{\phi}_h^n + \tilde{\phi}_h^n, \nabla \tilde{v}_h) + \left( \frac{1}{\eta} \tilde{A}^{-T} F[\tilde{c}_h^n, \tilde{c}_h^{n-1}], \tilde{v}_h \right) = 0, \quad \forall \tilde{v}_h \in V_h. \]

(3.12)

Taking \( \tilde{v}_h = \tilde{\phi}_h^n - \tilde{\phi}_h^{n-1} \), we immediately obtain the following result:

**Theorem 3.4.** Scheme (3.12) is unconditionally energy-stable, and

\[
E(\tilde{\phi}_h^n) + \frac{\gamma}{k} \| \tilde{c}_h^n - \tilde{c}_h^{n-1} \|_0^2 = E(\tilde{\phi}_h^{n-1}).
\]

This theorem satisfies the unconditionally energy-stability of the modified Crank-Nicolson scheme. However, it is necessary to solve a nonlinear system, the existence and uniqueness for which can only be numerically validated under a condition \( k \leq C\eta^2 \) for a certain constant \( C > 0 \). We refer to [12] for proof of the two-phase case and the numerical tests for the \( N \)-phase case in Section 4.

3.2. Numerical schemes for \( N \)-phase Cahn-Hilliard equations

We will discuss the numerical schemes for \( N \)-phase Cahn-Hilliard equations. In this subsection, we denote \( V_h, Q_h \) as the finite element subspace of \( H_1(T\Sigma) \). By virtue of (2.36), the strong form of the \( N \)-phase Cahn-Hilliard equations (2.28) turn out to be

\[
\begin{cases}
PA^{-T} A^{-1} \frac{\partial \tilde{\phi}}{\partial t} = \nabla \cdot \left[ M_0 (A^{-1} P)^T \tilde{A}_c A^{-1} P \nabla \tilde{w} \right], & \text{in } \Omega \times (0, T), \\
PA^{-T} A^{-1} \tilde{w} = -\nabla \cdot (\eta \tilde{A} \nabla \tilde{\phi}) + \frac{1}{\eta} PF \frac{\partial F}{\partial \tilde{c}}, & \text{in } \Omega \times (0, T), \\
(\nabla \tilde{\phi})_\nu = (\nabla \tilde{w})_\nu = 0, & \text{on } \partial \Omega \times (0, T).
\end{cases}
\]

(3.13)
3.2.1. First-order semi-implicit scheme

To make the scheme energy stable, we give the following first-order semi-implicit scheme for N-phase Cahn-Hilliard equations:

\[
\begin{aligned}
\left( A^{-1}(\bar{\phi}_h^n - \bar{\phi}_h^{n-1}), A^{-1}\bar{\eta}_h \right) + k(M_0 A_c^{-1} \nabla \bar{w}_h^{n}, A^{-1} \nabla \bar{\eta}_h) &= 0, \quad \forall \bar{\eta}_h \in Q_h, \\
-(A^{-1} \bar{w}_h^n, A^{-1} \bar{v}_h^n) + (\eta A \nabla \bar{\phi}_h^n, \nabla \bar{v}_h^n) + \left( \frac{1}{\eta} A^{-1} \frac{\partial F(\bar{\phi}_h^{n-1})}{\partial \bar{c}} , \bar{v}_h^n \right) &= 0, \quad \forall \bar{v}_h \in V_h.
\end{aligned}
\]  

(3.14)

Theorem 3.5. For (3.14), if \( Q_h \subset V_h \), then energy-stability holds when

\[ k \leq \frac{8\lambda_{c,\text{min}}^2}{M_0 L_1^2 \eta^3}, \]  

where \( \lambda_{c,\text{min}} \) is the minimal eigenvalue of \( \tilde{A}_c \) on \( T\Sigma_c \).

Proof. Taking \( \bar{\eta}_h = \bar{w}_h \) and \( \bar{v}_h = \bar{\phi}_h^n - \bar{\phi}_h^{n-1} \) in (3.14), we obtain

\[
k(M_0 A_c^{-1} \nabla \bar{w}_h^n, A^{-1} \nabla \bar{w}_h^n) + (\eta A \nabla \bar{\phi}_h^n, \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1})) + \left( \frac{1}{\eta} A^{-1} \frac{\partial F(\bar{\phi}_h^{n-1})}{\partial \bar{c}} , \bar{c}_h^n - \bar{c}_h^{n-1} \right) = 0.
\]

With the help of the Taylor expansion around \( \bar{\phi}_h^{n-1} \) and the fact that

\[
(A \nabla \bar{\phi}_h^n, \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1})) = \frac{1}{2} \left( A \nabla \bar{\phi}_h^n, \nabla \bar{\phi}_h^n \right) - \frac{1}{2} \left( A \nabla \bar{\phi}_h^{n-1}, \nabla \bar{\phi}_h^{n-1} \right) + \frac{1}{2} \left( A \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1}), \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1}) \right),
\]

we have

\[
E(\bar{\phi}_h^n) - E(\bar{\phi}_h^{n-1}) = \left( \frac{1}{2\eta} H(\bar{\xi}(c_h^n - c_h^{n-1}), c_h^n - c_h^{n-1}) \right) \\
\quad - k \left( M_0 A_c^{-1} \nabla \bar{w}_h^n, A^{-1} \nabla \bar{w}_h^n \right) - \left( \frac{\eta}{2} A \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1}), \nabla (\bar{\phi}_h^n - \bar{\phi}_h^{n-1}) \right) \\
\leq \frac{L_1}{2\eta} \| c_h^n - c_h^{n-1} \|_0^2 + \frac{1}{k} \left( M_0 A_c \nabla \bar{c}_h^n, \nabla \bar{c}_h^n \right) - \left( \frac{\eta}{2} A_c \nabla (c_h^n - c_h^{n-1}), \nabla (c_h^n - c_h^{n-1}) \right),
\]

(3.16)

where \( \bar{w}_{c,h} = A^{-1} \bar{w}_h \in H^1(T\Sigma_c) \). If \( Q_h \subset V_h \), then \( \bar{\eta}_h \) can be taken as \( \bar{\phi}_h^n - \bar{\phi}_h^{n-1} \) in order to obtain

\[
k \left( M_0 A_c^{-1} \nabla \bar{w}_h^n, \nabla (c_h^n - c_h^{n-1}) \right) = -\frac{1}{k} \| c_h^n - c_h^{n-1} \|_0^2.
\]

Then,

\[
k \left( M_0 A_c \nabla \bar{c}_h^n, \nabla (c_h^n - c_h^{n-1}) \right) + \left( \frac{\eta}{2} A_c \nabla (c_h^n - c_h^{n-1}), \nabla (c_h^n - c_h^{n-1}) \right) \\
= \frac{k}{M_0} \left( A_c (M_0 A_c^{-1} \nabla \bar{w}_h^n), (M_0 A_c^{-1} \nabla \bar{w}_h^n) \right) + \left( \frac{\eta}{2} A_c \nabla (c_h^n - c_h^{n-1}), \nabla (c_h^n - c_h^{n-1}) \right) \\
\geq -2\lambda_{c,\text{min}} \sqrt{\frac{\eta k}{2M_0}} \left( M_0 A_c \nabla \bar{c}_h^n, \nabla (c_h^n - c_h^{n-1}) \right) = \lambda_{c,\text{min}} \sqrt{\frac{2\eta}{M_0 k}} \| c_h^n - c_h^{n-1} \|_0^2.
\]

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Then, from \[3.16\],
\[ E(\tilde{\phi}_h^n) - E(\tilde{\phi}_h^{n-1}) \leq - (\lambda_{c,\min} \sqrt{\frac{2\eta}{M_0 k}} - \frac{L_1}{2\eta}) \|c_h^n - c_h^{n-1}\|^2, \]
which gives rise to the energy-stability when \[3.15\] holds. \[\square\]

3.2.2. Some nonlinear schemes

By applying the similar idea of the fully-implicit scheme for \(N\)-phase Allen-Cahn equations, we have the following first-order fully-implicit scheme for \(N\)-phase Cahn-Hilliard equations:

\[ \begin{align*}
& (A^{-1}(\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}), A^{-1}\tilde{q}_h^n) + k(M_0 \tilde{A}_c^+ A^{-1} \nabla \tilde{w}_h^n, A^{-1} \nabla \tilde{q}_h^n) = 0, \quad \forall \tilde{q}_h^n \in Q_h, \\
& -(A^{-1}\tilde{w}_h^n, A^{-1}\tilde{v}_h^n) + (\eta \tilde{A} \nabla \tilde{\phi}_h^n, \nabla \tilde{v}_h^n) + \left( \frac{1}{\eta} A^{-T} \frac{\partial F(\tilde{\phi}_h^n)}{\partial c}, \tilde{v}_h^n \right) = 0, \quad \forall \tilde{v}_h^n \in V_h.
\end{align*} \]  

(3.17)

And, the following theorem can be proved by slightly modifying the proof of Theorem 3.5.

**Theorem 3.6.** For \[3.17\], if \(Q_h \subset V_h\), then energy-stability holds when

\[ k \leq \frac{8\lambda_{c,\min}^2}{M_0 L_2^2 \eta^3}. \]  

(3.18)

Another naturally extended scheme for \(N\)-phase Cahn-Hilliard equations is the modified Crank-Nicolson scheme:

\[ \begin{align*}
& (A^{-1}(\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}), A^{-1}\tilde{q}_h^n) + k(M_0 \tilde{A}_c^+ A^{-1} \nabla \tilde{w}_h^n, A^{-1} \nabla \tilde{q}_h^n) = 0, \quad \forall \tilde{q}_h^n \in Q_h, \\
& -(A^{-1}\tilde{w}_h^n, A^{-1}\tilde{v}_h^n) + (\eta \tilde{A} \nabla \tilde{\phi}_h^n + \tilde{\phi}_h^{n-1}, \nabla \tilde{v}_h^n) + \left( \frac{1}{\eta} A^{-T} F(\tilde{\phi}_h^n, \tilde{c}_h^{n-1}), \tilde{v}_h^n \right) = 0, \quad \forall \tilde{v}_h^n \in V_h,
\end{align*} \]  

(3.19)

where \(F[\cdot, \cdot]\) is the finite difference of the nonlinear potential defined in \[3.10\] and \[3.11\], regarding to the homogeneous and inhomogeneous case, respectively. The following energy-stability can be proved, as expected.

**Theorem 3.7.** Scheme \[3.19\] is unconditionally energy-stable.

**Proof.** Taking \(\tilde{v}_h = \tilde{\phi}_h^n - \tilde{\phi}_h^{n-1}\) and \(\tilde{q}_h = \tilde{w}_h^n\) in \[3.19\], we have

\[ E(\tilde{\phi}_h^n) - E(\tilde{\phi}_h^{n-1}) = (A^{-1}\tilde{w}_h^n, A^{-1}(\tilde{\phi}_h^n - \tilde{\phi}_h^{n-1})) = -k(M_0 \tilde{A}_c^+ A^{-1} \nabla \tilde{w}_h^n, A^{-1} \nabla \tilde{w}_h^n) \leq 0. \]

This completes the proof. \[\square\]

We note that nonlinear schemes \[3.17\] and \[3.19\] for \(N\)-phase Cahn-Hilliard equations require the nonlinear solver at each time step, the convergence of which is difficult to verify. Intuitively, one needs to balance the energy stability of the numerical scheme and the convergence of the solver at each time step. In the numerical tests, we will focus on the semi-implicit scheme for \(N\)-phase Cahn-Hilliard equations.
4. Numerical Results

In this section, we introduce a series of numerical experiments to illustrate the characteristics of the schemes for our \( N \)-phase model. With the special choice of \( \mathbf{A} \) in (2.39), we know that

\[
H^1(T\Sigma) = \{ \vec{v} \in H^1(\mathbb{R}^N) \mid v_N = 0 \},
\]

which can be discretized by the piecewise linear Lagrangian element for the first \( N - 1 \) components. Suppose that the domain is subdivided by a shape-regular simplicial grid \( T_h = \{ K \} \). Then, in the numerical experiments, we apply

\[
V_h = Q_h = \{ \vec{v}_h \in H^1(\mathbb{R}^N) \mid v_i|_K \in P_1(K), 1 \leq i \leq N - 1, v_N = 0 \}.
\]

4.1. \( N \)-phase Allen-Cahn: Grain growth on the unit square domain

In order to validate the numerical algorithm for \( N \)-phase Allen-Cahn equations, we consider the grain growth on the unit square domain \( \Omega = [0, 1] \times [0, 1] \) with \( N = 5 \). The uniform mesh with \( h = 1/256 \) is used for computation. The initial condition here is a randomly chosen superposition of 1,000 circular grains, whose radii range from 0.01 to 0.04. We set the characteristic scale of the interfacial thickness \( \eta = 0.005 \) and the interfacial surface tension \( \sigma_{ij} = 1 \) so that the coefficient matrix \( \tilde{\mathbf{A}} = O(1) \) is computed by (2.12). The nonlinear potential is chosen as (2.37). The parameter is \( \gamma = \eta \).

First, we illustrate the energy-stability of different schemes. The time step size is chosen as \( k = 2 \times 10^{-5} \) for the semi-implicit scheme (3.5), the fully-implicit scheme (3.6), and the modified Crank-Nicolson scheme (3.12). The initial conditions for these schemes are the same. For the nonlinear scheme in each time step, the numerical solution on previous step \( \phi_{n-1}^h \) is used as the initial guess, and the standard Newton solver is applied with the stopping criteria that the residual is less than \( 10^{-5} \) times the initial residual. Figure 4.1 shows the initial condition and evolution of the phases computed by the modified Crank-Nicolson scheme. Similar to the results in [26, 27], we observe fast separation in the beginning and slower dynamics in the course of the evolution. The evolution of the Liapunov free-energy for each scheme is depicted in Figure 4.2. All the schemes can be observed to be energy-stable, and the respective dissipation rates of the fully-implicit and modified Crank-Nicolson schemes are very similar.

4.2. \( N \)-phase Cahn-Hilliard: Spinodal decomposition – the phase separation of a three-component mixture

The second numerical experiment is the phase separation of a three-phase mixture by spinodal decomposition. Similar tests are also studied in [25, 27, 28]. The initial conditions are random perturbations of state \( \vec{c} = \vec{\rho} \) with the maximum amplitude of 0.04, that is,

\[
\vec{c} = \begin{pmatrix}
\rho_1 + 0.06(2\xi_1 - \xi_2 - \xi_3)/3 \\
\rho_2 + 0.06(-\xi_1 + 2\xi_2 - \xi_3)/3 \\
\rho_3 + 0.06(-\xi_1 - \xi_2 + 2\xi_3)/3
\end{pmatrix},
\]

where \( \xi_i \sim \mathcal{U}[0, 1] \) are the random variables that obey the uniform distribution. A \( 160 \times 160 \times 2 \) uniform triangular grid is used on the computational domain \( \Omega = [0, 1] \times [0, 1] \). We take \( \eta = 0.01 \), \( M_0 = \frac{3}{2\sqrt{2}} \), and the nonlinear potential as (2.38) with \( s = 0 \). The time step size is set to be \( k = 1 \times 10^{-6} \).
Figure 4.1: $N$-phase Allen-Cahn equations: Evolution of the phases for $N = 5$ by modified Crank-Nicolson scheme

Figure 4.2: $N$-phase Allen-Cahn equations: Evolution of energy for $N = 5$
In the first three tests, the homogeneous surface tension $\sigma_{ij} = 1$ is applied with different states $\vec{\rho}$. For the uniform state $\vec{\rho} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})^T$, the result is presented in Figure 4.3a. As expected, the three phases have similar dynamics evolution, as the pairwise surface tensions and composition are completely symmetric with respect to the four phases. When the initial state is non-uniform, spinodal decomposition takes place and the system separates into spatial regions rich in some phases and poor in others. For $\vec{\rho} = (\frac{1}{4}, \frac{1}{4}, \frac{1}{2})^T$, the early states of spinodal decomposition are observed in Figure 4.3b. When $\vec{\rho} = (\frac{1}{5}, \frac{1}{5}, \frac{3}{5})^T$, the phase 3 (blue) in Figure 4.3c dominates the evolution, which leads to spinodal decomposition.

Thanks to our generalized multiphase models, we are able to simulate the spinodal decomposition for the inhomogeneous surface tension case. Here, we set $\sigma_{13} = 1.69$ and the others are $\sigma_{ij} = 1$. As shown in Figure 4.3d–4.3f, the phase 1 (red) and phase 3 (blue) tend to repel each other due to the relatively large surface tension of each.

![Figure 4.3](image-url)

Figure 4.3: N-phase Cahn-Hilliard equations: Evolution of spinodal decomposition with different surface tensions, $t = 500k = 5 \times 10^{-4}$

4.3. N-phase Cahn-Hilliard: Triple junctions in a quaternary system

The last experiment numerically simulates the evolution of the triple junctions in a quaternary system. In [25], the authors proposed a test for the homogeneous surface tension case. Here, we intend to demonstrate the effect of pairwise surface tensions, especially for the inhomogeneous case.
For all the experiments for triple junctions, we simulate how a T-shaped triple junction approaches a local equilibrium state under the effect of pairwise surface tensions. A 100 × 100 × 2 uniform triangular grid is used on the computational domain Ω = [0, 1] × [0, 1]. In the semi-implicit scheme (3.14), the parameters are chosen as η = 0.02. The mobility are set as M₀ = \( \frac{3}{2\sqrt{2}} \). The initial profile and corresponding coloring are depicted in Figure 4.4a and 4.4b, respectively. The solutions are computed until numerically stationary. Even though the time step size can be set small enough to guarantee the energy stability, we observe in our experiments that it may vary according to the current state. In general, when the phases evolving fast or approaching to the topological change, the time step size should be set small. Otherwise, it can be set larger than the theoretical constraint (3.15) to speed up the simulation.

In Figure 4.4c–4.4f, we display the evolution of the interface for the case in which \( \sigma_{ij} = 1 \). The stabilization parameter in the nonlinear potential (2.38) is set as s = 30, and the minimal time step size is set as \( k = 5 \times 10^{-8} \). For this case with homogeneous surface tension, we observe that the triple junction angles approach the true value 120° as they approach a local equilibrium state. We then compute two inhomogeneous surface tension cases as follows:

- **Inhomogeneous case 1:**
  \[
  \sigma_{ij} = \begin{cases} 
  1.69, & (i, j) = (1, 2), \\
  1, & \text{else}. 
  \end{cases}
  \]

- **Inhomogeneous case 2:**
  \[
  \sigma_{ij} = \begin{cases} 
  2.56, & (i, j) = (1, 2), \\
  1, & \text{else}. 
  \end{cases}
  \]

It is easy to check that these two sets of surface tensions satisfy the condition in Theorem 2.3. Thus, \( \tilde{\Lambda} \) is SPD on the tangent space \( T\Sigma \). As can be seen from Figure 4.4g–4.4j, for the inhomogeneous case 1, the interface between phases 1 and 2 becomes smaller and smaller due to the relatively large surface tension. Moreover, the inhomogeneous case 2 encounters the situation with \( \sigma_{12} > \sigma_{13} + \sigma_{23} \) and \( \sigma_{12} > \sigma_{14} + \sigma_{24} \), which corresponds to the total wetting \( \text{[1]} \) that the phase 1 and 2 will be penetrated by phase 3 and 4, as shown in Figure 4.4k-4.4n.

5. Concluding Remarks

In this paper, we presented multiphase Allen-Cahn and Cahn-Hilliard models and their finite element discretizations accounting for the effect of pairwise surface tensions. The free-energy functional with a coefficient matrix in the capillary term was set up for the generalized phase variables. By checking the consistency with the two-phase model, we gave a set of linear equations between the coefficient matrix and pairwise surface tensions. Thanks to the relationship between the symmetric matrix space and simplex, we proved the solvability of the coefficient matrix on the tangent space of solution manifold — an \( (N - 1) \)-dimensional hyperplane. Furthermore, we gave two sufficient and necessary conditions for the SPD of the coefficient matrix — conditions that are fundamental to the well-posedness of \( N \)-phase Allen-Cahn and \( N \)-phase Cahn-Hilliard models presented.

Our derivation of the \( N \)-phase Allen-Cahn and Cahn-Hilliard equations stems from the formulation of the free-energy functional and the gradient flows on the solution manifold. With the introduction of an induced inner product on the tangent space, the dynamics of concentrations of both models are inherently invariant, that is, independent of the choice of phase variables. Based
Figure 4.4: \( N \)-phase Cahn-Hilliard equations: Evolution of triple junctions with different surface tensions.
on this nice property, a special choice of phase variables is used in the numerical simulation to clarify the tangent space. We proposed semi-implicit, fully-implicit, and modified Crank-Nicolson schemes in the finite element framework for $N$-phase Allen-Cahn equations, such that the energy-stability properties are similar to the two-phase model. We also numerically verified the efficiency and energy-stability of each scheme by simulating the grain growth on the unit square domain. For the finite element discretization of $N$-phase Cahn-Hilliard equations, the semi-implicit, fully-implicit, and modified Crank-Nicolson schemes were also discussed. Further, the effect of inhomogeneous surface tensions on the spinodal decomposition was investigated. Finally, we carried out numerical experiments focused on the evolution of triple junctions in order to establish and demonstrate the ability of these models to deal with inhomogeneous surface tensions.

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