International Journal of Heat and Mass Transfer 87 (2015) 111–118

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Investigations on several numerical methods for the non-local Allen–Cahn equation ☆

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ARTICLE INFO

Article history:
Received 31 October 2014
Received in revised form 15 February 2015
Accepted 20 March 2015

Keywords:
Non-local Allen–Cahn equation
Mass conservation
Finite difference method
Operator splitting method
Fourier spectral method

ABSTRACT

This paper investigates some numerical methods for solving the non-local Allen–Cahn equation with a space–time dependent Lagrange multiplier. Several types of methods, including the Crank–Nicolson finite difference method, the finite difference operator splitting method, and the Fourier spectral operator splitting method are proposed respectively. Comparisons are made among these methods in terms of accuracy and computational efficiency for solving different types of problems. Numerical results show that the Fourier spectral operator splitting method is very efficient because of its spectral accuracy in space, especially for simulation of long time dynamics.

1. Introduction

Allen–Cahn equation was introduced in [1] to model phase transitions in iron alloys. It has been widely applied to various problems, such as crystal growth [2], image analysis [3,4] and phase separation [5], etc. Compared to large amount of studies for the classical Allen–Cahn equation [6–9], there are few numerical results on non-local Allen–Cahn equation. In 1992, Rubinstein and Sternberg [10] first proposed non-local Allen–Cahn equation, which is related to the mean-curvature flow with the constraint of constant volume enclosed by the evolving curve.

In this paper, we focus on the initial-boundary value problem for the non-local Allen–Cahn equation,

$$\begin{cases} \frac{\partial u(\mathbf{x},t)}{\partial t} = \Delta u(\mathbf{x},t) - \frac{1}{\epsilon^2}[f(u) - \beta(u,t)], & (\mathbf{x},t) \in \Omega \times (0,T], \\ \nabla u(\mathbf{x}) \cdot n_\Omega = 0, & \mathbf{x} \in \partial\Omega, \\ u(\mathbf{x},0) = u_0(x,y), & \mathbf{x} \in \Omega. \end{cases} \tag{1}$$

Here Ω, T and n denote a bounded domain, finite time and the unit outer normal vector on the domain boundary, respectively. The small parameter ϵ is related to the thickness of the interface layer which can develop in parts of the solution with steep gradient. The function $f(u) = F'(u)$ and $F(u) = \frac{1}{4}(u^2-1)^2$ is a double-well potential with equal well-depth, taking its global minimum value at $u = \pm 1$. In other words, the two stable zeros of $F'(u)$ have 'balanced' stability. Consequently, the values -1 and 1 of the function u prevail in Ω whereas the transition between them forms a thin interface layer. This allows to understand u as an indicator of the two components in a binary mixture. Meanwhile, we assume the initial data $|u_0| \leqslant 1$, which follows from the maximum principe that $|u| \leqslant 1$ in [11].

The term $\beta(u,t)$ can be understood as a Lagrange multiplier for the mass constraint

$$\frac{d}{dt}\int_\Omega u(\mathbf{x},t)d\mathbf{x} = 0. \tag{2}$$

There are mainly two kinds of representations for $\beta(u,t)$:

$$\mathbf{I}: \quad \beta(u,t) = \frac{1}{|\Omega|}\int_\Omega f(u)d\mathbf{x}$$

and

$$\mathbf{II}: \quad \beta(u,t) = \frac{\sqrt{4F(u)}}{\int_\Omega \sqrt{4F(u)}d\mathbf{x}}\int_\Omega f(u)d\mathbf{x}.$$

Both formulations have been widely used in [9,13–16]. Notice that the mass conservation Eq. (2) is ensured by the Lagrange multiplier **I** or **II** in Eq. (1). However, since the Lagrange multiplier **I** is only a function of time variable, Brassel and Bretin [12] concluded

☆ This work is in part supported by the Scientific Research Foundation of Huaqiao University (No. 14BS313), the Distinguished Young Scholars Fund of Xinjiang Province (No. 2013711010), NCET-13-0988, and the NSF of China (Nos. 11271313, 61163027, 11362021).

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.03.071
0017-9310/

that Eq. (1) with the Lagrange multiplier **II** has better volume preservation property than the case **I**, which also has been observed in [13]. Recently, for the Allen–Cahn equation with the Lagrange multiplier **II**, Alfaro and Alifrangis [11] performed formal asymptotic expansions of the solution, then proved the convergence to a weak volume preserving motion by mean curvature via energy estimates. Kim et al. [16] proposed an unconditionally stable numerical scheme for the same problem. However, their scheme is only first-order accurate in time and second-order accurate in space.

The aim of this paper is to obtain a robust and efficient approach for non-local Allen–Cahn equation (1) with the Lagrange multiplier **II** using finite difference method and Fourier spectral method in [17,18] respectively. First, we introduce a second-order Crank–Nicolson (CN) nonlinear scheme. However, for the nonlinear case, we need use an iterative method to solve the resulting algebraic system. In order to overcome this drawback, we further propose an operator splitting method. The non-local Allen–Cahn equation was divided into three parts: linear equation, nonlinear equation and nonlocal equation. The linear equation was solved using a CN scheme, then the nonlinear part was solved analytically, last the nonlocal equation was solved explicitly. Note that the previous methods are only second-order accuracy both in time and space. In order to construct higher-order scheme, we further investigate the performance of the Fourier spectral spatial discretization for the linear equation in the second method. To the best of the authors' knowledge, we have not found similar result for the non-local Allen–Cahn equation in the literature. It is worth to point out that in this paper we restrict our attention on the two-dimensional (2D) case with Neumann boundary conditions, while the developed techniques can be easily extended to the other boundary conditions and the three-dimensional (3D) case.

The rest of the paper is organized as follows. In Section 2, three numerical methods are introduced for non-local Allen–Cahn equation with the Lagrange multiplier **II**. Comparisons are made among them in terms of accuracy and computational efficiency for solving different types of problems in Section 3. Numerical results show that the Fourier spectral operator splitting method is highly efficient because of its spectral accuracy in space. Especially one 3D test problem is presented to illustrate the availability of this method. Finally, conclusions are drawn in Section 4.

2. Three numerical methods for non-local Allen–Cahn equation

In this section we consider three types of numerical methods for the solution of Eq. (1) with the Lagrange multiplier **II**.

2.1. A CN finite difference scheme (*M1*)

We first introduce some notations which will be used throughout the paper.

Define the domain $\Omega = (a,b)^2$ is partitioned by

$$\Omega_h = \{(x_i,y_j) = (a+(i+0.5)h, b+(j+0.5)h),\ 0 \leqslant i,j \leqslant (N-1)\},$$

where $h = (b-a)/N$ is a uniform grid size. For $m = 0$ to M, let $u_{ij}^m = u(x_i,y_j,m\tau)$ with the time step $\tau = T/M$.

For the grid function $u = \{u_{ij} | 0 \leqslant i,j \leqslant N-1\}$ on Ω_h, denote

$$[D_x u]_{ij} = \frac{u_{i-1,j} - 2u_{ij} + u_{i+1,j}}{h^2}, \quad [D_y u]_{ij} = \frac{u_{ij-1} - 2u_{ij} + u_{ij+1}}{h^2}.$$

Now, we approximate the Lagrange multiplier **II** in Eq. (1) by the following formula:

$$\beta_{ij}^m = \frac{\sum_{i,j=0}^{N-1} f(u_{ij}^m)}{\sum_{i,j=0}^{N-1}\sqrt{4F(u_{ij}^m)}}\sqrt{4F(u_{ij}^m)} + \mathcal{O}(h^2). \tag{3}$$

Combining the CN method, we get the following finite difference scheme for Eq. (1):

$$\begin{aligned}\textbf{M1}: \frac{u_{ij}^{m+1} - u_{ij}^m}{\tau} &= \frac{1}{2}\left\{[D_x u^{m+1}] + [D_y u^{m+1}] + [D_x u^m] + [D_y u^m]\right\}_{ij} \\ &\quad - \frac{1}{2\varepsilon^2}\left(f(u_{ij}^{m+1}) + f(u_{ij}^m)\right) + \frac{1}{2\varepsilon^2}(\beta_{ij}^{m+1} + \beta_{ij}^m)\end{aligned}$$

with boundary conditions

$$\begin{cases}(d_x u)_{-\frac{1}{2}j}^m = 0, \quad (d_x u)_{N-\frac{1}{2}j}^m = 0, \\ (d_y u)_{i,-\frac{1}{2}}^m = 0, \quad (d_y u)_{i,N-\frac{1}{2}}^m = 0.\end{cases} \tag{4}$$

It is well known that the CN scheme is an unconditionally stable, implicit scheme with second-order accuracy in time [21,22]. So method **M1** in this paper is unconditionally stable. The nonlinear term in scheme **M1** is treated using the following fixed point iteration: Define

$$u_{ij}^{m+1,0} = \begin{cases} u_{ij}^m, & m = 0, \\ 2u_{ij}^m - u_{ij}^{m-1}, & m = 1, \\ 3u_{ij}^m - 3u_{ij}^{m-1} + u_{ij}^{m-2}, & m > 1 \end{cases}$$

and for $l = 1,2,\ldots,L$, find $u_{ij}^{m+1,l}$ such that

$$\begin{aligned}\frac{u_{ij}^{m+1,l} - u_{ij}^m}{\tau} &= \frac{1}{2}\left\{[D_x u^{m+1,l}] + [D_y u^{m+1,l}] + [D_x u^m] + [D_y u^m]\right\}_{ij} \\ &\quad - \frac{1}{2\varepsilon^2}\left(f(u_{ij}^{m+1,l-1}) + f(u_{ij}^m)\right) + \frac{1}{2\varepsilon^2}(\beta_{ij}^{m+1,l-1} + \beta_{ij}^m),\end{aligned}$$

where L is to be chosen. The computations are terminated when the discrete residual in L^2-norm or L^∞-norm is reduced by a factor of 10^{-10}.

Moreover, the following result shows that scheme **M1** conserves the mass balance, which overcomes the shortcomings of the linearized finite difference scheme.

Theorem 2.1. *Suppose U^{m+1} is the solution of* **M1**. *Then we have the following conservation of mass*

$$\sum_{i,j=0}^{N-1} U_{ij}^{m+1} = \sum_{i,j=0}^{N-1} U_{ij}^m, \quad 0 \leqslant m \leqslant M-1.$$

Proof. It follows from scheme **M1** that

$$\begin{aligned}\frac{\sum_{i,j=0}^{N-1}(u_{ij}^{m+1} - u_{ij}^m)}{\tau} &= \frac{1}{2}\sum_{i,j=0}^{N-1}\left[D_x u^{m+1} + D_y u^{m+1} + D_x u^m + D_y u^m\right]_{ij} \\ &\quad - \frac{1}{2\varepsilon^2}\sum_{i,j=0}^{N-1}\left(f(u_{ij}^{m+1}) + f(u_{ij}^m)\right) + \frac{1}{2\varepsilon^2}\sum_{i,j=0}^{N-1}(\beta_{ij}^{m+1} + \beta_{ij}^m).\end{aligned}$$

Applying the boundary conditions (4), the above equation becomes

$$\frac{\sum_{i,j=0}^{N-1}(u_{ij}^{m+1} - u_{ij}^m)}{\tau} = -\frac{1}{2\varepsilon^2}\sum_{i,j=0}^{N-1}\left(f(u_{ij}^{m+1}) + f(u_{ij}^m)\right) + \frac{1}{2\varepsilon^2}\sum_{i,j=0}^{N-1}(\beta_{ij}^{m+1} + \beta_{ij}^m).$$

Combining with the specific form of β_{ij}^m in (3), the desired result is obtained. □

Notice that scheme **M1** is nonlinear, so we need employ iteration method to solve this system for each time step. Especially, for the small ϵ case, the transition layer will move slowly enough such that a longer time is required to resolve the dynamics. In order to reduce the amount of work, an operator splitting method