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A NUMERICAL METHOD FOR SOLVING ALLEN-CAHN **EQUATION**[†]

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ABSTRACT. We propose a numerical method for solving Allen-Cahn equation, in both one-dimensional and two-dimensional cases. The new scheme that is explicit, stable, and easy to compute is obtained and the proposed method provides a straightforward and effective way for nonlinear evolution equations.

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1. Introduction

Allen-Cahn equation was originally introduced by Allen and Cahn [1], and can be regarded as a simple model for the process of phase separation of a binary alloy at a fixed temperature. This equation has been widely applied to various problems, such as image analysis [2, 3], the motion by mean curvature flows [4], crystal growth [5]. In particular, it has become a basic model equation for the diffuse interface approach developed to study phase transitions and interfacial dynamics in materials science [6]. Thus, an efficient and accurate numerical method of this equation has practical significance, and has drawn the attention of many people.

Various numerical methods have been used to solve Allen-Cahn equation, and among them are the finite difference method [11, 7, 8], the finite element method [9, 10], etc. In addition, Yang [12] considered the stabilized semi-implicit (in time) scheme and the splitting scheme for this equation. Kessler et al. [13] presented a posteriori error estimate for the given equation, in which the dependence on ϵ^{-1} is no longer exponential, only polynomial.

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Recently, Abduwali et al. introduced the Local Crank-Nicolson method [14] and the Modified Local Crank-Nicolson (MLCN) method [15] for the heat conduction equation. The MLCN method transforms the partial differential equation into ordinary differential equations, and uses the Trotter product formula to approximate the coefficient matrix of these ordinary differential equations. The MLCN solver separates this matrix into some small-block matrices, and employs the Crank-Nicolson method to obtain the time updated solution. The MLCN is an explicit difference scheme with simple computation and is unconditionally stable.

In this paper, Allen-Cahn equation, in both one-dimensional and two dimensional cases, is considered. The MLCN is developed to solve this nonlinear equation. Moreover, a new difference scheme for the Allen-Cahn equation is formed. Our work in this paper, is not only used to solve the Allen-Cahn equation, but can also be used to develop the MLCN for other nonlinear evolution equations.

2. New scheme for one-dimensional Allen-Cahn equation

Consider one-dimensional Allen-Cahn equation

$$\frac{\partial u}{\partial t} - \gamma \frac{\partial^2 u}{\partial x^2} + f(u) = 0, \quad (x, t) \in [0, 1] \times [0, T], \tag{1}$$

with the initial condition

$$u(x,0) = u_0(x), \quad x \in [0,1],$$

and boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t \in (0,T),$$

where γ is positive number. f is

$$f(u) := F'(u)$$
 and $F(u) = \frac{1}{4}(u^2 - 1)^2$,

which will be assumed throughout this paper.

For Eq. (1), using central difference quotient instead of differential term of space, we obtain the following semi-discrete equation:

$$\frac{dV(t)}{dt} = \frac{1}{h^2}AV(t). \tag{2}$$

Let h=1/M be the mesh width in space and set $x_i=ih$ for $i=1,2,\ldots,M-1$. Moreover, V(t) in Eq. (2) is in the form $V(t)=(v(x_1,t),v(x_2,t),\ldots,v(x_{M-1},t))^T$. $v(x_i,t)$ is the approximate solution of $u(x_i,t), v_i:=v(x_i,t)$ and A is $(M-1)\times (M-1)$ tri-diagonal matrix

$$A = \begin{pmatrix} a_1 & \gamma & & & & 0 \\ \gamma & a_2 & \gamma & & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma & a_{M-2} & \gamma & \\ 0 & & \gamma & a_{M-1} \end{pmatrix}, \tag{3}$$

where $a_i = -2\gamma - h^2(v_i^2 - 1), i = 1, 2, \dots, M - 1.$

The solution of Eq. (2) with initial vector

 $V(0) = (v(x_1, 0), v(x_2, 0), \dots, v(x_{M-1}, 0))^T$ can be expressed as

$$V(t) = \exp(\frac{t}{h^2}A)V(0). \tag{4}$$

Let $\tau = T/N$ be the mesh width in time and set $t_n = n\tau$ for n = 1, 2, ..., N. Moreover, $V(t_n)$ can be written in the form $V(t_n) = (v(x_1, t_n), v(x_2, t_n), ..., v(x_{M-1}, t_n))^T$ and $v_i^n := v(x_i, t_n)$. The nonlinear system (4) can be linearized by allowing the nonlinearities to lag one time step behind. Thus we have

$$V(t_{n+1}) = \exp(\frac{\tau}{h^2}A)V(t_n), \tag{5}$$

where

$$A = \begin{pmatrix} a_1^n & \gamma & & & & 0 \\ \gamma & a_2^n & \gamma & & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma & a_{M-2}^n & \gamma & \\ & 0 & & \gamma & a_{M-1}^n \end{pmatrix}, \tag{6}$$

and $a_i^n = -2\gamma - h^2((v_i^n)^2 - 1), i = 1, 2, \dots, M - 1.$

Consider the Crank-Nicolson scheme for the Allen-Cahn equation

$$\frac{v_i^{n+1} - v_i^n}{\tau} = \frac{\gamma}{2h^2} \left(v_{i+1}^{n+1} - 2v_i^{n+1} + v_{i-1}^{n+1} + v_{i+1}^n - 2v_i^n + v_{i-1}^n \right) - \left((v_i^n)^2 - 1 \right) \frac{v_i^{n+1} + v_i^n}{2}.$$
(7)

Note that Eq. (7) can be rewritten as

$$-\lambda \gamma v_{i+1}^{n+1} + \left(1 - \lambda a_i^n\right) v_i^{n+1} - \lambda \gamma v_{i-1}^{n+1} = \lambda \gamma v_{i+1}^n + \left(1 + \lambda a_i^n\right) v_i^n + \lambda \gamma v_{i-1}^n,$$

where the mesh ratio $\lambda = \frac{\tau}{2h^2}$. Its matrix form is

$$V(t_{n+1}) = ((I - \lambda A)^{-1}(I + \lambda A))V(t_n).$$
(8)

Using (5) and (8), we obtain the approximation as follows:

$$\exp(\frac{\tau}{h^2}A) \approx (I - \lambda A)^{-1}(I + \lambda A). \tag{9}$$

From (9), we know that we should consider the approximation of $\exp(\frac{\tau}{\hbar^2}A)$ in order to obtain a new numerical method. Thus, we introduce a lemma on Trotter product formula.

Lemma 1. Let the matrix A can be denoted as $A = \sum_{i=1}^{M-1} A_i$. Then

$$\exp\left(\frac{t}{h^2}A\right) = \lim_{\delta \to \infty} \left(\prod_{i=1}^{M-1} \exp\left(\frac{tA_i}{\delta h^2}\right)\right)^{\delta}, \ \delta = 1, 2, \dots,$$
 (10)

for any h, t.

It follows from Lemma 1

$$\exp\left(\frac{\tau}{h^2}A\right) \approx \prod_{i=1}^{M-1} \exp\left(\frac{\tau A_i}{h^2}\right),\tag{11}$$

so (11) is a new approximation. And in order to use this approximation, we split matrix A in (5) as follows:

$$A_{1} = \begin{pmatrix} a_{1}^{n} & \gamma & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & & & \\ 0 & \cdots & \gamma & a_{i}^{n} & \gamma & \cdots & 0 \\ & & \ddots & & \vdots \\ 0 & & & & 0 \end{pmatrix}, i = 2, 3, \dots, M - 2, \qquad (12)$$

$$\begin{pmatrix} 0 & \cdots & 0 & 0 & 0 \\ & & & \ddots & \vdots \\ 0 & & & & 0 \end{pmatrix}$$

$$A_{M-1} = \begin{pmatrix} 0 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & \gamma & a_{M-1}^n \end{pmatrix}.$$

For any $i, i = 1, 2, \dots, M - 1$, from (9) we obtain

$$\exp\left(\frac{\tau}{h^2}A_i\right) \approx (I - \lambda A_i)^{-1}(I + \lambda A_i). \tag{13}$$

Then applying (11) and (13), we see that

$$\exp\left(\frac{\tau}{h^2}A\right) \approx \prod_{i=1}^{M-1} (I - \lambda A_i)^{-1} (I + \lambda A_i). \tag{14}$$

Consequently, combination of (5) and (14) yields a new scheme, i.e.,

$$V_1(t_{n+1}) = \prod_{i=1}^{M-1} ((I - \lambda A_i)^{-1} (I + \lambda A_i)) V_1(t_n).$$
 (15)

In order to improve the numerical accuracy of (15), we define $B_i = A_{M-i}$. By substituting B_i into (15), we deduce that

$$V_2(t_{n+1}) = \prod_{i=1}^{M-1} ((I - \lambda B_i)^{-1} (I + \lambda B_i)) V_2(t_n).$$
 (16)

Next, take the mean value of (15) and (16), i.e., $V(t_{n+1}) = \frac{1}{2}(V_1(t_{n+1}) + V_2(t_{n+1}))$. Denoting the coefficient matrix of $V(t_n)$ by $C(\lambda)$, we have

$$V(t_{n+1}) = C(\lambda)V(t_n). \tag{17}$$

So, (17) is the new scheme. We refer to the above method as MLCN method.

The matrix $(I + \lambda A_i)$ can be denoted by a simple form:

$$(I + \lambda A_i) = \begin{pmatrix} I_{i-2} & & \\ & S_i & \\ & & I_{M-i-2} \end{pmatrix}, i = 2, 3, \dots, M-2,$$
 (18)

where I_i is an $i \times i$ identity matrix and

$$S_i = \left(\begin{array}{ccc} 1 & 0 & 0\\ \lambda \gamma & 1 + \lambda a_i & \lambda \gamma\\ 0 & 0 & 1 \end{array}\right).$$

Similar to (18), we have

$$(I - \lambda A_i)^{-1} = \begin{pmatrix} I_{i-2} & & \\ & R_i^{-1} & \\ & I_{M-i-2} \end{pmatrix}, i = 2, 3, \dots, M - 2,$$
 (19)

where

$$R_i^{-1} = \left(\begin{array}{ccc} 1 & 0 & 0 \\ \frac{\lambda \gamma}{1 - \lambda a_i} & \frac{1}{1 - \lambda a_i} & \frac{\lambda \gamma}{1 - \lambda a_i} \\ 0 & 0 & 1 \end{array} \right).$$

Thus, we obtain an explicit expression of $V(t_{n+1})$. Clearly, (17) is an explicit scheme. Because we split A into some simple matrices as (12), we can obtain the inverse of the matrix in (17) exactly and easily. Therefore, it avoids solving the linear equations with large coefficient matrix, which is very important in numerical computation.

Theorem 1. Let the matrix A be written as $A = \sum_{i=1}^{M-1} A_i$ and suppose $\gamma > \frac{h^2(1-(v_i^n)^2)}{2}$. Then, for the split method expressed by (12), the difference scheme (17) is stable.

Proof. Let μ_i be any eigenvalue of matrix A_i , and η_i be any eigenvalue of matrix $(I - \lambda A_i)^{-1}(I + \lambda A_i)$. Noticing that $\gamma > \frac{h^2(1 - (v_i^n)^2)}{2}$, we have $\mu_i \leq 0$, and $|\eta_i| = \frac{|1 + \lambda \mu_i|}{|1 - \lambda \mu_i|} \leq 1$. Thus, $\prod_{i=1}^{M-1} |\eta_i| \leq 1$.

Therefore, the absolute value of any eigenvalue of the coefficient matrix $C(\lambda)$ of difference scheme (17) is not greater than 1. By the definition of stability, the new difference scheme is stable.

3. New scheme for two-dimensional Allen-Cahn equation

Consider two-dimensional Allen-Cahn equation

$$u_t = \gamma \Delta u - f(u), \quad (x, y) \in \Omega, \ t \in [0, T], \tag{20}$$

with the initial condition

$$u(x, y, 0) = u_0(x, y), \quad (x, y) \in \Omega,$$
 (21)

and boundary condition

$$u = 0, \quad (x, y) \in \partial\Omega, \ t \in (0, T],$$
 (22)

where $\Omega=(0,1)\times(0,1),\ \partial\Omega$ is the boundary of domain Ω and γ is positive number.

Like one-dimensional version, for Eq. (20), by using central difference quotient instead of differential term of space, we obtain the following semi-discrete equation:

$$\frac{dV(t)}{dt} = \frac{1}{h^2}AV(t),\tag{23}$$

Let x-direction and y-direction have the same mesh width in space, h = 1/M. Set $x_i = ih$ and $y_j = jh$ for i, j = 1, 2, ..., M-1. Moreover, V(t) in Eq. (23) is in the form $V(t) = (v(x_1, y_1, t), v(x_1, y_2, t), ..., v(x_1, y_{M-1}, t), v(x_2, y_1, t), v(x_2, y_2, t), ..., v(x_2, y_{M-1}, t), ..., v(x_{M-1}, y_1, t), v(x_{M-1}, y_2, t), ..., v(x_{M-1}, y_{M-1}, t))^T$. $v(x_i, y_j, t)$ is the approximate solution of $u(x_i, y_j, t), v_{ij} := v(x_i, y_j, t)$ and A is $(M-1)^2 \times (M-1)^2$ block tri-diagonal matrix

$$A = \begin{pmatrix} H_1 & \gamma I & & & 0 \\ \gamma I & H_2 & \gamma I & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma I & H_{M-2} & \gamma I \\ & 0 & & \gamma I & H_{M-1} \end{pmatrix}, \tag{24}$$

where H_i are $(M-1) \times (M-1)$ tri-diagonal matrices for $i = 1, 2, \dots, M-1$,

$$H_{i} = \begin{pmatrix} a_{i1} & \gamma & & & & 0 \\ \gamma & a_{i2} & \gamma & & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma & a_{i,M-2} & \gamma & \\ 0 & & & \gamma & a_{i,M-1} \end{pmatrix},$$

and $a_{ij} = -4\gamma - h^2(v_{ij}^2 - 1), j = 1, 2, \dots, M - 1.$

The solution of Eq. (23) with initial vector $V(0) = (v(x_1,y_1,0),v(x_1,y_2,0),\ldots,v(x_1,y_{M-1},0),v(x_2,y_1,0),v(x_2,y_2,0),\ldots,v(x_2,y_{M-1},0),\ldots,v(x_{M-1},y_1,0),v(x_{M-1},y_1,0),\ldots,v(x_{M-1},y_2,0),\ldots,v(x_{M-1},y_{M-1},0))^T$ can be expressed as

$$V(t) = \exp\left(\frac{t}{h^2}A\right)V(0). \tag{25}$$

Let $\tau=T/N$ be the mesh width in time and set $t_n=n\tau$ for $n=1,2,\ldots,N$. Moreover, $V(t_n)$ can be written in the form $V(t_n)=(v(x_1,y_1,t_n),v(x_1,y_2,t_n),\ldots,v(x_1,y_{M-1},t_n),v(x_2,y_1,t_n),v(x_2,y_2,t_n),\ldots,v(x_2,y_{M-1},t_n),\ldots,v(x_{M-1},y_1,t_n),v(x_{M-1},y_2,t_n),\ldots,v(x_{M-1},y_{M-1},t_n)]^T$, and $v_{ij}^n:=v(x_i,y_j,t_n)$. The nonlinear system (25) can be linearized by allowing the nonlinearities to lag one time step behind. Thus we have

$$V(t_{n+1}) = \exp(\frac{\tau}{h^2}A)V(t_n). \tag{26}$$

where

$$A = \begin{pmatrix} H_1 & \gamma I & & & 0 \\ \gamma I & H_2 & \gamma I & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma I & H_{M-2} & \gamma I \\ & 0 & & \gamma I & H_{M-1} \end{pmatrix}, \tag{27}$$

and

$$H_{i} = \begin{pmatrix} a_{i1}^{n} & \gamma & & & & & \\ \gamma & a_{i2}^{n} & \gamma & & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma & a_{i,M-2}^{n} & \gamma & \\ 0 & & & \gamma & a_{i,M-1}^{n} \end{pmatrix},$$

and $a_{ij}^n = -4\gamma - h^2((v_{ij}^n)^2 - 1), j = 1, 2, \dots, M - 1$

In order to obtain an approximate solution, we split the matrix A in (26) as follows:

$$A_{M-1,M-1} = \begin{pmatrix} 0 \cdots 0 & 0 & 0 \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 \cdots & 0 & 0 & 0 \cdots & 0 & 0 \\ 0 \cdots & 0 & \gamma & 0 \cdots & 0 & \gamma & a_{M-1,M-1}^n \end{pmatrix},$$

for i = 2, 3, ..., M - 2.

Similar to one-dimensional version, using the Trotter product formula and (28), we deduce an iterative formula as follows

$$V_1(t_{n+1}) = \prod_{i,j=1}^{M-1} ((I - \lambda A_{ij})^{-1} (I + \lambda A_{ij})) V_1(t_n).$$
 (29)

In order to improve the numerical accuracy of (29), we define $B_{ij} = A_{M-i,M-j}$. Then substituting it into (29), we deduce that

$$V_2(t_{n+1}) = \prod_{i,j=1}^{M-1} ((I - \lambda B_{ij})^{-1} (I + \lambda B_{ij})) V_2(t_n).$$
 (30)

Next, take the mean value of (29) and (30), i.e., $V(t_{n+1}) = \frac{1}{2}(V_1(t_{n+1}) + V_2(t_{n+1}))$. Denoting the coefficient matrix of $V(t_n)$ by $C(\lambda)$, we have

$$V(t_{n+1}) = C(\lambda)V(t_n). \tag{31}$$

So, (31) is the new scheme. We refer (31) as MLCN scheme. The matrix $(I + \lambda A_{ii})$ can be written in a simple form:

$$(I + \lambda A_{ii})$$

$$= \begin{pmatrix} 1 & & & & & & & & & & \\ \vdots & & & \ddots & & & & & & \\ 0 & \cdots & \lambda \gamma & \cdots & \lambda \gamma & 1 + a_{ii} & \lambda \gamma & \cdots & \lambda \gamma & \cdots & 0 \\ & & & \ddots & & & \vdots \\ & & & & & \ddots & & \vdots \end{pmatrix}, \quad (32)$$

$$i = 2, 3, \dots, M - 2.$$

 $(I - \lambda A_{ii})^{-1}$ can also be written in a simple form as follow:

$$\begin{pmatrix}
1 & & & & & & & & & & & \\
\vdots & & & \ddots & & & & & & \\
0 & \cdots & \frac{\lambda\gamma}{1-a_{ii}} & \cdots & \frac{\lambda\gamma}{1-a_{ii}} & \frac{1}{1-a_{ii}} & \frac{\lambda\gamma}{1-a_{ii}} & \cdots & \frac{\lambda\gamma}{1-a_{ii}} & \cdots & 0 \\
& & & & \ddots & & & \vdots \\
0 & & & & & \ddots & & \vdots
\end{pmatrix}, (33)$$

$$i = 2, 3, \dots, M - 2.$$

For the case i = 1 and M - 1, the matrices can also be rewritten. Here, for simplicity, we omit the details.

Thus, we obtain an explicit expression of $V(t_{n+1})$. Clearly, (31) is an explicit scheme. Because we split A into some simple matrices as (28), we can obtain the inverse of the matrix in (31) exactly and easily.

Theorem 2. Let the matrix A be written as $A = \sum_{i,j=1}^{M-1} A_{ij}$ and suppose $\gamma > \frac{h^2(1-(v_{ij}^n)^2)}{4}$. Then, for the split method expressed by (28), the difference scheme (31) is stable.

The proof of this theorem is similar to that of one-dimensional version, so we omit it.

4. Conclusions

The new numerical method (MLCN) for one-and two-dimensional Allen-Cahn equations has been presented. It is shown that the method is an explicit and stable difference scheme. Moreover, it avoids solving the linear equations with large coefficient matrix, which is very important in numerical computation. The advantages of the proposed method are that it is very easy to use it to solve Allen-Cahn equation and it can exhibit the dynamics property of the given equation well. Therefore, it is suggested to use the MLCN to get the numerical solution of the Allen-Cahn equation effectively.

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