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A structure-preserving explicit numerical scheme for the Allen–Cahn equation with a logarithmic potential

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ABSTRACT

This paper presents a stability analysis of a structure-preserving explicit finite difference method (FDM) for the Allen–Cahn (AC) equation with a logarithmic potential that has two arguments. Firstly, we compute the temporal step constraint that guarantees that if the initial condition is bounded by the two arguments of the minimum, then the numerical solutions are always bounded by them, i.e., the explicit numerical scheme satisfies the maximum principle. Secondly, we compute the temporal step constraint that guarantees that the discrete total energy of the system is non-increasing over time. To validate the preservation of the maximum principle and the decrease in discrete total energy, we perform numerical experiments.

1. Introduction

In this study, we investigate a fully explicit finite difference method (FDM) to solve the following Allen–Cahn (AC) equation [2] with a logarithmic potential and the homogeneous Neumann boundary condition:

$$\frac{\partial c(\mathbf{x},t)}{\partial t} = -F'(c(\mathbf{x},t)) + \epsilon^2 \Delta c(\mathbf{x},t), \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{1}$$

$$\mathbf{n} \cdot \nabla c(\mathbf{x},t) = 0, \quad \mathbf{x} \in \partial\Omega, \quad t > 0, \tag{2}$$

where $c(\mathbf{x},t)$ is the phase field concentration at spatial position $\mathbf{x}$ and time t, ϵ is a small positive parameter related to the thickness of the interfacial transition layer, $F(c)$ is a potential, and $\mathbf{n}$ is an outward unit normal vector on the boundary $\partial\Omega$. The double-well potential [5,11,23,32,36,38] is a general form of potential energy within the phase-field equations. On the other hand, in the case of the logarithmic Flory–Huggins energy potential [30,37], it becomes challenging to analyze due to logarithmic nonlinearity and singularity that

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occurs near the phase-field concentration values of 0 and 1. However, from a physics point of view, the Flory–Huggins energy potential is considered more realistic than the double-well potential [24]. In [28], a maximum bound principle preserving linear method for the conservative AC equation with the Flory–Huggins potential is proposed.

The AC equation models the phenomenon of phase separation occurring in binary alloys [34]. The AC equation has been used as a basic mathematical model for numerous problems, demonstrating its extensive utility [4,12,29]. Extensive research has been conducted on accurate and efficient numerical methods for solving the AC equation [3,6–8,10,17,21]. Furthermore, various studies on the AC equation with the logarithmic Flory–Huggins potential are being actively studied [18,35,37]. Research on structure-preserving numerical schemes for solving the AC equation has been conducted [9,16,40]. From the total free energy functional,

$$\mathcal{E}(c) = \int_{\Omega} \left(F(c) + \frac{\epsilon^2}{2} |\nabla c|^2 \right) \mathrm{d}\mathbf{x}, \tag{3}$$

the AC equation (1) can be derived by an L^2-gradient flow of the energy functional in Eq. (3). By differentiating the energy functional Eq. (3) with respect to the time variable t and applying the homogeneous Neumann boundary condition (2), we obtain the following

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(c) &= \int_{\Omega} \left(\frac{\partial c}{\partial t} F'(c) + \frac{\epsilon^2}{2} \nabla \frac{\partial c}{\partial t} \cdot \nabla c \right) \mathrm{d}\mathbf{x} \\ &= \int_{\Omega} \left(c_t F'(c) - \epsilon^2 \Delta c \right) \mathrm{d}\mathbf{x} = -\int_{\Omega} (c_t)^2 \, \mathrm{d}\mathbf{x} \le 0. \end{aligned} \tag{4}$$

In this study, we consider the following logarithmic Flory–Huggins energy potential:

$$F(c) = \theta \left[c \ln(c) + (1-c) \ln(1-c) \right] + 2\theta_c c(1-c), \quad \text{for } 0 < c < 1, \tag{5}$$

where θ is the absolute temperature and θ_c is the critical temperature [19]. Both parameters θ and θ_c are constant. We assume that $\theta_c = 1$ for simplicity, i.e.,

$$F(c) = \theta \left[c \ln(c) + (1-c) \ln(1-c) \right] + 2c(1-c), \quad \text{for } 0 < c < 1. \tag{6}$$

Equation (1) can be rewritten as follows:

$$\frac{\partial c(\mathbf{x},t)}{\partial t} = -\theta[\ln(c(\mathbf{x},t)) - \ln(1-c(\mathbf{x},t))] - 2(1-2c(\mathbf{x},t)) + \epsilon^2 \Delta c(\mathbf{x},t). \tag{7}$$

Several implicit stability-preserving numerical schemes have been developed to solve the AC equation. Uzunca and Karasözen [33] proposed a linear implicit method preserving the energy dissipation law for the AC equation. Li and Song [26] analyzed a reduced-order energy-stability-preserving iterative method for the AC equation with a double-well potential. Li and Wang [27] analyzed a conditional energy stable Crank–Nicolson scheme and proposed an unconditional energy-stable scheme with a stability term for the AC equation. Song et al. [31] proposed a modified Crank–Nicolson method preserving the maximum-principle for the phase-field model. Recently, there have been many research results with fully explicit numerical schemes for the AC equation [1,11,13,15,20,22,39,41]. In particular, Fu et al. [9] proposed Runge–Kutta methods preserving the maximum bound property and the energy dissipation law for the AC equation. Zhang et al. [40] proposed a third-order practically unconditionally structure-preserving method for the modified conservative AC equation.

In general, implicit or semi-implicit numerical schemes for partial differential equations (PDEs) can use sufficiently large time steps while maintaining stability. However, we need to use small time steps for accurate numerical solutions. In the case of the AC equation, which is a second-order PDE, the time step restriction for stability is comparable to the time step constraint imposed by the accuracy requirement. Therefore, the time step constraint for the explicit numerical scheme of the AC equation is not severe. The main purpose of this paper is to investigate the time step restrictions for the explicit numerical scheme that satisfy the maximum principle and a decrease in the discrete total energy of the system over time.

The outline of this paper is summarized as follows. In Section 2, a computational scheme is introduced for the AC equation with the logarithmic potential. In Section 3, the robustness of the proposed scheme is validated through computational experiments, and the results of these experiments are provided. Finally, the conclusion is drawn in Section 4.

2. Methodology

Now, we introduce discretization of the AC equation and investigate the temporal step restrictions, which satisfy the maximum principle and a decrease in the discrete total energy of the system over time, for the fully explicit FDM of the AC equation with a logarithmic potential.

To simplify the description, we focus on the AC equation with a logarithmic potential in $\Omega = (L_x, U_x)$. Higher-dimensional analysis can be done in a straightforward manner. We define a number of spatial grid points as N, the spatial uniform grid size as $h = (U_x - L_x)/N$, and $\Omega_h = \{x_i = L_x + (i-0.5)h,\ 1 \le i \le N\}$. Let Δt be the time step size and the numerical approximations $c_i^n := c(x_i, n\Delta t)$. A final time T is discretized as $T = N_t \Delta t$ where N_t is a total number of time steps. We denote a discrete operator ∇_h as $\nabla_h c_{i+1/2}^n = (c_{i+1}^n - c_i^n)/h$. In Ω_h, the zero Neumann boundary condition is provided as $\nabla_h c_{1/2}^n = \nabla_h c_{N+1/2}^n = 0$, for $n = 1, \dots, N_t$. Let $\Delta_h c_i^n = (\nabla_h c_{i+1/2}^n - \nabla_h c_{i-1/2}^n)/h = (c_{i-1}^n - 2c_i^n + c_{i+1}^n)/h^2$ be a discrete Laplacian operator and $\|\boldsymbol{c}^n\|_\infty = \max_{1\le i\le N} |c_i^n|$ be a discrete maximum norm, where $\boldsymbol{c}^n = (c_1^n, c_2^n, \cdots, c_N^n)$. The convergence accuracies in time and space for the AC equation (1) with a logarithmic potential can be expressed as follows:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \mathcal{O}(\Delta t) = \theta \left(\ln\left(1 - c_i^n\right) - \ln c_i^n\right) - 2\left(1 - 2c_i^n\right) + \epsilon^2 \Delta_h c_i^n + \mathcal{O}(h^2). \tag{8}$$

Therefore, we consider the following fully explicit method for approximating the AC equation:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = \theta \left(\ln\left(1 - c_i^n\right) - \ln c_i^n\right) - 2\left(1 - 2c_i^n\right) + \frac{\epsilon^2}{h^2}\left(c_{i-1}^n - 2c_i^n + c_{i+1}^n\right). \tag{9}$$

2.1. Discrete maximum principle

Let c_α and c_β be the two arguments of the minimum of the logarithmic potential (5) with $0 < c_\alpha \le \frac{1}{2} \le c_\beta < 1$.

Theorem 1. *Suppose that the initial values satisfy* $0 \le c_\alpha \le c_i^0 \le c_\beta \le 1$, *for* $1 \le i \le N$. *Then, for all* $n \ge 0$, *the numerical solutions of the scheme* (9) *satisfy* $0 < c_\alpha \le c_i^{n+1} \le c_\beta < 1,\ \text{for } 1 \le i \le N$, *if* Δt *satisfies*

$$\Delta t \le \frac{h^2}{Mh^2 + 2\epsilon^2}, \tag{10}$$

where $M = \max\left(F''\left(c_\alpha\right), F''\left(c_\beta\right)\right)$.

Proof. Equation (9) can be rewritten as

$$c_i^{n+1} = c_i^n + \Delta t \left(\theta \left(\ln \left(1 - c_i^n \right) - \ln c_i^n \right) - 2 \left(1 - 2c_i^n \right) + \frac{\epsilon^2}{h^2} \left(c_{i-1}^n - 2c_i^n + c_{i+1}^n \right) \right). \tag{11}$$

The proof is divided into three distinct cases.

Case 1. $c_i^n = \dfrac{1}{2}$

From Eq. (11) and $0 \le c_\alpha \le \dfrac{1}{2} \le c_\beta \le 1$, the numerical solution satisfies

$$\frac{1}{2} + \frac{\epsilon^2 \Delta t}{h^2} (2c_\alpha - 1) \le c_i^{n+1} = \frac{1}{2} + \frac{\epsilon^2 \Delta t}{h^2} \left(c_{i-1}^n - 1 + c_{i+1}^n \right) \le \frac{1}{2} + \frac{\epsilon^2 \Delta t}{h^2} (2c_\beta - 1).$$

Therefore, $c_\alpha \le c_i^{n+1} \le c_\beta$ provided that Δt satisfies $\Delta t \le \dfrac{h^2}{2\epsilon^2}$.

Case 2. $c_i^n = c_\beta$ *or* c_α

First, we consider when $c_i^n = c_\beta$. The numerical solution (11) is rewritten as

$$c_i^{n+1} = c_\beta + \frac{\epsilon^2 \Delta t}{h^2} \left(c_{i-1}^n - 2c_\beta + c_{i+1}^n \right).$$

Because $c_{i-1}^n - 2c_\beta + c_{i+1}^n \le 0$, we have that $c_i^{n+1} \le c_\beta$. If $c_{i-1}^n - 2c_\beta + c_{i+1}^n = 0$, the time step is not subject to any constraints or limitations; otherwise, i.e., $c_{i-1}^n - 2c_\beta + c_{i+1}^n < 0$, then $\Delta t \le \dfrac{h^2}{2\epsilon^2}$ results in $c_i^{n+1} \ge c_\beta + \frac{1}{2}(2c_\alpha - 2c_\beta) = c_\alpha$. Therefore, we have that $c_\alpha \le c_i^{n+1} \le c_\beta$.

Similarly, when $c_i^n = c_\alpha$, we have $c_\alpha \le c_i^{n+1} \le c_\beta$ with $\Delta t \le \dfrac{h^2}{2\epsilon^2}$ as well.

Case 3. $\dfrac{1}{2} < c_i^n < c_\beta$ *or* $c_\alpha < c_i^n < \dfrac{1}{2}$

Let $\dfrac{1}{2} < c_i^n < c_\beta$. In Eq. (11), if $\theta \left(-\ln c_i^n + \ln \left(1 - c_i^n \right) \right) - 2 \left(1 - 2c_i^n \right) + \dfrac{\epsilon^2}{h^2} \left(c_{i-1}^n - 2c_i^n + c_{i+1}^n \right) \ge 0$, then we always have $c_i^{n+1} \ge c_\alpha$. From Eq. (11), since $\dfrac{1}{2} < c_i^n < c_\beta$, we can obtain the following inequality

$$c_i^{n+1} \le c_i^n + \Delta t \left(\theta \left(-\ln c_i^n + \ln \left(1 - c_i^n \right) \right) - 2 \left(1 - 2c_i^n \right) + \frac{\epsilon^2}{h^2} \left(2c_\beta - 2c_i^n \right) \right).$$

Next, we want to determine the condition of Δt which satisfies

$$c_i^n + \Delta t \left(\theta \left(-\ln c_i^n + \ln \left(1 - c_i^n \right) \right) - 2 \left(1 - 2c_i^n \right) + \frac{\epsilon^2}{h^2} \left(2c_\beta^n - 2c_i^n \right) \right) \le c_\beta.$$

Then, it can be rewritten as

$$\Delta t \left(F'(c_\beta) - F'(c_i^n) + \frac{2\epsilon^2}{h^2} \left(c_\beta - c_i^n \right) \right) \le c_\beta - c_i^n \tag{12}$$

where $F'(c_\beta) = 0$. By dividing both sides of (12) by $(c_\beta - c_i^n) > 0$, we have

$$\Delta t\left(\frac{F'\left(c_\beta\right)-F'\left(c_i^n\right)}{c_\beta-c_i^n}+\frac{2\epsilon^2}{h^2}\right)\leq 1.$$

Therefore, we obtain the following constraint for Δt.

$$\Delta t\leq\frac{1}{\dfrac{F'\left(c_\beta\right)-F'\left(c_i^n\right)}{c_\beta-c_i^n}+\dfrac{2\epsilon^2}{h^2}}.$$

Here, the $\dfrac{F'\left(c_\beta\right)-F'\left(c_i^n\right)}{c_\beta-c_i^n}$ since $0<\dfrac{F'\left(c_\beta\right)-F'\left(c_i^n\right)}{c_\beta-c_i^n}<F''\left(c_\beta\right)$, we have the following time step condition

$$\Delta t\leq\frac{h^2}{F''\left(c_\beta\right)h^2+2\epsilon^2}.$$

Similarly, when the right hand side of Eq. (11) is less than or equal to c_i^n, then $c_i^{n+1}\leq c_\beta$ is always valid. From Eq. (11), we take the following inequality

$$c_i^{n+1}\geq c_i^n+\Delta t\left(\theta\left(-\ln c_i^n+\ln\left(1-c_i^n\right)\right)-2\left(1-2c_i^n\right)+\frac{\epsilon^2}{h^2}\left(2c_\alpha-2c_i^n\right)\right). \tag{13}$$

From the inequality (13), to satisfy that $c_\alpha\leq c_i^{n+1}$, we consider the following inequality

$$c_i^n+\Delta t\left(\theta\left(-\ln c_i^n+\ln\left(1-c_i^n\right)\right)-2\left(1-2c_i^n\right)+\frac{\epsilon^2}{h^2}\left(2c_\alpha^n-2c_i^n\right)\right)\geq c_\alpha. \tag{14}$$

Since $F'\left(c_\alpha\right)=0$ and $c_\alpha-c_i^n<0$, it can be rewritten as

$$\Delta t\left(\frac{F'\left(c_\alpha\right)-F'\left(c_i^n\right)}{c_\alpha-c_i^n}+\frac{2\epsilon^2}{h^2}\right)\leq 1.$$

Then, since $F'\left(c_\alpha\right)>F'\left(c_i^n\right)$ on $c_\alpha<\dfrac{1}{2}<c_i^n$, we get the following condition

$$\Delta t\leq\frac{h^2}{2\epsilon^2}.$$

Now, we consider that $c_\alpha<c_i^n<\dfrac{1}{2}$. Similarly, in Eq. (11), if $\theta\left(-\ln c_i^n+\ln\left(1-c_i^n\right)\right)-2\left(1-2c_i^n\right)+\dfrac{\epsilon^2}{h^2}\left(c_{i-1}^n-2c_i^n+c_{i+1}^n\right)\leq 0$, then we have $c_i^{n+1}\leq c_\beta$. We want to find the condition of Δt satisfying that

$$c_i^n+\Delta t\left(\theta\left(-\ln c_i^n+\ln\left(1-c_i^n\right)\right)-2\left(1-2c_i^n\right)+\frac{\epsilon^2}{h^2}\left(2c_\alpha^n-2c_i^n\right)\right)\geq c_\alpha.$$

Then, we obtain that

$$\Delta t\left(\frac{F'\left(c_\alpha\right)-F'\left(c_i^n\right)}{c_\alpha-c_i^n}+\frac{2\epsilon^2}{h^2}\right)\leq 1.$$

Here, since $0<\dfrac{F'\left(c_\alpha\right)-F'\left(c_i^n\right)}{c_\alpha-c_i^n}<F''\left(c_\alpha\right)$, the following condition is derived

$$\Delta t \le \frac{h^2}{F''(c_\alpha)\,h^2 + 2\epsilon^2}.$$

Lastly, when $\theta\left(-\ln c_i^n + \ln\left(1 - c_i^n\right)\right) - 2\left(1 - 2c_i^n\right) + \frac{\epsilon^2}{h^2}\left(c_{i-1}^n - 2c_i^n + c_{i+1}^n\right) > 0$, then $c_i^{n+1} \ge c_\alpha$ always holds true. From Eq. (11), we consider the following inequality

$$c_i^n + \Delta t\left(\theta\left(-\ln c_i^n + \ln\left(1 - c_i^n\right)\right) - 2\left(1 - 2c_i^n\right) + \frac{\epsilon^2}{h^2}\left(2c_\beta^n - 2c_i^n\right)\right) \le c_\beta.$$

It can be rewritten as

$$\Delta t\left(\frac{F'(c_\beta) - F'(c_i^n)}{c_\beta - c_i^n} + \frac{2\epsilon^2}{h^2}\right) \le 1.$$

Therefore, since $F'(c_\beta) < F'(c_i^n)$ on $c_i^n < \frac{1}{2} < c_\beta$, we can derive the following condition

$$\Delta t \le \frac{h^2}{2\epsilon^2}. \quad \square$$

We note that a critical time step is denoted by

$$\delta t(M, h, \epsilon) := \frac{h^2}{Mh^2 + 2\epsilon^2},$$

where $M = \max(F''(c_\alpha), F''(c_\beta))$.

2.2. Energy stability analysis

We now examine the energy stability of the explicit Euler FDM, which considers the AC equation with a logarithmic potential, while adhering to the analyzed time step constraint (10) on Ω. The analysis described here follows a comparable procedure as presented in [11,14]. We denote the discrete l_2-inner product as $\langle \boldsymbol{c}, \boldsymbol{\psi} \rangle_h = h\sum_{i=1}^{N} c_i\psi_i$. As a result of the free energy functional (3), we obtain a discrete energy functional $\mathcal{E}_h(\boldsymbol{c}^n)$ and decompose it into two parts as shown below

$$\begin{aligned}\mathcal{E}_h(\boldsymbol{c}^n) = h\sum_{i=1}^{N}\left[\theta\left(c_i^n \ln c_i^n + \left(1 - c_i^n\right)\ln\left(1 - c_i^n\right)\right) + 2c_i^n\left(1 - c_i^n\right)\right] \\ + \frac{h\epsilon^2}{2}\sum_{i=1}^{N-1}\left|\nabla_h c_{i+\frac{1}{2}}^n\right|^2 = \mathcal{E}^{(1)}(\boldsymbol{c}^n) + \mathcal{E}^{(2)}(\boldsymbol{c}^n),\end{aligned} \tag{15}$$

where $\mathcal{E}^{(1)}(\boldsymbol{c}^n) = h\sum_{i=1}^{N}\left[\theta\left(c_i^n \ln c_i^n + \left(1 - c_i^n\right)\ln\left(1 - c_i^n\right)\right) + 2c_i^n\left(1 - c_i^n\right)\right]$ and $\mathcal{E}^{(2)}(\boldsymbol{c}^n) = \frac{h\epsilon^2}{2}\sum_{i=1}^{N-1}\left|\nabla_h c_{i+\frac{1}{2}}^n\right|^2$. Then, we can describe the fully explicit scheme as the gradient of discrete total energy by

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = -\frac{1}{h}\nabla\mathcal{E}_h(\boldsymbol{c}^n)_i, \quad \text{for} \quad i = 1, \cdots, N. \tag{16}$$

For the discrete energy functionals $\mathcal{E}^{(1)}(\boldsymbol{c})$ and $\mathcal{E}^{(2)}(\boldsymbol{c})$ in (15), we consider the following Hessian matrices $\mathbf{H}^{(1)}$ and $\mathbf{H}^{(2)}$, which are defined as the Jacobian of $\nabla\mathcal{E}^{(1)}(\boldsymbol{c})$ and $\nabla\mathcal{E}^{(2)}(\boldsymbol{c})$.

$$\left\{\mathbf{H}^{(1)}, \mathbf{H}^{(2)}\right\} = \left\{\nabla^2 \mathcal{E}^{(1)}(\boldsymbol{c}), \nabla^2 \mathcal{E}^{(2)}(\boldsymbol{c})\right\}$$
$$= \left\{ h \begin{pmatrix} F''(c_1) & & & & 0 \\ & F''(c_2) & & & \\ & & \ddots & & \\ & & & F''(c_{N-1}) & \\ 0 & & & & F''(c_N) \end{pmatrix}, h\epsilon^2 \begin{pmatrix} 1 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & -1 & 1 \end{pmatrix} \right\},$$

where $F''(c) = \dfrac{\theta}{c} + \dfrac{\theta}{1-c} - 4$. Here, the homogeneous Neumann boundary condition is applied. Then, for $k = 1, 2, \ldots, N$, the eigenvalues of $\mathbf{H}^{(1)}$ and $\mathbf{H}^{(2)}$ are

$$\lambda_k^{(1)} = h\left(\frac{\theta}{c_k} + \frac{\theta}{1-c_k} - 4\right), \quad \lambda_k^{(2)} = \frac{4\epsilon^2}{h}\sin^2\frac{(k-1)\pi}{2N},$$

respectively. Let $\mathbf{v}_k = \mathbf{w}_k/|\mathbf{w}_k|$ be the orthonormal eigenvector corresponding to the eigenvalues $\lambda_k^{(2)}$, where

$$\mathbf{w}_k = \left(\cos\frac{(k-1)\pi}{2N}, \cos\frac{3(k-1)\pi}{2N}, \cdots, \cos\frac{(2N-1)(k-1)\pi}{2N}\right).$$

Then, we can express $\boldsymbol{c}^{n+1} - \boldsymbol{c}^n$ with terms of $\mathbf{v}_k$ as

$$\boldsymbol{c}^{n+1} - \boldsymbol{c}^n = \sum_{k=1}^{N} \alpha_k \mathbf{v}_k.$$

Theorem 2. *Assume that the AC equation with a logarithmic potential satisfies the zero Neumann boundary condition. If the initial condition satisfies $0 \le c_\alpha \le c_i^0 \le c_\beta \le 1$, for $1 \le i \le N$, then the discrete energy decreasing property is satisfied by the numerical solutions acquired through the fully explicit Euler method* (9)

$$\mathcal{E}_h(\boldsymbol{c}^{n+1}) \le \mathcal{E}_h(\boldsymbol{c}^n),$$

if the time step satisfies:

$$\Delta t \le \frac{h^2}{Mh^2 + 2\epsilon^2} \tag{17}$$

where $M = \max\left(F''(c_\alpha), F''(c_\beta)\right)$

Proof. We can obtain $\mathcal{E}_h(\boldsymbol{c}^{n+1})$ by applying the Taylor expansion at $\boldsymbol{c}^n$ up to the second order as

$$\mathcal{E}_h(\boldsymbol{c}^{n+1}) = \mathcal{E}_h(\boldsymbol{c}^n) + \left\langle \frac{1}{h}\nabla\mathcal{E}_h(\boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h$$
$$+ \left\langle \frac{1}{2h}\nabla^2\mathcal{E}_h(\xi)(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h,$$

where $\xi = \alpha\boldsymbol{c}^n + (1-\alpha)\boldsymbol{c}^{n+1}$ and $0 \le \alpha \le 1$. Then, we have the following equation,

$$\mathcal{E}_h(\boldsymbol{c}^{n+1}) - \mathcal{E}_h(\boldsymbol{c}^n) = \left\langle \frac{1}{h}\nabla\mathcal{E}_h(\boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h$$
$$+ \left\langle \frac{1}{2h}\nabla^2\mathcal{E}_h(\xi)(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h. \tag{18}$$

By using the Hessian matrix and Eq. (16), Eq. (18) can be rewritten as

$$
\begin{aligned}
&\mathcal{E}(\mathbf{c}^{n+1}) - \mathcal{E}(\mathbf{c}^n) \\
&= -\left\langle \frac{\boldsymbol{c}^{n+1} - \boldsymbol{c}^n}{\Delta t}, \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h + \left\langle \frac{1}{2h}\left(\mathbf{H}^{(1)} + \mathbf{H}^{(2)}\right)(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h \\
&= -\frac{1}{\Delta t}\left\langle \boldsymbol{c}^{n+1} - \boldsymbol{c}^n, \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h + \frac{1}{2}\left\langle \frac{1}{h}\mathbf{H}^{(1)}(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h \\
&\quad + \left\langle \frac{1}{2h}\mathbf{H}^{(2)}(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h \\
&\le -\frac{1}{\Delta t}\left\langle \boldsymbol{c}^{n+1} - \boldsymbol{c}^n, \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h + \frac{m}{2}\left\langle \boldsymbol{c}^{n+1} - \boldsymbol{c}^n, \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h \\
&\quad + \left\langle \frac{1}{2h}\mathbf{H}^{(2)}(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h \qquad (19) \\
&= \sum_{k,l=1}^{N} \left\langle \left[-\frac{1}{\Delta t} + \frac{m}{2} + \frac{1}{2h}\lambda_k^{(2)} \right] \alpha_k \mathbf{v}_k, \alpha_l \mathbf{v}_l \right\rangle_h \\
&= \sum_{k,l=1}^{N} \left\langle \left[-\frac{1}{\Delta t} + \frac{m}{2} + \frac{2\epsilon^2}{h^2}\sin^2\frac{(k-1)\pi}{2N} \right] \alpha_k \mathbf{v}_k, \alpha_l \mathbf{v}_l \right\rangle_h \\
&= \sum_{k=1}^{N} \left[-\frac{1}{\Delta t} + \frac{m}{2} + \frac{2\epsilon^2}{h^2}\sin^2\frac{(k-1)\pi}{2N} \right] \alpha_k^2, \qquad (20)
\end{aligned}
$$

where $m = \max_{1 \le p \le N}(\lambda_p^{(1)}/h)$. We note that in Eq. (19), the following has been used:

$$
\begin{aligned}
&\left\langle \frac{1}{h}\mathbf{H}^{(1)}(\boldsymbol{c}^{n+1} - \boldsymbol{c}^n), \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h = \sum_{k,l=1}^{N} \left\langle \frac{1}{h}\mathbf{H}^{(1)}(d_k \mathbf{e}_k), d_l \mathbf{e}_l \right\rangle_h \\
&= \sum_{k,l=1}^{N} \left\langle \frac{\lambda_k^{(1)}}{h}(d_k \mathbf{e}_k), d_l \mathbf{e}_l \right\rangle_h \le \sum_{k,l=1}^{N} \max_{1 \le p \le N}\left(\frac{\lambda_p^{(1)}}{h}\right)\left\langle d_k \mathbf{e}_k, d_l \mathbf{e}_l \right\rangle_h \\
&= \frac{m}{2}\left\langle \boldsymbol{c}^{n+1} - \boldsymbol{c}^n, \boldsymbol{c}^{n+1} - \boldsymbol{c}^n \right\rangle_h,
\end{aligned}
$$

where $\mathbf{e}_k = (0, \ldots, 0, \underset{\text{k-th position}}{\underset{\uparrow}{1}}, 0, \ldots, 0)$ is a standard basis and $\mathbf{c}^{n+1} - \mathbf{c}^n = \sum_{k=1}^{N} d_k \mathbf{e}_k$. If the time step satisfies $\Delta t \le \frac{h^2}{Mh^2 + 2\epsilon^2}$, where $M = \max\left(F''(c_\alpha), F''(c_\beta)\right)$, then the following inequality can be derived from Eq. (20):

$$
\mathcal{E}_h(\boldsymbol{c}^{n+1}) - \mathcal{E}_h(\boldsymbol{c}^n) \le \sum_{k=1}^{N} \alpha_k^2 \left(\frac{1}{2}M + \frac{2\epsilon^2}{h^2} - \frac{Mh^2 + 2\epsilon^2}{h^2} \right) = -\frac{M}{2}\sum_{k=1}^{N} \alpha_k^2 \le 0.
$$

Here, we have used $m = \max_{1 \le p \le N}(\lambda_p^{(1)}/h) \le M$. □

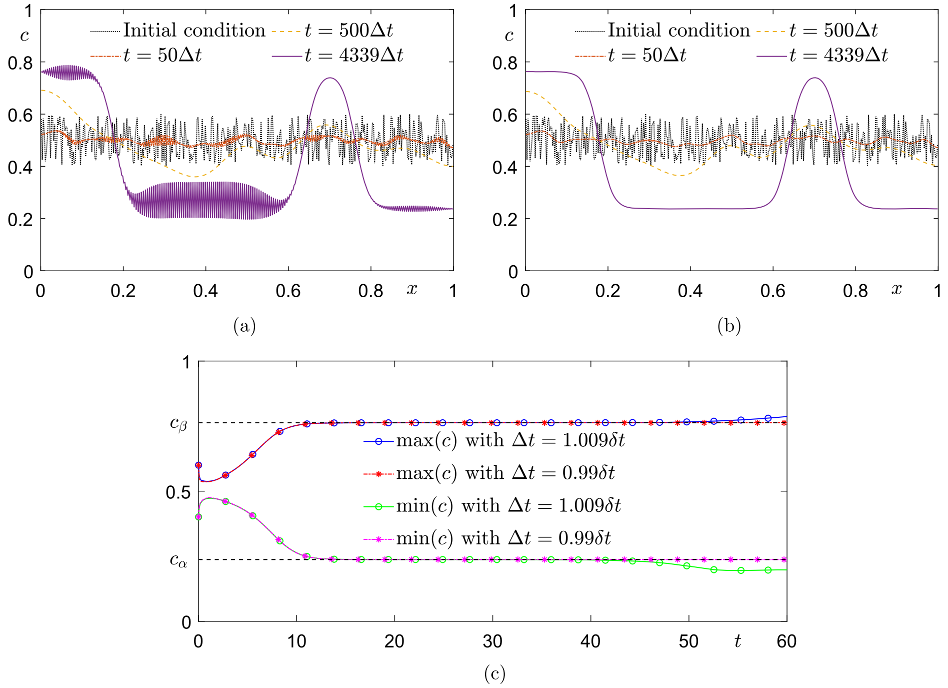

Fig. 1. (a) is evolution of c with $\Delta t = 1.009\delta t$. (a) is evolution of c with $\Delta t = 0.99\delta t$. (c) is evolution results of $\max(c)$ and $\min(c)$ with $\Delta t = 1.009\delta t$ and $\Delta t = 0.99\delta t$.

3. Structure-preservation

By observing the maximum principle and discrete energy decrease of the numerical solution, we demonstrate the structure-preservation of the numerical solution with the proposed critical time step for the AC equation. We set the initial condition as follows:

$$c(x, 0) = 0.2\text{rand}(x) + 0.4 \quad \text{on} \quad \Omega = (0, 1),$$

where $\text{rand}(x)$ is a random value between 0 and 1. For the computational tests, the parameters used are $\theta = 0.9$, $N = 400$, and $\epsilon = 0.015$. We define discrete maximum and minimum values of the numerical solution as $\max(c) = \max_{1\le i\le N} c_i$ and $\min(c) = \min_{1\le i\le N} c_i$, respectively.

To validate that the proposed analyzed time-step restriction $\delta t = (h^2/(Mh^2 + 2\epsilon^2))$ guarantees the maximum principle of the numerical solution, we consider two time steps $\Delta t = 1.009\delta t$ and $\Delta t = 0.99\delta t$. Fig. 1 shows profiles of $c(x, t)$ and evolutions of $\max(c)$ and $\min(c)$ with $\Delta t = 1.009\delta t$ and $\Delta t = 0.99\delta t$. When we use the time step as $1.009\delta t$, we obtain an oscillated numerical solution, which does not preserve the structure. We investigate the temporal variation of discrete total energy. The discrete total energy functional is defined as follows:

$$\mathcal{E}_h(c^n) = h\sum_{i=1}^{N} F(c_i^n) + \frac{\epsilon^2}{2}\left((c_1^n - c_0^n)^2 + \sum_{i=1}^{N-1}(c_{i+1}^n - c_i^n)^2 + (c_{N+1}^n - c_N^n)^2\right).$$

The initial condition and parameters are the same as in the previous numerical test. Fig. 2 shows the variation in total energy over time for $\Delta t = 1.009\delta t$ and $\Delta t = 0.99\delta t$. From the result of Fig. 2, we can observe that the proposed time-step restriction δt is a critical value, which preserves the structure of the numerical solution for the explicit scheme of the AC equation.

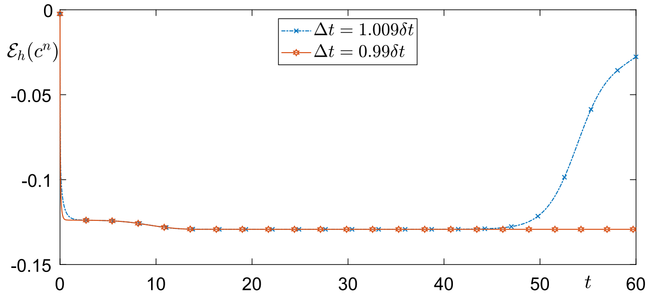

Fig. 2. The discrete total energy variation.

4. Conclusions

When using a small time step size for high accuracy in numerical solutions, the explicit Euler method is one of the simplest and fastest methods. Moreover, considering that the logarithmic Flory–Huggins potential represents the physics involved, the time step analysis of the explicit Euler FDM that preserves the structure of the AC equation using the logarithmic potential becomes significant. We presented a stability analysis of a structure-preserving explicit FDM for the AC equation with a logarithmic potential that has two arguments of the minimum. First, we computed the temporal step constraint which guarantees that if the initial condition is bounded by the two arguments of the minimum, then the numerical solutions are always bounded by them, i.e., the explicit numerical scheme satisfies the maximum principle. Second, we proved that the computed critical time step guarantees that the discrete total energy of the system is non-increasing over time. Numerical experiments, demonstrating the preservation of the maximum principle and the decrease in discrete total energy of the numerical solution, were performed. As future work, we will apply the current methodology to the AC equation with a high-order polynomial free energy [25].

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