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Linear relaxation schemes for the Allen–Cahn-type and Cahn–Hilliard-type phase field models

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ABSTRACT

This letter introduces novel linear relaxation schemes for solving the phase field models, particularly the Allen–Cahn (AC) type and Cahn–Hilliard (CH) type equations. The proposed schemes differ from existing schemes for the phase field models in the literature. The resulting semi-discrete schemes are linear by discretizing the AC and CH models on staggered time meshes. Only a linear algebra problem needs to be solved at each time marching step after the spatial discretization. Furthermore, our proposed schemes are shown to be unconditionally energy stable, i.e., the numerical solutions respect energy dissipation laws without restriction on the time steps. Several numerical examples are provided to illustrate the power of the proposed linear relaxation schemes for solving phase field models.

1. Introduction

The phase field method has been widely exploited in various fields, investigating interface dynamics, new material preparation, polymers and others. Generally, the phase field models are proposed following energy variation laws by introducing a phase variable ϕ, a free energy functional $E(\phi)$, and a semi-positive definite mobility operator $\mathcal{G}$, such that the phase field models can be written as

$$\partial_t \phi = -\mathcal{G}\frac{\delta E}{\delta \phi}, \tag{1.1}$$

with $\frac{\delta E}{\delta \phi}$ the variational derivative of E with respect to ϕ. Given a specific free energy E and a mobility operator $\mathcal{G}$, a phase field model will be derived by following (1.1). The generic phase field model in (1.1) is also known as a gradient flow system. Considering the regular domain Ω, we introduce notations of the inner product and the L^2 norm over Ω as $(f,g) = \int_\Omega fg d\mathbf{x}$, and $\|f\| = \sqrt{(f,f)}$, for all $f, g \in L^2(\Omega)$. One of its intrinsic properties is the so-called energy dissipation law

$$\frac{dE}{dt} = \Big(\frac{\delta E}{\delta \phi}, \frac{\partial \phi}{\partial t}\Big) = -\Big(\frac{\delta E}{\delta \phi}, \mathcal{G}\frac{\delta E}{\delta \phi}\Big) \leq 0,$$

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where we have assumed all the boundary integrals vanish. Such assumptions can be justified given proper Neumann or periodic boundary conditions.

Because the gradient flow system in (1.1) is usually highly nonlinear, the analytical solutions are not accessible in general, making numerical approximation a better option. Developing effective, accurate, and stable schemes for the phase field models has been an active topic for decades. In the past few years, some noticeable achievements have been made, including the invariant energy quadratization (IEQ) method [1–4], the scalar auxiliary variable (SAV) method [4,5] and relaxation approaches [6,7]. The first step of the IEQ-type and SAV-type methods is to introduce one or several auxiliary variables. Then the original system is translated to one equivalent PDE system. Based on the equivalent system, people can construct high-order structure-preserving numerical schemes by discretizing the time derivative of the auxiliary variable equations.

Inspired by the scheme for nonlinear schrödinger equation [8], we propose a novel linear relaxation scheme for phase field models or gradient flow systems. Unlike the IEQ-type and SAV-type methods, we do not need to take the time derivative of the auxiliary variables, making the schemes more consistent with the original PDE problem. To better explain our idea, we focus on the broadly used Allen–Cahn (AC) equation and the Cahn–Hilliard (CH) equation with the double-well bulk potentials in this letter. However, we emphasize that our idea can be easily applied to several other phase field models with minor adjustments.

The rest of this letter is organized as follows. We first introduce the linear relaxation schemes for the AC and CH equations in Section 2, followed by the proofs to show the schemes' energy stability properties. Then, we present several numerical tests to illustrate the schemes' effectiveness in Section 3. In the end, we draw a brief conclusion.

2. Linear relaxation schemes

2.1. Linear relaxation schemes for the AC equation

Consider the Allen–Cahn equation

$$\partial_t \phi = \varepsilon^2 \Delta \phi - (\phi^3 - \phi), \tag{2.1}$$

with its free energy $E(\phi) = \int_\Omega \Big[\frac{\varepsilon^2}{2}|\nabla \phi|^2 + \frac{1}{4}(\phi^2-1)^2\Big] d\mathbf{x}$. We introduce the relaxation variable

$$q = \phi^2 - 1 - \gamma, \tag{2.2}$$

where γ is a stabilization parameter [9]. Unlike the IEQ or SAV methods that take the time derivatives for (2.2), we try to discretize (2.2) on a staggered time meshes. The linear relaxation numerical scheme is proposed as

$$\frac{\phi^{n+1}-\phi^n}{\delta t} = \varepsilon^2 \Delta \frac{\phi^{n+1}+\phi^n}{2} - q^{n+\frac{1}{2}} \frac{\phi^{n+1}+\phi^n}{2} - \gamma \frac{\phi^{n+1}+\phi^n}{2}, \tag{2.3}$$

$$\frac{q^{n+\frac{1}{2}} + q^{n-\frac{1}{2}}}{2} = (\phi^n)^2 - 1 - \gamma. \tag{2.4}$$

The scheme above is second-order in time. Now, we will show its energy stability property.

Theorem 2.1. *The scheme (2.3)–(2.4) is energy stable, with the following energy law*

$$E(\phi^{n+1}, q^{n+\frac{1}{2}}) - E(\phi^n, q^{n-\frac{1}{2}}) = -\delta t \|\mu^{n+\frac{1}{2}}\|^2, \quad n \geq 0.$$

with the chemical potential $\mu^{n+\frac{1}{2}}$ defined as

$$\mu^{n+\frac{1}{2}} := -\varepsilon^2 \Delta \frac{\phi^{n+1}+\phi^n}{2} + q^{n+\frac{1}{2}} \frac{\phi^{n+1}+\phi^n}{2} + \gamma \frac{\phi^{n+1}+\phi^n}{2}, \tag{2.5}$$

and the free energy $E(\phi,q)$ defined as

$$E(\phi,q)=\frac{\varepsilon^2}{2}\|\nabla\phi\|^2+\frac{\gamma}{2}\|\phi\|^2+\Big(\frac{1}{2}q(\phi^2-1-\gamma)-\frac{1}{4}q^2,1\Big)-\frac{2\gamma+\gamma^2}{4}|\Omega|. \tag{2.6}$$

Proof. Multiplying (2.4) with $q^{n+\frac{1}{2}}-q^{n-\frac{1}{2}}$ leads us to

$$\frac{1}{2}\Big(q^{n+\frac{1}{2}}\Big)^2-\frac{1}{2}\Big(q^{n-\frac{1}{2}}\Big)^2=\Big((\phi^n)^2-1-\gamma\Big)\Big(q^{n+\frac{1}{2}}-q^{n-\frac{1}{2}}\Big). \tag{2.7}$$

Multiplying (2.3) with $\delta t\mu^{n+\frac{1}{2}}$, we get

$$\Big(\phi^{n+1}-\phi^n,-\varepsilon^2\Delta\frac{\phi^{n+1}+\phi^n}{2}+q^{n+\frac{1}{2}}\frac{\phi^{n+1}+\phi^n}{2}+\gamma\frac{\phi^{n+1}+\phi^n}{2}\Big)=-\delta t\|\mu^{n+\frac{1}{2}}\|^2.$$

i.e.

$$\begin{aligned}&\frac{\varepsilon^2}{2}(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2)+\frac{\gamma}{2}\Big(\|\phi^{n+1}\|^2-\|\phi^n\|^2\Big)\\&\quad+\frac{1}{2}\Big(q^{n+\frac{1}{2}}(\phi^{n+1})^2,1\Big)-\frac{1}{2}\Big(q^{n+\frac{1}{2}}(\phi^n)^2,1\Big)=-\delta t\|\mu^{n+\frac{1}{2}}\|^2.\end{aligned}$$

Notice the fact

$$\begin{aligned}q^{n+\frac{1}{2}}\Big[(\phi^{n+1})^2-(\phi^n)^2\Big]&=q^{n+\frac{1}{2}}\Big[(\phi^{n+1})^2-(\phi^n)^2\Big]+q^{n-\frac{1}{2}}\Big[(\phi^n)^2-(\phi^n)^2\Big]\\&=q^{n+\frac{1}{2}}\Big((\phi^{n+1})^2-1-\gamma\Big)-q^{n-\frac{1}{2}}\Big((\phi^n)^2-1-\gamma\Big)-(q^{n+\frac{1}{2}}-q^{n-\frac{1}{2}})\Big((\phi^n)^2-1-\gamma\Big).\end{aligned} \tag{2.8}$$

Applying (2.7) to (2.8) and multiplying $\frac{1}{2}$ on both sides, we arrive at

$$\frac{1}{2}q^{n+\frac{1}{2}}\Big[(\phi^{n+1})^2-(\phi^n)^2\Big]=\frac{1}{2}q^{n+\frac{1}{2}}\Big((\phi^{n+1})^2-1-\gamma\Big)-\frac{1}{2}q^{n-\frac{1}{2}}\Big((\phi^n)^2-1-\gamma\Big)-\frac{1}{4}\Big(q^{n+\frac{1}{2}}\Big)^2+\frac{1}{4}\Big(q^{n-\frac{1}{2}}\Big)^2.$$

Finally, we have

$$\begin{aligned}&\frac{\varepsilon^2}{2}(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2)+\frac{\gamma}{2}\Big(\|\phi^{n+1}\|^2-\|\phi^n\|^2\Big)+\frac{1}{2}\Big(q^{n+\frac{1}{2}}((\phi^{n+1})^2-1-\gamma),1\Big)\\&\quad-\frac{1}{2}\Big(q^{n-\frac{1}{2}}((\phi^n)^2-1-\gamma),1\Big)-\frac{1}{4}\|q^{n+\frac{1}{2}}\|^2+\frac{1}{4}\|q^{n-\frac{1}{2}}\|^2=-\delta t\|\mu^{n+\frac{1}{2}}\|^2.\end{aligned}$$

This indicates

$$E(\phi^{n+1},q^{n+\frac{1}{2}})-E(\phi^n,q^{n-\frac{1}{2}})=-\delta t\|\mu^{n+\frac{1}{2}}\|^2,\quad n\ge 0.$$

The proof is complete. □

Remark 2.1. *Here we briefly explain that the modified free energy in (2.6) is consistent with the original energy. Intuitively, we shall have*

$$\begin{aligned}&E(\phi^{n+1},q^{n+\frac{1}{2}})\\=\;&\frac{\varepsilon^2}{2}\|\nabla\phi^{n+1}\|^2+\frac{\gamma}{2}\|\phi^{n+1}\|^2+\Big(\frac{1}{2}q^{n+\frac{1}{2}}((\phi^{n+1})^2-1-\gamma)-\frac{1}{4}(q^{n+\frac{1}{2}})^2,1\Big)\\\approx\;&\frac{\varepsilon^2}{2}\|\nabla\phi^{n+1}\|^2+\frac{\gamma}{2}\|\phi^{n+1}\|^2+\Big(\frac{1}{2}\frac{(\phi^{n+1})^2-1-\gamma+(\phi^n)^2-1-\gamma}{2}((\phi^{n+1})^2-1-\gamma)\\&\quad-\frac{1}{4}\Big(\frac{(\phi^{n+1})^2-1-\gamma+(\phi^n)^2-1-\gamma}{2}\Big)^2,1\Big)\\=\;&\frac{\varepsilon^2}{2}\|\nabla\phi^{n+1}\|^2+\frac{\gamma}{2}\|\phi^{n+1}\|^2+\frac{1}{4}\|(\phi^{n+1})^2-1-\gamma\|^2-\frac{2\gamma+\gamma^2}{4}|\Omega|\\=\;&\frac{\varepsilon^2}{2}\|\nabla\phi^{n+1}\|^2+\frac{1}{4}\|(\phi^{n+1})^2-1\|^2\\=\;&E(\phi^{n+1}).\end{aligned}$$

2.2. Linear relaxation schemes for the CH equation

Consider the Cahn–Hilliard equation

$$\partial_t \phi = M \Delta \mu, \tag{2.9}$$
$$\mu = -\varepsilon^2 \Delta \phi + (\phi^3 - \phi), \tag{2.10}$$

with its free energy $E = \int_\Omega \left[\frac{\varepsilon^2}{2} |\nabla \phi|^2 + \frac{1}{4}(\phi^2 - 1)^2 \right] d\mathbf{x}$. Similarly as (2.2), we introduce the same relaxation variable

$$q = \phi^2 - 1 - \gamma, \tag{2.11}$$

where γ is a stabilization parameter [9]. We use the same strategy in the AC model to discretize q as represented in (2.11) on staggered time grids. The linear relaxation numerical scheme is proposed as

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = M \Delta \frac{\mu^{n+1} + \mu^n}{2}, \tag{2.12}$$
$$\frac{\mu^{n+1} + \mu^n}{2} = -\varepsilon^2 \Delta \frac{\phi^{n+1} + \phi^n}{2} + q^{n+\frac{1}{2}} \frac{\phi^{n+1} + \phi^n}{2} + \gamma \frac{\phi^{n+1} + \phi^n}{2}, \tag{2.13}$$
$$\frac{q^{n+\frac{1}{2}} + q^{n-\frac{1}{2}}}{2} = (\phi^n)^2 - 1 - \gamma. \tag{2.14}$$

The scheme above is second-order in time. Next, we present its energy stability property.

Theorem 2.2. *The scheme (2.12)–(2.14) is energy stable with the following energy law*

$$E(\phi^{n+1}, q^{n+\frac{1}{2}}) - E(\phi^n, q^{n-\frac{1}{2}}) = -\delta t \|\nabla \mu^{n+\frac{1}{2}}\|^2, \quad n \geq 0,$$

where the chemical potential is defined as

$$\mu^{n+\frac{1}{2}} := -\varepsilon^2 \Delta \frac{\phi^{n+1} + \phi^n}{2} + q^{n+\frac{1}{2}} \frac{\phi^{n+1} + \phi^n}{2} + \gamma \frac{\phi^{n+1} + \phi^n}{2}, \tag{2.15}$$

and the free energy is defined as

$$E(\phi, q) = \frac{\varepsilon^2}{2} \|\nabla \phi\|^2 + \frac{\gamma}{2} \|\phi\|^2 + \left(\frac{1}{2} q(\phi^2 - 1 - \gamma) - \frac{1}{4} q^2, 1 \right) - \frac{2\gamma + \gamma^2}{4} |\Omega|. \tag{2.16}$$

The proof of Theorem 2.2 is similar to Theorem 2.1. We have omitted it due to space limitations.

3. Numerical results

In the rest of this section, we use $\gamma = 2.0$ for numerical tests. Detailed discussions on the choices of γ are skipped due to space limitations. Interested readers are encouraged to refer to our earlier work [9]. We use the finite element method for spatial discretization and choose piecewise linear polynomial bases for simplicity. And the homogeneous Neumann boundary conditions are considered for all cases below.

Firstly, we test the convergence order of the proposed relaxation schemes. Consider the domain $\Omega = [0, 1] \times [0, 1]$. For an easy convergence test, we manufacture the exact solution $\phi(x, y, t) = \cos(\pi x) \cos(\pi y) \exp(-t)$ by adding forcing terms on the right hand sides of (2.1) and (2.9)–(2.10). Therefore the initial condition is given as $\phi(x, y, 0) = \cos(\pi x) \cos(\pi y)$. Assume the parameter $\epsilon = 1$ for the AC model, and $\epsilon = 1$, $M = 1$ for the CH model. For different mesh size h and $\delta t = h$, we calculate the errors at $t = 1$, as summarized in Tables 3.1 and 3.2. We could easily observe that the proposed relaxation schemes reach second-order time and second-order spatial accuracy in both the L^2-norm and the L^∞-norm.

Table 3.1
Convergence test results for ϕ for the AC equation.

h	Convergence rates in space				Convergence rates in time			
	L^∞	rate	L^2	Rate	L^∞	rate	L^2	rate
1/8	1.33e−01	–	1.10e−01	–	1.33e−01	–	1.10e−01	–
1/16	3.38e−02	2.0	2.70e−02	2.0	3.38e−02	2.0	2.70e−02	2.0
1/32	8.70e−03	2.0	6.72e−03	2.0	8.70e−03	2.0	6.72e−03	2.0
1/64	2.25e−03	2.0	1.68e−03	2.0	2.25e−03	2.0	1.68e−03	2.0
1/128	5.87e−04	2.0	4.19e−04	2.0	5.87e−04	2.0	4.19e−04	2.0

Table 3.2
Convergence test results for ϕ for the CH equation.

h	Convergence rates in space				Convergence rates in time			
	L^∞	rate	L^2	Rate	L^∞	rate	L^2	rate
1/16	3.50e−01	–	3.30e−01	–	3.50e−01	–	3.30e−01	–
1/32	8.59e−02	2.0	8.24e−02	2.0	8.59e−02	2.0	8.24e−02	2.0
1/64	2.14e−02	2.0	2.06e−02	2.0	2.14e−02	2.0	2.06e−02	2.0
1/128	5.36e−03	2.0	5.15e−03	2.0	5.36e−03	2.0	5.15e−03	2.0
1/256	1.35e−03	2.0	1.29e−03	2.0	1.35e−03	2.0	1.29e−03	2.0

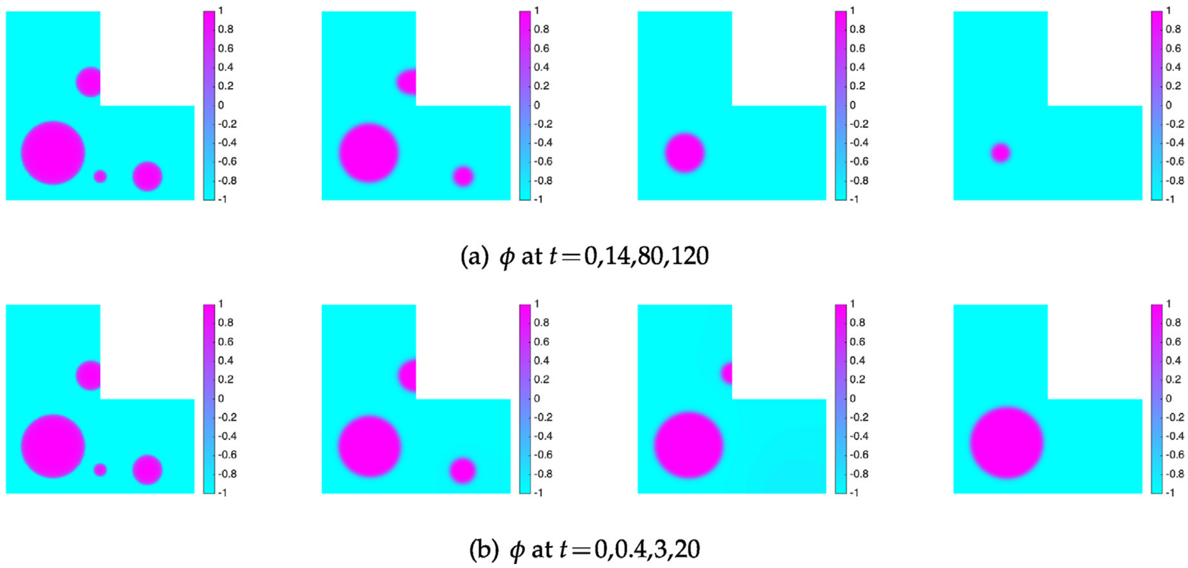
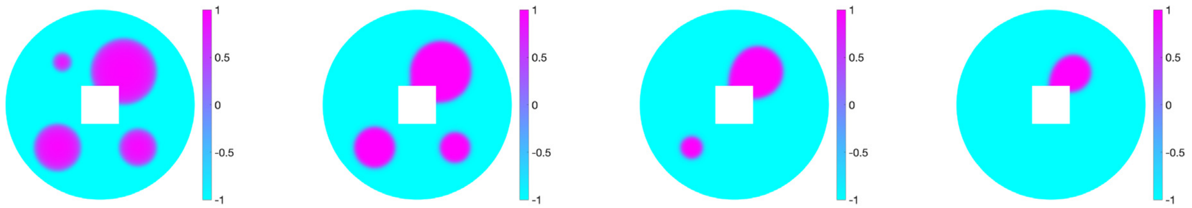


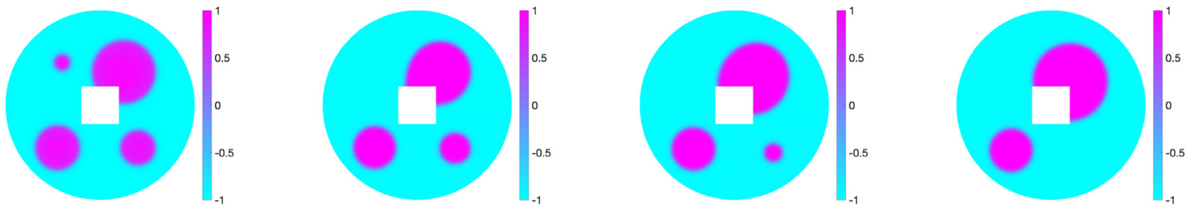
Fig. 3.1. Coarsening dynamics in a L-shape domain. In (a), the dynamics is driven by the AC model. We set $\delta t = 0.01$, and the profiles of ϕ at $t = 0, 14, 80, 120$ are shown; In (b), the dynamics is driven by the CH model. We set $\delta t = 0.001$, and the profiles of ϕ at $t = 0, 0.4, 3, 20$ are shown.

Secondly, we consider problems in the L-shape domain, with the maximum border length as one. Similarly with the benchmark problem in [10], we set up four disks in the 2D domain as an initial condition shown in the first column of Fig. 3.1(a) and (b). The parameters are $\epsilon = 0.01$ in the AC model and $\epsilon = 0.01$, $M = 0.1$ in CH model, respectively. It is known that the disks will eventually disappear in the dynamics process driven by the AC equation as the total volume is not conserved, which is observed as shown in Fig. 3.1(a). For the dynamics driven by the CH model, it is known that the total volume is conserved, so a large disk will eventually form. These dynamics are observed in Fig. 3.1(b). This numerical example illustrates the effectiveness and accuracy of the proposed relaxation schemes.

Next, we consider the circular domain with one square hole inside. We use the same initial condition as the example above. Specifically, we set up four disks in the 2D domain as an initial condition, as shown in Fig. 3.2(a) and (b). The parameters are $\epsilon = 0.04$ for the AC model and $\epsilon = 0.04$, $M = 0.1$ for the CH



(a) ϕ at $t = 0,10,50,100$



(b) ϕ at $t = 0,10,50,100$

Fig. 3.2. Coarsening dynamics in a circular domain. In (a), the dynamics is driven by the AC equation. We set $\delta t = 0.1$, and the profiles of ϕ at $t = 0, 10, 50, 100$ are shown; In (b), the dynamics is driven by the CH equation. We set $\delta t = 0.01$, and the profiles of ϕ at $t = 0, 10, 50, 100$ are shown.

model, respectively. Similarly, we observe the shrinking of disks in the dynamics driven by the AC model, as shown in Fig. 3.2(a), and the formation of a large disk in the dynamics driven by the CH model, as shown in Fig. 3.2(b).

4. Conclusion

In this letter, we propose novel linear relaxation schemes for the Allen–Cahn-type and Cahn–Hilliard-type phase-field models. The relaxation schemes differ from existing numerical schemes for phase field models. The main idea is to introduce one proper auxiliary variable and discretize the transformed PDEs on a staggered time mesh. We present rigorous proofs to show the unconditional energy stable property of the novel relaxation scheme for solving the AC and CH equations. Numerical examples further illustrate the effectiveness and accuracy of the proposed linear relaxation scheme. The proposed idea could be readily applied to some other phase field models or gradient flow PDEs, which will be further investigated in our later research.

Data availability

No data was used for the research described in the article.

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