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Comparison study of numerical methods for solving the Allen–Cahn equation

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ABSTRACT

The goal of this paper is to present a brief review and a critical comparison of the performance of several numerical schemes for solving the Allen–Cahn equation representing a model for antiphase domain coarsening in a binary mixture. Explicit, fully implicit, Crank–Nicolson, and unconditionally gradient stable schemes are considered. In this paper, we show the solvability conditions of the numerical schemes and the decreasing property of total energy using eigenvalues of the Hessian matrix of the energy functional. We also present the pointwise boundedness of the numerical solution for the Allen–Cahn equation. To compare the accuracy and numerical efficiency of these methods, numerical experiments such as traveling wave and motion by mean curvature are performed. Numerical results show that Crank–Nicolson and nonlinearly stabilized splitting schemes are almost close to the analytic solution. However, if a large time step is used in the numerical test, we have only two results with linearly and nonlinearly stabilized splitting schemes in spite of having large gaps between analytic solution and numerical results. The other numerical schemes except for linearly and nonlinearly stabilized splitting schemes have unstable results when large time step is used.

1. Introduction

In this paper, we shall present a brief review and a critical comparison of the performance of several numerical schemes for solving the Allen–Cahn (AC) equation [1]:

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

where $\Omega \subset \mathbb{R}^d$ $(d=1,2,3)$ is a domain. $\phi(\mathbf{x},t)$ is the difference between the concentrations of the two mixtures' components and $F(\phi) = 0.25(\phi^2-1)^2$. The parameter ϵ is the gradient energy coefficient related to the interfacial energy. The boundary condition is

$$\mathbf{n}\cdot\nabla\phi = 0 \text{ on } \partial\Omega, \tag{2}$$

where $\mathbf{n}$ denotes the normal vector on $\partial\Omega$. The AC equation is the L^2-gradient flow of the following total free energy functional:

$$\mathcal{E}(\phi) = \int_\Omega \left(\frac{F(\phi)}{\epsilon^2} + \frac{1}{2}|\nabla\phi|^2\right) d\mathbf{x}. \tag{3}$$

Differentiating the energy $\mathcal{E}(\phi)$ with respect to t gives

$$\begin{aligned}\frac{d}{dt}\mathcal{E}(\phi) &= \int_\Omega \left(\frac{F'(\phi)}{\epsilon^2}\phi_t + \nabla\phi\cdot\nabla\phi_t\right) d\mathbf{x} \\ &= \int_\Omega \left(\frac{F'(\phi)}{\epsilon^2} - \Delta\phi\right)\phi_t\, d\mathbf{x} = -\int_\Omega (\phi_t)^2\, d\mathbf{x} \leqslant 0,\end{aligned} \tag{4}$$

where the integration by parts and the boundary condition (2) are used. Therefore, the total energy is non-increasing in time. The AC Eq. (1) was originally introduced as a mathematical model for antiphase domain coarsening in a binary alloy [1]. The equilibrium configuration of the Ginzburg–Landau free energy functional has been applied to a wide range of problems such as phase transitions [2], coupled with the Navier–Stokes equation [3,4], energy minimizers [5], a gradient flow of a lower semicontinuous convex function [6], the motion by mean curvature flows [7], image analysis [8–12], crystal growth [13], anisotropic equations [14,15], vector-valued Allen–Cahn equation [12,16,17], precipitation and dissolution [18], pattern dynamics of reaction–diffusion equations [19,20], and degenerate diffusion [21]. Error estimates and stability were also studied in [22,23]. In addition, high accuracy solution for the AC equation is discussed in [24,25] and the conservative AC equation is also studied [26,27].

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This paper is organized as follows. In Section 2, we describe numerical analysis such as solvability, the total energy decrease, and the boundedness of the numerical solution. We present the numerical results in Section 3. In Section 4, we conclude.

2. Numerical analysis

We present various numerical schemes for the AC equation. For simplicity, we discretize the AC equation in one-dimensional space $\Omega = (a, b)$. Higher dimensional discretizations are similarly defined. Let N be a positive even integer, $h = (b-a)/N$ be the uniform mesh size, and $\Omega_h = \{x_i = (i-0.5)h, 1 \leqslant i \leqslant N\}$ be the set of cell-centers. Let ϕ_i^n be approximations of $\phi(x_i, n\Delta t)$, where $\Delta t = T/N_t$ is the time step, T is the final time, N_t is the total number of time steps, and $\boldsymbol{\phi}^n = (\phi_1^n, \phi_2^n, \ldots, \phi_N^n)$. Let a discrete differentiation operator be $\nabla_h \phi^n_{i+\frac{1}{2}} = (\phi^n_{i+1} - \phi^n_i)/h$, then the zero Neumann boundary condition (2) is defined as

$$\nabla_h \phi^n_{\frac{1}{2}} = \nabla_h \phi^n_{N+\frac{1}{2}} = 0. \tag{5}$$

We then define a discrete Laplacian by $\Delta_h \phi_i = \left(\nabla_h \phi_{i+\frac{1}{2}} - \nabla_h \phi_{i-\frac{1}{2}}\right)\big/ h$ and discrete l_2-inner products by

$$\langle \boldsymbol{\phi}, \boldsymbol{\psi} \rangle_h = h\sum_{i=1}^{N} \phi_i \psi_i \quad \text{and} \quad (\nabla_h \boldsymbol{\phi}, \nabla_h \boldsymbol{\psi})_h = h\sum_{i=0}^{N} \nabla_h \phi_{i+\frac{1}{2}} \nabla_h \psi_{i+\frac{1}{2}}.$$

Note that a discrete summation by parts holds with the boundary condition (5), i.e., $\langle \Delta_h \boldsymbol{\phi}, \boldsymbol{\psi} \rangle_h = \langle \boldsymbol{\phi}, \Delta_h \boldsymbol{\psi} \rangle_h = -(\nabla_h \boldsymbol{\phi}, \nabla_h \boldsymbol{\psi})_h$. We also define the discrete norms as $\|\boldsymbol{\phi}\|_h^2 = \langle \boldsymbol{\phi}, \boldsymbol{\phi} \rangle_h$ and $\|\boldsymbol{\phi}\|_\infty = \max_{1 \leqslant i \leqslant N} |\phi_i|$. We consider the following six numerical schemes for Eq. (1) and compare their accuracy and performance by using numerical experiments:

$$\text{Explicit} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{\phi_i^n - (\phi_i^n)^3}{\epsilon^2} + \Delta_h \phi_i^n, \tag{6}$$

$$\text{Implicit} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{\phi_i^{n+1} - (\phi_i^{n+1})^3}{\epsilon^2} + \Delta_h \phi_i^{n+1}, \tag{7}$$

$$\text{Crank–Nicolson} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{\phi_i^{n+1} - (\phi_i^{n+1})^3}{2\epsilon^2} + \frac{1}{2}\Delta_h \phi_i^{n+1} + \frac{\phi_i^n - (\phi_i^n)^3}{2\epsilon^2} + \frac{1}{2}\Delta_h \phi_i^n, \tag{8}$$

$$\text{Nonlinear splitting} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{\phi_i^n - (\phi_i^{n+1})^3}{\epsilon^2} + \Delta_h \phi_i^{n+1}, \tag{9}$$

$$\text{Linear splitting} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{3\phi_i^n - 2\phi_i^{n+1} - (\phi_i^n)^3}{\epsilon^2} + \Delta_h \phi_i^{n+1}, \tag{10}$$

where $i = 1, \ldots, N$.

2.1. Solvability of the schemes

Let us consider the following discrete AC equation:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{-\alpha(\phi_i^{n+1})^3 - (1-\alpha)(\phi_i^n)^3 + \beta\phi_i^{n+1} + (1-\beta)\phi_i^n}{\epsilon^2} + \Delta_h(\gamma\phi_i^{n+1} + (1-\gamma)\phi_i^n), \tag{11}$$

where α, β, and γ are real numbers. Note that

$$\text{Explicit} \quad \alpha = \beta = \gamma = 0, \tag{12}$$

$$\text{Implicit} \quad \alpha = \beta = \gamma = 1, \tag{13}$$

$$\text{Crank–Nicolson} \quad \alpha = \beta = \gamma = \frac{1}{2}, \tag{14}$$

$$\text{Nonlinear splitting} \quad \alpha = 1,\ \beta = 0,\ \gamma = 1, \tag{15}$$

$$\text{Linear splitting} \quad \alpha = 0,\ \beta = -2,\ \gamma = 1. \tag{16}$$

Here, the explicit scheme is uniquely solvable in Eq. (11). Therefore, we focus on the solvability of the other four schemes.

Bearing in mind that we want to have Eq. (11) as the Euler equation of a functional, we consider the following functional

$$G(\boldsymbol{\phi}) = \frac{1}{2\Delta t}\|\boldsymbol{\phi} - \boldsymbol{\phi}^n\|_h^2 + \left\langle \frac{\alpha\boldsymbol{\phi}^3}{4\epsilon^2} + \frac{(1-\alpha)(\boldsymbol{\phi}^n)^3}{\epsilon^2} - \frac{\beta\boldsymbol{\phi}}{2\epsilon^2} - \frac{(1-\beta)\boldsymbol{\phi}^n}{\epsilon^2}, \boldsymbol{\phi} \right\rangle_h + \frac{\gamma}{2}\|\nabla_h \boldsymbol{\phi}\|_h^2 + (1-\gamma)(\nabla_h \boldsymbol{\phi}^n, \nabla_h \boldsymbol{\phi})_h. \tag{17}$$

Here, we define the notation by $\boldsymbol{\phi}\boldsymbol{\psi} = (\phi_1\psi_1, \phi_2\psi_2, \ldots, \phi_N\psi_N)$. Let $\boldsymbol{\phi}^*$ and $\boldsymbol{\psi} \neq \mathbf{0}$ be fixed vectors and s be a real number variable. We consider a quartic polynomial H in s by

$$\begin{aligned} H(s) &= G(\boldsymbol{\phi}^* + s\boldsymbol{\psi}) \\ &= G(\boldsymbol{\phi}^*) + s\left\langle \frac{\boldsymbol{\phi}^* - \boldsymbol{\phi}^n}{\Delta t} + \frac{\alpha(\boldsymbol{\phi}^*)^3}{\epsilon^2} + \frac{(1-\alpha)(\boldsymbol{\phi}^n)^3}{\epsilon^2} - \frac{\beta\boldsymbol{\phi}^*}{\epsilon^2} - \frac{(1-\beta)\boldsymbol{\phi}^n}{\epsilon^2} - \Delta_h(\gamma\boldsymbol{\phi}^* + (1-\gamma)\boldsymbol{\phi}^n), \boldsymbol{\psi} \right\rangle_h \\ &\quad + s^2\left\langle \frac{\boldsymbol{\psi}}{2\Delta t} + \frac{(3\alpha(\boldsymbol{\phi}^*)^2 - \beta)\boldsymbol{\psi}}{2\epsilon^2} - \frac{\gamma\Delta_h\boldsymbol{\psi}}{2}, \boldsymbol{\psi} \right\rangle_h + s^3\left\langle \frac{\alpha\boldsymbol{\phi}^*\boldsymbol{\psi}^2}{\epsilon^2}, \boldsymbol{\psi} \right\rangle_h \\ &\quad + s^4\left\langle \frac{\alpha\boldsymbol{\psi}^3}{4\epsilon^2}, \boldsymbol{\psi} \right\rangle_h. \end{aligned} \tag{18}$$

And the second derivative is derived as

$$H''(s) = \left(\frac{1}{\Delta t} - \frac{\beta}{\epsilon^2}\right)\langle \boldsymbol{\psi}, \boldsymbol{\psi} \rangle_h + \frac{3\alpha}{\epsilon^2}\langle (\boldsymbol{\phi}^* + s\boldsymbol{\psi})^2, \boldsymbol{\psi}^2 \rangle_h + \gamma\|\nabla_h \boldsymbol{\psi}\|_h^2. \tag{19}$$

If the parameters satisfy $\alpha \geqslant 0$, $\beta < \epsilon^2/\Delta t$, and $\gamma \geqslant 0$, then $H''(s)$ has a strictly positive value. It means that the polynomial H is strictly convex and $G(\boldsymbol{\phi})$ is bounded below. Thus, there is the unique minimizer $\boldsymbol{\phi}^*$, i.e., $G(\boldsymbol{\phi}^*) \leqslant G(\boldsymbol{\phi})$ for all $\boldsymbol{\phi}$. Since $\boldsymbol{\phi}^*$ is the critical point, we have,

$$H'(0) = \left\langle \frac{\boldsymbol{\phi}^* - \boldsymbol{\phi}^n}{\Delta t} + \frac{\alpha(\boldsymbol{\phi}^*)^3}{\epsilon^2} + \frac{(1-\alpha)(\boldsymbol{\phi}^n)^3}{\epsilon^2} - \frac{\beta\boldsymbol{\phi}^*}{\epsilon^2} - \frac{(1-\beta)\boldsymbol{\phi}^n}{\epsilon^2} - \gamma\Delta_h\boldsymbol{\phi}^* - (1-\gamma)\Delta_h\boldsymbol{\phi}^n, \boldsymbol{\psi} \right\rangle_h = 0. \tag{20}$$

Since Eq. (19) holds regardless of $\boldsymbol{\psi}$, we have

$$\frac{\boldsymbol{\phi}^* - \boldsymbol{\phi}^n}{\Delta t} = \frac{-\alpha(\boldsymbol{\phi}^*)^3 - (1-\alpha)(\boldsymbol{\phi}^n)^3 + \beta\boldsymbol{\phi}^* + (1-\beta)\boldsymbol{\phi}^n}{\epsilon^2} + \Delta_h(\gamma\boldsymbol{\phi}^* + (1-\gamma)\boldsymbol{\phi}^{\mathbf{n}}). \tag{21}$$

Next, we want to show that the minimizer is unique. Let us assume $\hat{\boldsymbol{\phi}}$ is another minimizer, i.e., $G(\hat{\boldsymbol{\phi}}) = G(\boldsymbol{\phi}^*)$ and $\boldsymbol{\psi} = \hat{\boldsymbol{\phi}} - \boldsymbol{\phi}^* \neq \mathbf{0}$. By using the strict convexity of H, we have

$$G(\boldsymbol{\phi}^* + 0.5\boldsymbol{\psi}) = H(0.5) < \frac{H(0) + H(1)}{2} = \frac{G(\boldsymbol{\phi}^*) + G(\hat{\boldsymbol{\phi}})}{2} = G(\boldsymbol{\phi}^*),$$

which leads to a contradiction that $\boldsymbol{\phi}^*$ is the minimizer.

For linearly and nonlinearly stabilized splitting schemes, $H''(s) > 0$ is satisfied with any time step size. Crank–Nicolson and implicit schemes holds if $\Delta t < 2\epsilon^2$ and $\Delta t < \epsilon^2$, respectively. From now on, we define the unique minimizer as $\boldsymbol{\phi}^{n+1}$ and it satisfies Eq. (21).