NUMERICAL APPROXIMATIONS FOR A THREE COMPONENT CAHN-HILLIARD PHASE-FIELD MODEL BASED ON THE INVARIANT ENERGY QUADRATIZATION METHOD

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Abstract. How to develop efficient numerical schemes while preserving the energy stability at the discrete level is a challenging issue for the three component Cahn-Hillard phase-field model. We develop in this paper first and second order temporal approximation schemes based on the "Invariant Energy Quadratization" method, where all nonlinear terms are treated semi-explicitly. Consequently, the resulting numerical schemes lead to a symmetric positive definite linear system to be solved at each time step. We rigorously prove that the proposed schemes are unconditional energy stable. Various 2D and 3D numerical simulations are presented to demonstrate the stability and the accuracy of the schemes.

Key words. Phase-field model; Chan-Hilliard, Three phase; Unconditional Energy Stability; Invariant Energy Quadratization.

1. Introduction.

The phase-field (i.e. the diffuse-interface) approach is a robust modeling approach to simulate the free interface problem (cf. [?,?,?,?,?,?,?,?,?,?,?,?], and the references therein). Its essential idea is to use one (or more) continuous phase-field variable(s) to describe different phases in the multi-components system, and represents the interfaces by thin, smooth transition layers. The constitutive equations for those phase-field variables can be derived from the energetic variational formalism, the governing system of equations is thereby well-posed and thermo-dynamically consistent. Consequently, one can carry out mathematical analyses to show solution existence and uniqueness in appropriate functional spaces, and to develop convergent numerical schemes.

For the two phase system, the commonly used free energy for the system consists of (i) a double-well bulk part which promotes either of the two phases in the bulk, yielding a hydrophobic contribution to the free energy; and (ii) a conformational capillary entropic term that promotes hydrophilicity in the multiphase material system. The competition between the hydrophilic and hydrophobic part in the free energy forms the mechanism for the coexistence of two distinctive phases in the two-phase system. The corresponding binary system can be modeled either by the Allen–Cahn equation (second order) or the Cahn–Hilliard equation (fourth order). For both of these two models, there have been many theoretical analysis, algorithm developments and numerical simulations (cf. [?, ?, ?, ?]).

The generalization from the two-phase system to multi-phases have been studied by many (cf. [?,?,?,?,?,?,?,?,?,?,?,?,?]). Specifically, for the system with three components, the general framework is to adopt three independent phase variables (c_1, c_2, c_3) while imposing a hyperplane link condition among the three variables $(c_1 + c_2 + c_3 = 1)$. The free energy is simply a summation of the original double-well energy for each phase variable [?, ?, ?]. Moreover, in order to ensure the boundedness (from below) of the free energy, especially for the total spreading case where one of the coefficients for the bulk energy becomes negative, an extra sixth order polynomial term is needed [?, ?], which

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couples the three phase variables altogether.

In general, it is very challenging to develop energy stable schemes to solve the three components Cahn-Hilliard phase-field system, since all three phase variables are nonlinearly coupled. We emphasize that the preservation of energy stability laws is critical for numerical methods to capture the correct long time dynamics of the system. Furthermore, the energy-law preserving schemes provide flexibility for dealing with stiffness issue in phase-filed models. Simple fully implicit or semi-implicit schemes often lead to quite severe stability conditions so they are not efficient in practice [?, ?, ?, ?, ?].

Although a variety of numerical algorithms have been developed for the three phase Cahn-Hilliard model, most of the existing methods are either first-order accurate in time, and/or are not energy stable. We refer to [?] for a summary on recent advances about the three-phase models and their numerical approximations. In particular, the authors of [?] concluded that (i) the fully implicit discretization of the six-order polynomial term leads to non convergence of the Newton linearization method for the total spreading case; (ii) it is questionable to establish convex-concave decomposition for the six order polynomial term; and (iii) A semi-implicit scheme is the best choice if it can preserve the energy dissipation law (a desired property known as unconditionally energy stable) for any time step, and the existence and the convergence can be thereby proved. However, the semi-implicit schemes proposed in [?] are nonlinear, thus they require some efficient iterative solvers in the implementations.

The main focus of this paper is to develop linear and unconditionally energy stable schemes to solve the three component Cahn-Hilliard system. Instead of using convex splitting, or various tricky Taylor expansions to discretize the nonlinear potentials, we adopt the *Invariant Energy Quadratization* (IEQ) approach, where we introduce some nonlinear transformations to enforce the free energy density as an invariant, quadratic functionals in terms of new, auxiliary variables. The IEQ method has been successfully applied in the context of other models in the authors' other work, for example, the surfactant model, crystal model, or vesicle model, (cf. [?, ?, ?, ?, ?, ?]). However, application of IEQ method to the three component model is faced with new challenges due to the nonlinearities in the Lagrange multiplier term, and the sixth order polynomial potential.

The essential idea of the IEQ method is to transform the free energy into a quadratic form (since the nonlinear potential is usually bounded from below) of a new variable via a change of variables. The new, equivalent system still retains a similar energy dissipation law in terms of the new variable. For the time-continuous case, the energy law of the new reformulated system is equivalent to the energy law of the original system. One great advantage of such reformulation is that all nonlinear terms can be treated semi-explicitly, which in turn leads to a linear system. Moreover, the resulting linear system is symmetric positive definite, thus it can be solved efficiently with simple iterative methods such as CG or other Krylov subspace methods. Using this new strategy, we develop a series of linear and energy stable numerical schemes, without introducing artificial stabilizers as in [?, ?] or using convex splitting (cf. [?, ?, ?, ?]).

In summary, the new numerical schemes that we develop in this paper possess the following properties: (i) the schemes are *accurate* (up to second order in time); (ii) they are *unconditionally energy stable* ; and (iii) they are *efficient and easy to implement* (lead to symmetric positive definite linear system at each time step). To the best of our knowledge, the proposed schemes are the first such schemes for solving the three-phase Cahn-Hilliard phase-field system that can have all these desired properties.

The rest of the paper is organized as follows. In Section 2, we give a brief introduction of the model. In Section 3, we construct numerical schemes and prove their unconditional energy stability and solvability in the time discrete case. In Section 4, we conduct numerical convergence tests and present various numerical simulations of dendritic crystal growth in 2D and 3D to demonstrate the accuracy and efficiency of the proposed schemes. Finally, some concluding remarks are presented in Section 5.

2. Model System. We now introduce the three component Cahn-Hilliard phase-field model proposed in [**?**, **?**]. Let Ω be a smooth, open bounded, connected domain in $\mathbb{R}^d$, $d = 2, 3$. Let c_i $(i = 1, 2, 3)$ be the $i-th$ phase function (or order parameter) which represents the volume fraction of the $i-$th component in the mixture, i.e.,

$$c_i = \begin{cases} 1 & \text{inside the i-th component,} \\ 0 & \text{outside the i-th component.} \end{cases} \tag{2.1}$$

In the phase-field framework, a thin (of thickness ϵ) but smooth layer is used to connect between the interface between 0 and 1. The three unknowns c_1, c_2, c_3 are linked though the relationship:

$$c_1 + c_2 + c_3 = 1. \tag{2.2}$$

This is the link condition for the vector $\mathbf{c} = (c_1, c_2, c_3)$, where it belongs to the hyperplane

$$S = \{(c_1, c_2, c_3) \in \mathbb{R}^3, c_1 + c_2 + c_3 = 1\}. \tag{2.3}$$

In the two-phase model, the free energy of the mixture is as follows,

$$E^{diph}(c) = \int_\Omega \Big(\frac{3}{4}\sigma\epsilon|\nabla c|^2 + 12\frac{\sigma}{\epsilon}c^2(1-c)^2\Big)dx, \tag{2.4}$$

where σ is the surface tension parameter, the first term contributes to the "hydro-philic" type (tendency of mixing) of interactions between the materials and the second part, the double well bulk energy term represents the "hydro-phobic" type (tendency of separation) of interactions. As the consequence of the competition between the two types of interactions, the equilibrium configuration will include a diffusive interface with thickness proportional to the parameter ϵ; and, as ϵ approaches zero, we expect to recover the sharp interface separating the two different materials (cf., for instance, [**?**, **?**, **?**]).

There exist several generalizations from the two-phase model to the three-phase model [**?**, **?**, **?**]. we adopt below the approach in [**?**] where the free energy is defined as:

$$E^{triph}(c_1, c_2, c_3) = \int_\Omega \Big(\frac{3}{8}\Sigma_1\epsilon|\nabla c_1|^2 + \frac{3}{8}\Sigma_2\epsilon|\nabla c_2|^2 + \frac{3}{8}\Sigma_3\epsilon|\nabla c_3|^2 + \frac{12}{\epsilon}F(c_1, c_2, c_3)\Big)dx, \tag{2.5}$$

To be algebraically consistent with the two-phase systems, surface tensions $\sigma_{12}, \sigma_{13}, \sigma_{23}$ should verify the following conditions:

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk}, i = 1, 2, 3. \tag{2.6}$$

The nonlinear potential $F(c_1, c_2, c_3)$ is:

$$F(c_1, c_2, c_3) = \sigma_{12}c_1^2c_2^2 + \sigma_{13}c_1^2c_3^2 + \sigma_{23}c_2^2c_3^2 + c_1c_2c_3(\Sigma_1c_1 + \Sigma_2c_2 + \Sigma_3c_3) + 3\Lambda c_1^2c_2^2c_3^2. \tag{2.7}$$

Since c_1, c_2, c_3 satisfy the hyperplane link condition (2.2), the free energy can be rewritten as

$$F(c_1, c_2, c_3) = F_0(c_1, c_2, c_3) + P(c_1, c_2, c_3), \tag{2.8}$$

where

$$\begin{aligned} &F_0(c_1, c_2, c_3) = \frac{\Sigma_1}{2}c_1^2(1-c_1)^2 + \frac{\Sigma_2}{2}c_2^2(1-c_2)^2 + \frac{\Sigma_3}{2}c_3^2(1-c_3)^2, \\ &P(c_1, c_2, c_3) = 3\Lambda c_1^2c_2^2c_3^2, \end{aligned} \tag{2.9}$$

and Λ is a non negative constant.

Therefore, the time evolution of c_i is governed by the gradient of the energy E^{triph} with respect to the $H^{-1}(\Omega)$ gradient flow,

$$c_{it} = \frac{M_0}{\Sigma_i}\Delta\mu_i, \tag{2.10}$$

$$\mu_i = -\frac{3}{4}\epsilon\Sigma_i\Delta c_i + \frac{12}{\epsilon}\partial_i F + \beta,\ i = 1, 2, 3, \tag{2.11}$$

with the initial condition

$$c_i|_{(t=0)} = c_i^0,\ i = 1, 2, 3,\ c_1^0 + c_2^0 + c_3^0 = 1, \tag{2.12}$$

where β is the Lagrange multiplier to ensure the hyperplane link condition (2.2), that can be derived as

$$\beta = -\frac{4\Sigma_T}{\epsilon}\Big(\frac{1}{\Sigma_1}\partial_1 F + \frac{1}{\Sigma_2}\partial_2 F + \frac{1}{\Sigma_3}\partial_3 F\Big), \tag{2.13}$$

with

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_1} + \frac{1}{\Sigma_2} + \frac{1}{\Sigma_3}. \tag{2.14}$$

we consider in this paper either of the two type boundary conditions below:

$$\text{(i) all variables are periodic, or (ii) } \partial_{\mathbf{n}} c_i|_{\partial\Omega} = \nabla\mu_i \cdot \mathbf{n}|_{\partial\Omega} = 0,\ i = 1, 2, 3, \tag{2.15}$$

where $\mathbf{n}$ is the unit outward normal on the boundary $\partial\Omega$.

It is easily seen that the three chemical potentials (μ_1, μ_2, μ_3) are linked through the relation

$$\frac{\mu_1}{\Sigma_1} + \frac{\mu_2}{\Sigma_2} + \frac{\mu_3}{\Sigma_3} = 0. \tag{2.16}$$

Remark 2.1. *In the physical literature, the coefficient Σ_i is called the spreading coefficient of the phase i at the interface between phases j and k. Since Σ_i is determined by the surface tensions $\sigma_{i,j}$, it might not be always positive. If $\Sigma_i > 0$, the spreading is said to be "partial", and if $\Sigma_i < 0$, it is called "total".*

The following lemmas hold (cf. [**?**]):

LEMMA 2.1. *There exists $\underline{\Sigma} > 0$ such that*

$$\Sigma_1|\xi_1|^2 + \Sigma_1|\xi_1|^2 + \Sigma_1|\xi_1|^2 \geq \underline{\Sigma}\Big(|\xi_1|^2 + |\xi_2|^2 + |\xi_3|^2\Big),\ \forall \xi_1 + \xi_2 + \xi_3 = 0, \tag{2.17}$$

if and only if the following condition holds:

$$\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0, \Sigma_i + \Sigma_j > 0, \forall i \neq j. \tag{2.18}$$

LEMMA 2.2. *Let σ_{12}, σ_{13} and σ_{23} be three positive numbers and Σ_1, Σ_2 and Σ_3 defined by (2.6). For any $\Lambda > 0$, the bulk free energy $F(c_1, c_2, c_3)$ is bounded from below if c_1, c_2, c_3 is on the hyperplane S in 2D. Furthermore, the lower bound only depends on $\Sigma_1, \Sigma_2, \Sigma_3$ and Λ.*

Remark 2.2. *From Lemma 2.1, when (2.18) holds, the summation of the gradient entropy term* *is bounded from below since* $\nabla(c_1 + c_2 + c_3) = 0$, *i.e.,*

$$\Sigma_1\|\nabla c_1\|^2 + \Sigma_2\|\nabla c_2\|^2 + \Sigma_3\|\nabla c_3\|^2 \geq \underline{\Sigma}(\|\nabla c_1\|^2 + \|\nabla c_2\|^2 + \|\nabla c_3\|^2) \geq 0. \tag{2.19}$$

Remark 2.3. *The bulk part energy $F(c_1, c_2, c_3)$ defined in (2.8) has to be bounded from below as well. For partial spreading case ($\Sigma_i > 0\,\forall i$), one can drop the six order polynomial term by assuming $\Lambda = 0$ since $F_0(c_1, c_2, c_3) \geq 0$ is naturally bounded from below. For the total spreading case, Λ has to be non zero. Moreover, to ensure the non-negativity for F, Λ has to be large enough.*

For 3D case, it is shown in [?] that the bulk energy F is bounded from below when $P(c_1, c_2, c_3)$ takes the following form:

$$P(c_1, c_2, c_3) = 3\Lambda(c_1^2c_2^2c_3^3)(\phi_\alpha(c_1) + \phi_\alpha(c_2) + \phi_\alpha(c_3)) \tag{2.20}$$

where $\phi_\alpha(x) = \frac{1}{(1+x^2)^\alpha}$ *with* $0 < \alpha \leq \frac{8}{17}$.

Since (2.9) is commonly used in literature [?, ?], we adopt it as well for convenience. However, the numerical schemes we developed in this paper can deal with either (2.9) or (2.20).

Remark 2.4. *The system (2.10)-(2.11) is equivalent to the following system with two order parameters,*

$$\begin{cases} c_{it} = \dfrac{M_0}{\Sigma_i}\Delta\mu_i, \\ \mu_i = -\dfrac{3}{4}\epsilon\Sigma_i\Delta c_i + \dfrac{12}{\epsilon}\partial_i F + \beta, i = 1, 2, \\ c_3 = 1 - c_1 - c_2, \\ \dfrac{\mu_3}{\Sigma_3} = -(\dfrac{\mu_1}{\Sigma_1} + \dfrac{\mu_2}{\Sigma_2}). \end{cases} \tag{2.21}$$

We omit the detailed proof since it is quite similar to Theorem 3.1 in section 3.

The model equation (2.10)-(2.11) follows the dissipative energy law. More precisely, by taking the L^2 inner product of (2.10) with $-\mu_i$, and of (2.11) with c_{it}, and perform integration by parts, we obtain

$$-(c_{it}, \mu_i) = \frac{M_0}{\Sigma_i}\|\nabla\mu_i\|^2, \tag{2.22}$$

$$(\mu_i, c_{it}) = \frac{3}{4}\epsilon\Sigma_i(\nabla c_i, \partial_t\nabla c_i) + \frac{12}{\epsilon}(\partial_i F, c_{it}) + (\beta, c_{it}). \tag{2.23}$$

Taking summation of the two equalities for $i = 1, 2, 3$, and notice that $(\beta, (c_1+c_2+c_3)_t) = (\beta, (1)_t) = 0$, we obtain the energy dissipative law as

$$\frac{d}{dt}E^{triph}(c_1, c_2, c_3) = -M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3\|^2\Big). \tag{2.24}$$

Since (μ_1, μ_2, μ_3) satisfies the condition (2.16), if (2.18) holds, we can derive

$$-M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3\|^2\Big) \leq -M_0\underline{\Sigma}(\frac{\|\nabla\mu_1\|^2}{\Sigma_1^2} + \frac{\|\nabla\mu_2\|^2}{\Sigma_2^2} + \frac{\|\nabla\mu_3\|^2}{\Sigma_3^2}) \leq 0. \tag{2.25}$$

3. Numerical schemes. We develop in this section unconditionally energy stable and linear numerical schemes for solving the three component phase-field model (2.10)-(2.11). To this end, the main challenges are how to discretize: (i) the nonlinear term associated with the double well potential

F_0, (ii) the six order polynomial term P, (iii) the Lagrange multiplier term β especially for the total spreading case ($\Sigma_i < 0$).

For the two-phase Cahn-Hilliard model, the discretization of the nonlinear, cubic polynomial term induced from the double well potential had been well studied (cf. [?, ?, ?, ?, ?]). In summary, there are two commonly used techniques to discretize it in order to preserve the unconditional energy stability. The first is the so-called convex splitting approach [?], where the convex part of the potential is treated implicitly and the concave part is treated explicitly. The convex splitting approach is energy stable, however, it produces nonlinear schemes, thus the implementations are often complicated with potentially high computational costs.

The second technique is the so-called stabilization approach [?, ?], where the nonlinear term is treated explicitly. In order to preserve the energy law, a linear stabilizing term has to be added, and the magnitude of that term usually depends on the upper bound of the second order derivative of the G-L potential. The stabilized approach leads purely linear schemes, thus it is easy to implement and solve. However, it appears that second order schemes based on the stabilization are only conditionally energy stability [?]. On the other hand, the nonlinear potential may not satisfy the condition required for the stabilization. A feasible remedy is to make some reasonable revisions to the nonlinear potential in order to obtain a finite bound, for example, the quadratic order cut-off functions for the double well potential (cf. [?, ?, ?]). Such method is particularly reliable for those models with maximum principle. If the maximum principle does not hold, modified nonlinear potentials may lead to spurious solutions.

For the three component Cahn-Hillard model system, the above two approaches can not be easily applied. First, even though the convex-concave decomposition can be applied to F_0, it is not clear how to deal with the sixth order polynomial term [?]. Second, it is uncertain whether the solution of the system satisfies certain maximum principle so the condition required for stabilization is not satisfied.

We aim to develop numerical schemes that are efficient (linear system), stable (unconditionally energy stable), and accurate (ready for second order or even higher order in time). To this end, we use the IEQ approach, without worrying about whether the continuous/discrete maximum principle holds or a convexity/concavity splitting exists.

3.1. Transformed system. Since $F(c_1, c_2, c_3)$ is always bouned from below from Lemma 2.2 for 2D and Remark 2.3 for 3D. Therefore, we can rewrite the free energy functional $F(c_1, c_2, c_3)$ to the following equivalent form

$$F(c_1, c_2, c_3) = (F(c_1, c_2, c_3) + B) - B, \tag{3.1}$$

where B is some constant to ensure $F(c_1, c_2, c_3) + B > 0$. Furthermore, we define an auxiliary function as follows,

$$U = \sqrt{F(c_1, c_2, c_3) + B}. \tag{3.2}$$

In turn, the total free energy (2.5) can be rewritten as

$$E^{triph}(c_1, c_2, c_3, U) = \int_\Omega \Big(\frac{3}{8}\Sigma_1\epsilon|\nabla c_1|^2 + \frac{3}{8}\Sigma_2\epsilon|\nabla c_2|^2 + \frac{3}{8}\Sigma_3\epsilon|\nabla c_3|^2 + \frac{12}{\epsilon}U^2 - \frac{12}{\epsilon}B\Big)d\boldsymbol{x}, \tag{3.3}$$

Thus we could rewrite the system (2.10)-(2.11) to the following equivalent form:

$$c_{it} = \frac{M_0}{\Sigma_i}\Delta\mu_i, \tag{3.4}$$

$$\mu_i = -\frac{3}{4}\epsilon\Sigma_i\Delta c_i + \frac{24}{\epsilon}H_iU + \beta,\ i = 1,2,3, \tag{3.5}$$

$$U_t = H_1c_{1t} + H_2c_{2t} + H_3c_{3t}, \tag{3.6}$$

where

$$H_1 = \frac{\delta U}{\delta c_1} = \frac{1}{2}\frac{\frac{\Sigma_1}{2}(c_1 - c_1^2)(1-2c_1) + 6\Lambda c_1c_2^2c_3^2}{\sqrt{F+B}}, \tag{3.7}$$

$$H_2 = \frac{\delta U}{\delta c_2} = \frac{1}{2}\frac{\frac{\Sigma_2}{2}(c_2 - c_2^2)(1-2c_2) + 6\Lambda c_1^2c_2c_3^2}{\sqrt{F+B}}, \tag{3.8}$$

$$H_3 = \frac{\delta U}{\delta c_3} = \frac{1}{2}\frac{\frac{\Sigma_3}{2}(c_3 - c_3^2)(1-2c_3) + 6\Lambda c_1^2c_2^2c_3}{\sqrt{F+B}}, \tag{3.9}$$

$$\beta = -\frac{8}{\epsilon}\Sigma_T(\frac{1}{\Sigma_1}H_1 + \frac{1}{\Sigma_2}H_2 + \frac{1}{\Sigma_3}H_3)U. \tag{3.10}$$

The transformed system (3.4)- (3.6) in the variables c_1, c_2, c_3, U form a closed PDE system with the following initial conditions,

$$\begin{cases} c_i(t=0) = c_i^0, i = 1,2,3, \\ U(t=0) = U^0 = \sqrt{F(c_1^0, c_2^0, c_3^0) + B}. \end{cases} \tag{3.11}$$

Since the equations (3.6) for the new variables U is only ordinary differential equation with time, the boundary conditions of the new system (3.4)-(3.6) are still (2.15).

Remark 3.1. *The system (3.4)-(3.6) is equivalent to the following two order parameter system*

$$\begin{cases} c_{it} = \frac{M_0}{\Sigma_i}\Delta\mu_i, \\ \mu_i = -\frac{3}{4}\epsilon\Sigma_i\Delta c_i + \frac{24}{\epsilon}H_iU + \beta,\ i = 1,2, \end{cases} \tag{3.12}$$

with

$$\begin{aligned} &c_3 = 1 - c_1 - c_2, \\ &\frac{\mu_3}{\Sigma_3} = -(\frac{\mu_1}{\Sigma_1} + \frac{\mu_2}{\Sigma_2}). \end{aligned} \tag{3.13}$$

Since the proof is quite similar to Theorem 3.1, we omit the proof here.

We can easily obtain the energy law for the new system (3.4)-(3.6). Taking the L^2 inner product of (3.4) with $-\mu_i$, of (3.5) with $\partial_t c_i$, of (3.6) with $-\frac{24}{\epsilon}U$, taking the summation for $i = 1,2,3$, and noticing that $(\beta, \partial_t(c_1 + c_2 + c_3)) = 0$ from Remark 3.1, we still obtain the energy dissipation law as

$$\begin{aligned} \frac{d}{dt}E^{triph}(c_1, c_2, c_3, U) &= -M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3\|^2\Big) \\ &\le -M_0\Sigma_0(\frac{\|\nabla\mu_1\|^2}{\Sigma_1^2} + \frac{\|\nabla\mu_2\|^2}{\Sigma_2^2} + \frac{\|\nabla\mu_3\|^2}{\Sigma_3^2}) \le 0. \end{aligned} \tag{3.14}$$

Remark 3.2. *The new transformed system (3.4)- (3.6) is equivalent to the original system (2.10)-(2.11) since (3.2) can be obtained by integrating (3.6) with respect to the time. Therefore, the energy law (3.14) for the transformed system is exactly the same as the energy law (2.24) for the original system.*

We emphasize that we will develop energy stable numerical schemes for the new transformed system (3.4)- (3.6). The proposed schemes will a discrete energy law corresponding to (3.14) instead of the energy law for the original system (2.24).

Let $\delta t > 0$ denote the time step size and set $t^n = n\,\delta t$ for $0 \le n \le N$ with $T = N\,\delta t$. We also denote by $(f(\boldsymbol{x}), g(\boldsymbol{x})) = \int_\Omega f(\boldsymbol{x})g(\boldsymbol{x})d\boldsymbol{x}$ the L^2 inner product of any two functions $f(\boldsymbol{x})$ and $g(\boldsymbol{x})$, and by $\|f\| = \sqrt{(f,f)}$ the L^2 norm of the function $f(\boldsymbol{x})$.

3.2. First order scheme. We now present the first order time stepping scheme to solve the system (3.4)-(3.6) where the time derivative is discretized based on the first order backward Euler method.

Assumming that $(c_1, c_2, c_3, U)^n$ are already calculated, we compute $(c_1, c_2, c_3, U)^{n+1}$ from the following temporal discrete system:

$$\frac{c_i^{n+1} - c_i^n}{\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+1}, \tag{3.15}$$

$$\mu_i^{n+1} = -\frac{3}{4}\epsilon\Sigma_i\Delta c_i^{n+1} + \frac{24}{\epsilon}H_i^n U^{n+1} + \beta^{n+1},\ i = 1, 2, 3, \tag{3.16}$$

$$U^{n+1} - U^n = H_1^n(c_1^{n+1} - c_1^n) + H_2^n(c_2^{n+1} - c_2^n) + H_3^n(c_3^{n+1} - c_3^n), \tag{3.17}$$

where

$$H_1^n = \frac{1}{2}\frac{\frac{\Sigma_1}{2}(c_1^n - {c_1^n}^2)(1 - 2c_1^n) + 6\Lambda c_1^n {c_2^n}^2 {c_3^n}^2}{\sqrt{F(c_1^n, c_2^n, c_3^n) + B}}, \tag{3.18}$$

$$H_2^n = \frac{1}{2}\frac{\frac{\Sigma_2}{2}(c_2^n - {c_2^n}^2)(1 - 2c_2^n) + 6\Lambda {c_1^n}^2 c_2^n {c_3^n}^2}{\sqrt{F(c_1^n, c_2^n, c_3^n) + B}}, \tag{3.19}$$

$$H_3^n = \frac{1}{2}\frac{\frac{\Sigma_3}{2}(c_3^n - {c_3^n}^2)(1 - 2c_3^n) + 6\Lambda {c_1^n}^2 {c_2^n}^2 c_3^n}{\sqrt{F(c_1^n, c_2^n, c_3^n) + B}}, \tag{3.20}$$

$$\beta^{n+1} = -\frac{8}{\epsilon}\Sigma_T\Big(\frac{1}{\Sigma_1}H_1^n + \frac{1}{\Sigma_2}H_2^n + \frac{1}{\Sigma_3}H_3^n\Big)U^{n+1}. \tag{3.21}$$

The initial conditions are (3.11), and the boundary conditions are

$$\text{(i) all variables are periodic, or (ii) } \partial_{\mathbf{n}} c_i^{n+1}|_{\partial\Omega} = \nabla\mu_i^{n+1}\cdot\mathbf{n}|_{\partial\Omega} = 0,\ i = 1, 2, 3. \tag{3.22}$$

We immediately derive the following result which ensures the numerical solutions satisfy the hyperplane condition (2.2).

Theorem 3.1. *The system of (3.15)-(3.17) is equivalent to the following scheme with two order parameters,*

$$\frac{c_i^{n+1} - c_i^n}{\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+1}, \tag{3.23}$$

$$\mu_i^{n+1} = -\frac{3}{4}\epsilon\Sigma_1\Delta c_i^{n+1} + \frac{24}{\epsilon}H_i^n U^{n+1} + \beta^{n+1},\ i = 1, 2, \tag{3.24}$$

with

$$c_3^{n+1} = 1 - c_1^{n+1} - c_2^{n+1}, \tag{3.25}$$

$$\frac{\mu_3^{n+1}}{\Sigma_3} = -(\frac{\mu_1^{n+1}}{\Sigma_1} + \frac{\mu_2^{n+1}}{\Sigma_2}). \tag{3.26}$$

Proof. From (3.21), we can easily show that the following indentity holds,

$$\frac{24}{\epsilon}(\frac{H_1^n}{\Sigma_1} + \frac{H_2^n}{\Sigma_2} + \frac{H_3^n}{\Sigma_3})U^{n+1} + \beta^{n+1}(\frac{1}{\Sigma_1} + \frac{1}{\Sigma_2} + \frac{1}{\Sigma_3}) = 0. \tag{3.27}$$

- (i) We first assume that (3.23)-(3.26) are sastified, and derive (3.15)-(3.16). By taking the summation of (3.23) for $i = 1, 2$, and applying (3.25) and (3.26), we obtain

$$\frac{c_3^{n+1} - c_3^n}{\delta t} = \frac{M_0}{\Sigma_3}\Delta\mu_3^{n+1}. \tag{3.28}$$

  From (3.25), (3.26) and (3.27), we obtain

$$\begin{aligned} \mu_3^{n+1} &= -\Sigma_3(\frac{\mu_1^{n+1}}{\Sigma_1} + \frac{\mu_2^{n+1}}{\Sigma_2}) \\ &= -\Sigma_3\Big(- \frac{3}{4}\epsilon\Delta c_1^{n+1} - \frac{3}{4}\epsilon\Delta c_2^{n+1} + \frac{24}{\epsilon}(\frac{H_1^n}{\Sigma_1} + \frac{H_2^n}{\Sigma_2})U^{n+1} + \beta^{n+1}(\frac{1}{\Sigma_1} + \frac{1}{\Sigma_2})\Big) \\ &= \frac{3}{4}\epsilon\Sigma_3\Delta c_3^{n+1} + \frac{24}{\epsilon}H_3^n U^{n+1} + \beta^{n+1}. \end{aligned} \tag{3.29}$$

- (ii) We then assume that (3.15)-(3.16) are satisfied, and derive (3.23)-(3.26). By taking the summation of (3.15) for $i = 1, 2, 3$, we derive

$$\frac{S^{n+1} - S^n}{\delta t} = M_0\Delta\Theta^{n+1}, \tag{3.30}$$

  where $S^n = c_1^n + c_2^n + c_3^n$ and $\Theta^{n+1} = \frac{1}{\Sigma_1}\mu_1^{n+1} + \frac{1}{\Sigma_2}\mu_2^{n+1} + \frac{1}{\Sigma_3}\mu_3^{n+1}$. From (3.16) and (3.27), we derive

$$\Theta^{n+1} = -\frac{3}{4}\epsilon\Delta S^{n+1}. \tag{3.31}$$

  By taking the L^2 inner product of (3.30) with $-\Theta^{n+1}$, of (3.31) with $S^{n+1} - S^n$, and taking the summation of the two equalities above, we derive

$$\frac{3}{8}\epsilon(\|\nabla S^{n+1}\|^2 - \|\nabla S^n\|^2 + \|\nabla S^{n+1} - \nabla S^n\|^2) + \delta t M_0\|\nabla\Theta^{n+1}\|^2 = 0. \tag{3.32}$$

  Since $S^n = 1$, the lefthand side of (3.32) is a sum of non negative terms, thus $\nabla S^{n+1} = 0$, and $\nabla\Theta^{n+1} = 0$, i.e., the functions S^{n+1} and Θ^{n+1} are constants. Then (3.31) leads to $\Theta^{n+1} = 0$, and (3.30) leads to $S^{n+1} = S^n = 1$. Thus we obtain (3.25). By dividing Σ_i for (3.16) and taking the summation of it for $i = 1, 2, 3$, and applying (3.27) and (3.25), we obtain (3.26). □

Note that all nonlinear coefficient H_i of the new variables U are treated explicitly. Moreover, we can rewrite the equations (3.17) as follows:

$$U^{n+1} = H_1^n c_1^{n+1} + H_2^n c_2^{n+1} + H_3^n c_3^{n+1} + Q_1^n, \tag{3.33}$$

where $Q_1^n = U^n - H_1^n c_1^n - H_2^n c_2^n - H_3^n c_3^n$. Thus, the system (3.15)- (3.17) can be rewritten as

$$\frac{c_i^{n+1} - c_i^n}{\delta t} = \frac{M_0}{\Sigma_i} \Delta \mu_i^{n+1}, \tag{3.34}$$

$$\mu_i^{n+1} = -\frac{3}{4}\epsilon \Sigma_i \Delta c_i^{n+1} + \frac{24}{\epsilon} H_i^n (H_1^n c_1^{n+1} + H_2^n c_2^{n+1} + H_3^n c_3^{n+1}) \tag{3.35}$$
$$+\beta^{n+1} + \frac{24}{\epsilon} H_i^n Q_1^n, \ i = 1, 2, 3,$$

THEOREM 3.2. *Assuming (2.18), the linear system (3.34)-(3.35) for the variable $\Phi = (c_1^{n+1}, c_2^{n+1}, c_3^{n+1})^T$ is self-adjoint and positive definite.*

Proof. Taking the L^2 inner product of (3.34) with 1, we derive

$$\int_\Omega c_i^{n+1} d\boldsymbol{x} = \int_\Omega c_i^n d\boldsymbol{x} = \cdots = \int_\Omega c_i^0 d\boldsymbol{x}. \tag{3.36}$$

Let $\alpha_i^0 = \frac{1}{|\Omega|}\int_\Omega c_i^0 d\boldsymbol{x}$, $\gamma_i^0 = \frac{1}{|\Omega|}\int_\Omega \mu_i^{n+1} d\boldsymbol{x}$, and define

$$\widehat{c}_i^{n+1} = c_i^{n+1} - \alpha_i^0, \ \widehat{\mu}_i^{n+1} = \mu_i^{n+1} - \gamma_i^0. \tag{3.37}$$

Thus, from (3.34)-(3.35), $\widehat{c}_i^{n+1}$ and $\widehat{\mu}_i^{n+1}$ are the solutions for the following equations,

$$\frac{C_i}{M_0 \delta t} - \frac{1}{\Sigma_i} \Delta \mu_i = f_i^n, \tag{3.38}$$

$$\mu_i + \gamma_i^0 = -\frac{3}{4}\epsilon \Sigma_i \Delta C_i + \frac{24}{\epsilon} H_i^n P_1^{n+1} + \beta^{n+1} + g_i^n, \tag{3.39}$$

where $P_1^{n+1} = H_1^n C_1 + H_2^n C_2 + H_3^n C_3$ and

$$C_1 + C_2 + C_3 = 0, \int_\Omega C_i d\boldsymbol{x} = 0, \int_\Omega \mu_i d\boldsymbol{x} = 0. \tag{3.40}$$

We define the inverse Laplace operator $u \to v = \Delta^{-1} u$ by

$$\Delta v = u, \quad \int_\Omega v d\boldsymbol{x} = 0, \tag{3.41}$$
with the boundary conditions (2.15).

Applying $-\Delta^{-1}$ to (3.38) and using (3.39), we obtain

$$-\frac{\Sigma_i}{M_0 \delta t} \Delta^{-1} C_i - \frac{3}{4}\epsilon \Sigma_i \Delta C_i + \frac{24}{\epsilon} H_i^n P_1^{n+1} + \beta^{n+1} - \gamma_i^0 = -\Sigma_i \Delta^{-1} f_i^n - g_i^n, i = 1, 2, 3. \tag{3.42}$$

We express the above linear system (3.42) as $\mathbb{A}\mathbf{C} = \mathbf{b}$, where $\mathbf{C} = (C_1, C_2, C_3)^T$.

For any $\Phi = (\phi_1, \phi_2, \phi_3)^T, \Psi = (\psi_1, \psi_2, \psi_3)^T$ with $\sum_{i=1}^3 \phi_i = \sum_{i=1}^3 \psi_i = 0$ and $\int_\Omega \phi_i d\boldsymbol{x} = \int_\Omega \psi_i d\boldsymbol{x} = 0$, we can easily derive

$$(\mathbb{A}\Phi, \Psi) = (\Phi, \mathbb{A}\Psi), \tag{3.43}$$

thus $\mathbb{A}$ is self-adjoint. Meanwhile, we have

$$\begin{aligned}(\mathbb{A}\Phi,\Phi)=&\frac{1}{M_0\delta t}(\Sigma_1(-\Delta^{-1}\phi_1,\phi_1)+\Sigma_2(-\Delta^{-1}\phi_2,\phi_2)+\Sigma_3(-\Delta^{-1}\phi_3,\phi_3))\\&+\frac{3}{8}\epsilon(\Sigma_1\|\nabla\phi_1\|^2+\Sigma_2\|\nabla\phi_2\|^2+\Sigma_3\|\nabla\phi_3\|^2)+\frac{24}{\epsilon}\|H_1^n\phi_1+H_2^n\phi_2+H_3^n\phi_3\|^2\end{aligned} \tag{3.44}$$

Let $d_i=\Delta^{-1}\phi_i$, i.e.,

$$\Delta d_i=\phi_i,\quad \int_\Omega d_i d\boldsymbol{x}=0, \tag{3.45}$$

with periodic boundary conditions or $\partial_{\mathbf{n}}d_i|_{\partial\Omega}=0$. Therefore, we have

$$(-\Delta^{-1}\phi_i,\phi_i)=\|\nabla d_i\|^2. \tag{3.46}$$

Furthermore, $Z=d_1+d_2+d_3$ satisfies

$$\Delta Z=0, \tag{3.47}$$

$$quad\int_\Omega Z d\boldsymbol{x}=0, \tag{3.48}$$

with periodic boundary conditions or $\partial_{\mathbf{n}}Z|_{\partial\Omega}=0$. Thus $Z=d_1+d_2+d_3=0$. From (2.19), we derive

$$\begin{aligned}(\mathbb{A}\Phi,\Phi)\geq&\frac{1}{M_0\delta t}\underline{\Sigma}(\|\nabla d_1\|^2+\|\nabla d_2\|^2+\|\nabla d_3\|^2)+\frac{3}{8}\underline{\Sigma}\epsilon(\|\nabla\phi_1\|^2+\|\nabla\phi_2\|^2+\|\nabla\phi_3\|^2)\\&+\frac{24}{\epsilon}\|H_1^n\phi_1+H_2^n\phi_2+H_3^n\phi_3\|^2\geq 0,\end{aligned} \tag{3.49}$$

∎

and $(\mathbb{A}\Phi,\Phi)=0$ if and only if $\Phi=0$. Thus we conclude the theorem.

The stability result of the first order scheme (3.15)-(3.17) is given below.

Theorem 3.3. *When* (2.18) *holds, the first order linear scheme* (3.15)-(3.17) *is unconditionally energy stable, i.e., satisfies the following discrete energy dissipation law:*

$$\frac{1}{\delta t}(E_{1st}^{n+1}-E_{1st}^n)\leq -M_0\underline{\Sigma}(\frac{\|\nabla\mu_1^{n+1}\|^2}{\Sigma_1^2}+\frac{\|\nabla\mu_2^{n+1}\|^2}{\Sigma_2^2}+\frac{\|\nabla\mu_3^{n+1}\|^2}{\Sigma_3^2}). \tag{3.50}$$

where E_{1st}^n is defined by

$$E_{1st}^n=\frac{3}{8}\Sigma_1\epsilon\|\nabla c_1^n\|^2+\frac{3}{8}\Sigma_2\epsilon\|\nabla c_2^n\|^2+\frac{3}{8}\Sigma_3\epsilon\|\nabla c_3^n\|^2+\frac{12}{\epsilon}\|U^n\|^2\geq 0,\forall n. \tag{3.51}$$

Proof. Taking the L^2 inner product of (3.15) with $-\delta t\mu_i^{n+1}$, we obtain

$$-(c_i^{n+1}-c_i^n,\mu_i^{n+1})=\delta t\frac{M_0}{\Sigma_i}\|\nabla\mu_i^{n+1}\|^2. \tag{3.52}$$

Taking the L^2 inner product of (3.16) with $c_i^{n+1}-c_i^n$ and applying the following identities

$$2(a-b,a)=|a|^2-|b|^2+|a-b|^2, \tag{3.53}$$

we derive

$$
\begin{aligned}
(\mu_i^{n+1}, c_i^{n+1}-c_i^n) =& \frac{3}{8}\epsilon\Sigma_i(\|\nabla c_i^{n+1}\|^2 - \|\nabla c_i^n\|^2 + \|\nabla c_i^{n+1}-\nabla c_i^n\|^2) \\
&+ \frac{24}{\epsilon}(H_i^n U^{n+1}, c_i^{n+1}-c_i^n) + (\beta^{n+1}, c_i^{n+1}-c_i^n).
\end{aligned} \tag{3.54}
$$

Taking the L^2 inner product of (3.17) with $\frac{24}{\epsilon}U^{n+1}$, we obtain

$$
\begin{aligned}
&\frac{12}{\epsilon}\Big(\|U^{n+1}\|^2 - \|U^n\|^2 + \|U^{n+1}-U^n\|^2\Big) \\
&= \frac{24}{\epsilon}\Big(\big(H_1^n(c_1^{n+1}-c_1^n), U^{n+1}\big) + \big(H_2^n(c_2^{n+1}-c_2^n), U^{n+1}\big) + \big(H_3^n(c_3^{n+1}-c_3^n), U^{n+1}\big)\Big).
\end{aligned} \tag{3.55}
$$

Combinning (3.51), (3.53), taking the summation for $i = 1, 2, 3$ and using (3.54) and (3.25), we have

$$
\begin{aligned}
&\frac{3}{8}\epsilon\sum_{i=1}^{3}\Sigma_i\Big(\|\nabla c_i^{n+1}\|^2 - \|\nabla c_i^n\|^2\Big) + \frac{3}{8}\epsilon\sum_{i=1}^{3}\Sigma_i\|\nabla c_i^{n+1}-\nabla c_i^n\|^2 \\
&+ \frac{12}{\epsilon}\Big(\|U^{n+1}\|^2 - \|U^n\|^2\Big) = -M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1^{n+1}\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2^{n+1}\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3^{n+1}\|^2\Big) \\
&\qquad\qquad \le -M_0\underline{\Sigma}(\|\nabla\mu_1^{n+1}\|^2 + \|\nabla\mu_2^{n+1}\|^2 + \|\nabla\mu_3^{n+1}\|^2).
\end{aligned} \tag{3.56}
$$

Noticing that $\sum_{i=1}^{3}\nabla c_i^{n+1} = 0$, we derive

$$
\sum_{i=1}^{3}\Big(\Sigma_i\|\nabla c_i^{n+1}-\nabla c_i^n\|^2\Big) \ge \underline{\Sigma}\sum_{i=1}^{3}\Big(\|\nabla c_i^{n+1}-\nabla c_i^n\|^2\Big) \ge 0. \tag{3.57}
$$

Therefore, the desired result (3.49) is obtained. □

3.3. Second order scheme based on Crank-Nicolson. We now present a second order time stepping scheme to solve the system (3.4)-(3.6).

Assumming that $(c_1, c_2, c_3, U)^n$ and $(c_1, c_2, c_3, U)^{n-1}$ are already calculated, we compute $(c_1, c_2, c_3, U)^{n+1}$ from the following temporal discrete system

$$
c_{it} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+\frac{1}{2}}, \tag{3.58}
$$

$$
\mu_i^{n+\frac{1}{2}} = -\frac{3}{4}\epsilon\Sigma_i\Delta\frac{c_i^{n+1}+c_i^n}{2} + \frac{24}{\epsilon}H_i^* U^{n+\frac{1}{2}} + \beta^{n+\frac{1}{2}}, i = 1, 2, 3, \tag{3.59}
$$

$$
U^{n+1} - U^n = H_1^*(c_1^{n+1}-c_1^n) + H_2^*(c_2^{n+1}-c_2^n) + H_3^*(c_3^{n+1}-c_3^n), \tag{3.60}
$$

where

$$
\begin{cases}
U^{n+\frac{1}{2}} = \dfrac{U^{n+1}+U^n}{2}, \\
c_i^* = \dfrac{3}{2}c_i^n - \dfrac{1}{2}c_i^{n-1}, \\
H_1^* = \dfrac{1}{2}\dfrac{\frac{\Sigma_1}{2}(c_1^*-{c_1^*}^2)(1-2c_1^*)+6\Lambda c_1^*{c_2^*}^2{c_3^*}^2}{\sqrt{F(c_1^*,c_2^*,c_3^*)+B}}, \\
H_2^* = \dfrac{1}{2}\dfrac{\frac{\Sigma_2}{2}(c_2^*-{c_2^*}^2)(1-2c_2^*)+6\Lambda {c_1^*}^2 c_2^*{c_3^*}^2}{\sqrt{F(c_1^*,c_2^*,c_3^*)+B}}, \\
H_3^* = \dfrac{1}{2}\dfrac{\frac{\Sigma_3}{2}(c_3^*-{c_3^*}^2)(1-2c_3^*)+6\Lambda {c_1^*}^2{c_2^*}^2 c_3^*}{\sqrt{F(c_1^*,c_2^*,c_3^*)+B}}, \\
\beta^{n+\frac{1}{2}} = -\dfrac{8}{\epsilon}\Sigma_T(\dfrac{1}{\Sigma_1}H_1^*+\dfrac{1}{\Sigma_2}H_2^*+\dfrac{1}{\Sigma_3}H_3^*)U^{n+\frac{1}{2}}.
\end{cases}
\tag{3.61}
$$

The initial conditions are (3.11), and the boundary conditions are

$$
\text{(i) all variables are periodic, or (ii) } \partial_{\mathbf{n}} c_i^{n+1}|_{\partial\Omega} = \nabla \mu_i^{n+\frac{1}{2}}\cdot \mathbf{n}|_{\partial\Omega} = 0,\ i=1,2,3. \tag{3.62}
$$

The following theorem ensures the numerical solution $(c_1^{n+1}, c_2^{n+1}, c_3^{n+1})$ always satisfies the hyperplane link condition (2.2).

Theorem 3.4. *The system (3.57)-(3.59) is equivalent to the following scheme with two order parameters,*

$$
\frac{c_i^{n+1}-c_i^n}{\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+\frac{1}{2}}, \tag{3.63}
$$

$$
\mu_i^{n+\frac{1}{2}} = -\frac{3}{4}\epsilon\Sigma_i\Delta\frac{c_i^{n+1}+c_i^n}{2} + \frac{24}{\epsilon}H_i^*U^{n+\frac{1}{2}} + \beta^{n+\frac{1}{2}}, i=1,2, \tag{3.64}
$$

with

$$
c_3^{n+1} = 1 - c_1^{n+1} - c_2^{n+1}, \tag{3.65}
$$

$$
\frac{\mu_3^{n+\frac{1}{2}}}{\Sigma_3} = -(\frac{\mu_1^{n+\frac{1}{2}}}{\Sigma_1} + \frac{\mu_2^{n+\frac{1}{2}}}{\Sigma_2}). \tag{3.66}
$$

Proof. The proof is omitted here since it is similar to that for Theorem 3.1. ∎

Similar to the first orders scheme, we can rewrite the system (3.59) as follows,

$$
U^{n+1} = H_1^*c_1^{n+1} + H_2^*c_2^{n+1} + H_3^*c_3^{n+1} + Q_2^n, \tag{3.67}
$$

where $Q_2^n = U^n - H_1^*c_1^n - H_2^*c_2^n - H_3^*c_3^n$. Thus, the system (3.57)- (3.59) can be rewritten as

$$
\frac{c_i^{n+1}-c_i^n}{\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+\frac{1}{2}}, \tag{3.68}
$$

$$
\begin{aligned}
\mu_i^{n+\frac{1}{2}} = -\frac{3}{4}\epsilon\Sigma_i\Delta\frac{c_i^{n+1}+c_i^n}{2} &+ \frac{24}{\epsilon}H_i^*(H_1^*c_1^{n+1}+H_2^*c_2^{n+1}+H_3^*c_3^{n+1}) \\
&+\beta^{n+\frac{1}{2}} + \frac{24}{\epsilon}H_i^*Q_2^n,\ i=1,2,3.
\end{aligned}
\tag{3.69}
$$

THEOREM 3.5. *The linear system* (3.67)-(3.68) *for the variable* $\Phi = (c_1^{n+1}, c_2^{n+1}, c_3^{n+1})^T$ *is self-adjoint and positive definite.*

Proof. The proof is omitted here since it is similar to that for Theorem 3.2. ∎

The stability result of the second order Crank-Nicolson scheme (3.57)-(3.59) is given below.

THEOREM 3.6. *Assuming* (2.18)*, the second order Crank-Nicolson scheme* (3.57)-(3.59) *is unconditionally energy stable and satisfies the following discrete energy dissipation law:*

$$\begin{aligned}\frac{1}{\delta t}(E_{cn}^{n+1} - E_{cn}^{n}) &= -M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1^{n+\frac12}\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2^{n+\frac12}\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3^{n+\frac12}\|^2\Big)\\ &\le -M_0\underline{\Sigma}\Big(\frac{\|\nabla\mu_1^{n+\frac12}\|^2}{\Sigma_1^2} + \frac{\|\nabla\mu_2^{n+\frac12}\|^2}{\Sigma_2^2} + \frac{\|\nabla\mu_3^{n+\frac12}\|^2}{\Sigma_3^2}\Big),\end{aligned} \tag{3.70}$$

where E_{cn}^n *that is defined by*

$$E_{cn}^n = \frac38\Sigma_1\epsilon\|\nabla c_1^n\|^2 + \frac38\Sigma_2\epsilon\|\nabla c_2^n\|^2 + \frac38\Sigma_3\epsilon\|\nabla c_3^n\|^2 + \frac{12}{\epsilon}\|U^{n+1}\|^2 \ge 0, \forall n. \tag{3.71}$$

Proof. Taking the L^2 inner product of (3.57) with $-\delta t\mu_i^{n+1}$, we obtain

$$-(c_i^{n+1} - c_i^n, \mu_i^{n+\frac12}) = \delta t\frac{M_0}{\Sigma_i}\|\nabla\mu_i^{n+\frac12}\|^2. \tag{3.72}$$

Taking the L^2 inner product of (3.58) with $c_i^{n+1} - c_i^n$, we obtain

$$\begin{aligned}(\mu_i^{n+\frac12}, c_i^{n+1} - c_i^n) &= \frac38\epsilon\Sigma_i(\|\nabla c_i^{n+1}\|^2 - \|\nabla c_i^n\|^2)\\ &\quad + \frac{24}{\epsilon}(H_i^* U^{n+\frac12}, c_i^{n+1} - c_i^n) + (\beta^{n+\frac12}, c_i^{n+1} - c_i^n).\end{aligned} \tag{3.73}$$

Taking the L^2 inner product of (3.17) with $\frac{24}{\epsilon}U^{n+\frac12}$, we obtain

$$\begin{aligned}&\frac{24}{\epsilon}\Big((H_1^*(c_1^{n+1} - c_1^n), U^{n+\frac12}) + (H_2^*(c_2^{n+1} - c_2^n), U^{n+\frac12}) + (H_3^*(c_3^{n+1} - c_3^n), U^{n+\frac12})\Big)\\ &= \frac{12}{\epsilon}(\|U^{n+1}\|^2 - \|U^n\|^2)\end{aligned} \tag{3.74}$$

Combinning (3.71), (3.72) for $i = 1, 2, 3$ and (3.73), we derive

$$\begin{aligned}&\frac38\epsilon\sum_{i=1}^{3}\Sigma_i\Big(\|\nabla c_i^{n+1}\|^2 - \|\nabla c_i^n\|^2\Big) + \frac{12}{\epsilon}\Big(\|U^{n+1}\|^2 - \|U^n\|^2\Big)\\ &\qquad = -M_0(\frac{1}{\Sigma_1}\|\nabla\mu_1^{n+\frac12}\|^2 + \frac{1}{\Sigma_1}\|\nabla\mu_1^{n+\frac12}\|^2 + \frac{1}{\Sigma_1}\|\nabla\mu_1^{n+\frac12}\|^2)\\ &\qquad \le -M_0\Sigma_0(\frac{\|\nabla\mu_1^{n+\frac12}\|^2}{\Sigma_1^2} + \frac{\|\nabla\mu_2^{n+\frac12}\|^2}{\Sigma_2^2} + \frac{\|\nabla\mu_3^{n+\frac12}\|^2}{\Sigma_3^2}).\end{aligned} \tag{3.75}$$

∎

Thus we obtain the desired result (3.69).

Notice that that the above scheme conserves the energy if $M_0 = 0$ as in the continuous case. In certain situation, additional dissipation is desirable. To this end, we develop another second order scheme based on the backward difference formula (BDF) which introduces additional dissipation.

3.4. Second order scheme based on BDF. Assumming that $(c_1, c_2, c_3, U)^n$ and $(c_1, c_2, c_3, U)^{n-1}$ are already calculated, we compute $(c_1, c_2, c_3, U)^{n+1}$ from the following discrete system:

$$\frac{3c_i^{n+1} - 4c_i^n + c_i^{n-1}}{2\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+1}, \tag{3.76}$$

$$\mu_i^{n+1} = -\frac{3}{4}\epsilon\Sigma_1\Delta c_i^{n+1} + \frac{24}{\epsilon}H_i^\dagger U^{n+1} + \beta^{n+1}, i = 1, 2, 3, \tag{3.77}$$

$$\begin{aligned} 3U^{n+1} - 4U^n + U^{n-1} = {} & H_1^\dagger(3c_1^{n+1} - 4c_1^n + c_1^{n-1}) \\ & + H_2^\dagger(3c_2^{n+1} - 4c_2^n + c_2^{n-1}) + H_3^\dagger(3c_3^{n+1} - 4c_3^n + c_3^{n-1}), \end{aligned} \tag{3.78}$$

where

$$\begin{cases} c_i^\dagger = 2c_i^n - c_i^{n-1} \\ H_1^\dagger = \dfrac{1}{2}\dfrac{\frac{\Sigma_1}{2}(c_1^\dagger - {c_1^\dagger}^2)(1 - 2c_1^\dagger) + 6\Lambda c_1^\dagger {c_2^\dagger}^2 {c_3^\dagger}^2}{\sqrt{F(c_1^\dagger, c_2^\dagger, c_3^\dagger) + B}} \\ H_2^\dagger = \dfrac{1}{2}\dfrac{\frac{\Sigma_2}{2}(c_2^\dagger - {c_2^\dagger}^2)(1 - 2c_2^\dagger) + 6\Lambda {c_1^\dagger}^2 c_2^\dagger {c_3^\dagger}^2}{\sqrt{F(c_1^\dagger, c_2^\dagger, c_3^\dagger) + B}} \\ H_3^\dagger = \dfrac{1}{2}\dfrac{\frac{\Sigma_3}{2}(c_3^\dagger - {c_3^\dagger}^2)(1 - 2c_3^\dagger) + 6\Lambda {c_1^\dagger}^2 {c_2^\dagger}^2 c_3^\dagger}{\sqrt{F(c_1^\dagger, c_2^\dagger, c_3^\dagger) + B}} \\ \beta^{n+1} = -\dfrac{8}{\epsilon}\Sigma_T(\dfrac{1}{\Sigma_1}H_1^\dagger + \dfrac{1}{\Sigma_2}H_2^\dagger + \dfrac{1}{\Sigma_3}H_3^\dagger)U^{n+1}. \end{cases} \tag{3.79}$$

The initial conditions are (3.11), and the boundary conditions are

$$\text{(i) all variables are periodic, or (ii) } \partial_{\mathbf{n}} c_i^{n+1}|_{\partial\Omega} = \nabla\mu_i^{n+1}\cdot\mathbf{n}|_{\partial\Omega} = 0,\ i = 1, 2, 3. \tag{3.80}$$

Similar to the first order scheme and the second order Crank-Nicolson scheme, the hyperplane link condition still holds for this scheme.

THEOREM 3.7. *The system* (3.75)-(3.77) *is equivalent to the following scheme with two order parameters,*

$$\frac{3c_i^{n+1} - 4c_i^n + c_i^{n-1}}{2\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+1}, \tag{3.81}$$

$$\mu_i^{n+1} = -\frac{3}{4}\epsilon\Sigma_i\Delta c_i^{n+1} + \frac{24}{\epsilon}H_i^\dagger U^{n+1} + \beta^{n+1}, i = 1, 2, \tag{3.82}$$

$$c_3^{n+1} = 1 - c_1^{n+1} - c_2^{n+1}, \tag{3.83}$$

$$\frac{\mu_3^{n+1}}{\Sigma_3} = -(\frac{\mu_1^{n+1}}{\Sigma_1} + \frac{\mu_2^{n+1}}{\Sigma_2}). \tag{3.84}$$

Proof. The proof is omitted here since it is similar to that for Theorem 3.1. ∎

Similar to the previous cases, we can rewrite the sysytem (3.77) as

$$U^{n+1} = H_1^\dagger c_1^{n+1} + H_2^\dagger c_2^{n+1} + H_3^\dagger c_3^{n+1} + Q_3^n \tag{3.85}$$

where $Q_3^n = U^\ominus - H_1^\dagger c_1^\ominus - H_2^\dagger c_2^\ominus - H_3^\dagger c_3^\ominus$ and $V^\ominus = \frac{4V^n - V^{n-1}}{3}$ for any variable V. Thus, the system (3.15)- (3.17) can be rewritten as

$$\frac{3c_i^{n+1} - 4c_i^n + c_i^{n-1}}{2\delta t} = \frac{M_0}{\Sigma_i}\Delta\mu_i^{n+1}, \tag{3.86}$$

$$\begin{aligned}\mu_i^{n+1} = &-\frac{3}{4}\epsilon\Sigma_i\Delta c_i^{n+1} + \frac{24}{\epsilon}H_i^\dagger(H_1^\dagger c_1^{n+1} + H_2^\dagger c_2^{n+1} + H_3^\dagger c_3^{n+1}) \\ &+\beta^{n+1} + \frac{24}{\epsilon}H_i^\dagger Q_3^n,\ i = 1,2,3,\end{aligned} \tag{3.87}$$

THEOREM 3.8. *The linear system* (3.85)-(3.86) *for the variable* $\Phi = (c_1^{n+1}, c_2^{n+1}, c_3^{n+1})^T$ *is self-adjoint and positive definite.*

Proof. The proof is omitted here since it is similar to that for Theorem 3.2. ∎

THEOREM 3.9. *The second order scheme* (3.75)-(3.77) *is unconditionally energy stable and satisfies the following discrete energy dissipation law:*

$$\begin{aligned}\frac{1}{\delta t}(E_{bdf}^{n+1} - E_{bdf}^n) &\le -M_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1^{n+1}\|^2 + \frac{1}{\Sigma_2}\|\nabla\mu_2^{n+1}\|^2 + \frac{1}{\Sigma_3}\|\nabla\mu_3^{n+1}\|^2\Big) \\ &\le -M_0\underline{\Sigma}\Big(\frac{\|\nabla\mu_1^{n+1}\|^2}{\Sigma_1^2} + \frac{\|\nabla\mu_2^{n+1}\|^2}{\Sigma_2^2} + \frac{\|\nabla\mu_3^{n+1}\|^2}{\Sigma_3^2}\Big),\end{aligned} \tag{3.88}$$

where E_{bdf}^n *is defined by*

$$\begin{aligned}E_{bdf}^n = &\frac{3}{8}\Sigma_1\epsilon\Big(\frac{\|\nabla c_1^n\|^2}{2} + \frac{\|2\nabla c_1^n - \nabla c_1^{n-1}\|^2}{2}\Big) + \frac{3}{8}\Sigma_2\epsilon\Big(\frac{\|\nabla c_2^n\|^2}{2} + \frac{\|2\nabla c_2^n - \nabla c_2^{n-1}\|^2}{2}\Big) \\ &+ \frac{3}{8}\Sigma_3\epsilon\Big(\frac{\|\nabla c_3^n\|^2}{2} + \frac{\|2\nabla c_3^n - \nabla c_3^{n-1}\|^2}{2}\Big) + \frac{12}{\epsilon}\Big(\frac{\|U^n\|^2}{2} + \frac{\|2U^n - U^{n-1}\|^2}{2}\Big) \ge 0, \forall n.\end{aligned} \tag{3.89}$$

Proof. Taking the L^2 inner product of (3.75) with $-2\delta t\mu_i^{n+1}$, we obtain

$$-(3c_i^{n+1} - 4c_i^n + c_i^{n-1}, \mu_i^{n+1}) = 2\delta t\frac{M_0}{\Sigma_i}\|\nabla\mu_i^{n+1}\|^2. \tag{3.90}$$

Taking the L^2 inner product of (3.75) with $3c_i^{n+1} - 4c_i^n + c_i^{n-1}$, and applying the following identities the following identity

$$2(3a - 4b + c, a) = |a|^2 - |b|^2 + |2a - b|^2 - |2b - c|^2 + |a - 2b + c|^2, \tag{3.91}$$

we derive

$$\begin{aligned}(\mu_i^{n+1}, 3c_i^{n+1} - 4c_i^n + c_i^{n-1}) = &\frac{3}{8}\epsilon\Sigma_i\Big(\|\nabla c_i^{n+1}\|^2 - \|\nabla c_i^n\|^2 + \|2\nabla c_i^{n+1} - \nabla c_i^n\|^2 - \|2\nabla c_i^n - \nabla c_i^{n-1}\|^2\Big) \\ &+ \frac{3}{8}\epsilon\Sigma_i\|\nabla c_i^{n+1} - 2\nabla c_i^n + \nabla c_i^{n-1}\|^2 \\ &+ \frac{24}{\epsilon}(H_i^\dagger U^{n+1}, 3c_i^{n+1} - 4c_i^n + c_i^{n-1}) + (\beta^{n+1}, 3c_i^{n+1} - 4c_i^n + c_i^{n-1}).\end{aligned} \tag{3.92}$$

Taking the L^2 inner product of (3.77) with $\frac{24}{\epsilon}U^{n+1}$, we obtain

$$\begin{aligned}&\frac{12}{\epsilon}\Big(\|U^{n+1}\|^2-\|U^n\|^2+\|2U^{n+1}-U^n\|^2-\|2U^n-U^{n-1}\|^2+\|U^{n+1}-2U^n+U^{n-1}\|^2\Big)\\&=\frac{24}{\epsilon}\Big((H_1^\dagger(3c_1^{n+1}-4c_1^n+c_1^{n-1}),U^{n+1})+(H_2^\dagger(3c_2^{n+1}-4c_2^n+c_2^{n-1}),U^{n+1})\\&+(H_3^\dagger(3c_3^{n+1}-4c_3^n+c_3^{n-1}),U^{n+1})\Big).\end{aligned}\tag{3.93}$$

Combinning (3.71), (3.72) for $i=1,2,3$ and (3.73), we derive

$$\begin{aligned}&\frac{3}{8}\epsilon\sum_{i=1}^3\Sigma_i\Big(\|\nabla c_i^{n+1}\|^2+\|2\nabla c_i^{n+1}-\nabla c_i^n\|^2\Big)-\frac{3}{8}\epsilon\sum_{i=1}^3\Sigma_i\Big(\|\nabla c_i^n\|^2+\|2\nabla c_i^n-\nabla c_i^{n-1}\|^2\Big)\\&\qquad+\frac{3}{8}\epsilon\sum_{i=1}^3\Sigma_i\Big(\|\nabla c_i^{n+1}-2\nabla c_i^n+\nabla c_i^{n-1}\|^2\Big)+\frac{12}{\epsilon}\Big(\|U^{n+1}\|^2+\|2U^{n+1}-U^n\|^2\Big)\\&\qquad-\frac{12}{\epsilon}\Big(\|U^n\|^2+\|2U^n-U^{n-1}\|^2\Big)+\frac{12}{\epsilon}\|U^{n+1}-2U^n+U^{n-1}\|^2\\&\qquad=-2\delta tM_0\Big(\frac{1}{\Sigma_1}\|\nabla\mu_1^{n+1}\|^2+\frac{1}{\Sigma_2}\|\nabla\mu_2^{n+1}\|^2+\frac{1}{\Sigma_3}\|\nabla\mu_3^{n+1}\|^2\Big)\\&\qquad\le-2\delta tM_0\underline{\Sigma}\Big(\frac{\|\nabla\mu_1^{n+1}\|^2}{\Sigma_1^2}+\frac{\|\nabla\mu_2^{n+1}\|^2}{\Sigma_2^2}+\frac{\|\nabla\mu_3^{n+1}\|^2}{\Sigma_3^2}\Big).\end{aligned}\tag{3.94}$$

Since $\sum_{i=1}^3(\nabla c_i^{n+1}-2\nabla c_i^n+\nabla c_i^{n-1})=0$, from Lemma 2.1, we have

$$\sum_{i=1}^3\Big\{\Sigma_i\|\nabla c_i^{n+1}-2\nabla c_i^n+\nabla c_i^{n-1}\|^2\Big\}\ge\underline{\Sigma}\sum_{i=1}^3\Big\{\|\nabla c_i^{n+1}-2\nabla c_i^n+\nabla c_i^{n-1}\|^2\Big\}\ge 0.\tag{3.95}$$

Therefore, we obtain (3.87) after we drop the unnecessary positive terms in (3.93). ◻

Remark 3.3. *From formal Taylor expansion, we find*

$$\begin{aligned}&\Big(\frac{\|\phi^{n+1}\|^2+\|2\phi^{n+1}-\phi^n\|^2}{2\delta t}\Big)-\Big(\frac{\|\phi^n\|^2+\|2\phi^n-\phi^{n-1}\|^2}{2\delta t}\Big)\\&\qquad\cong\Big(\frac{\|\phi^{n+2}\|^2-\|\phi^n\|^2}{2\delta t}\Big)+O(\delta t^2)\cong\frac{d}{dt}\|\phi(t^{n+1})\|^2+O(\delta t^2),\end{aligned}\tag{3.96}$$

and

$$\frac{\|\phi^{n+1}-2\phi^n+\phi^{n-1}\|^2}{\delta t}\cong O(\delta t^3)\tag{3.97}$$

for any variable ϕ. Therefore, the discrete energy law (3.87) is a second order approximation of $\frac{d}{dt}E^{triph}(\phi)$ in (3.14).

4. Numerical Simulations.

5. Concluding Remarks. We developed in this paper several efficient time stepping schemes that are linear and unconditionally energy stable for the three component Cahn-Hilliard phase-field model based on a novel IEQ approach. The proposed schemes bypass the difficulties encountered in the convex splitting and the stabilized approach and enjoy the following desirable properties: (i) *accurate* (up to second order in time); (ii) *unconditionally energy stable*; and (iii) *easy to implement* (one only solves linear equations at each time step). Moreover, the resulting linear system at each time step is symmetric, positive definite so that it can be efficiently solved by any Krylov subspace methods with suitable (e.g., block-diagonal) pre-conditioners.

To the best of our knowledge, these new schemes are the first schemes which are linear and unconditionally energy stable for the three component Cahn-Hilliard phase-field model. Although we considered only time discretization in this study, the results can be carried over to any consistent finite-dimensional Galerkin approximations since the proofs are all based on a variational formulation with all test functions in the same space as the space of the trial functions.