Some Efficient Numerical Solutions of Allen-Cahn Equation with Non-Periodic Boundary Conditions

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Abstract: This paper presents some numerical methods for Allen-Cahn equation using different time stepping and space discretization methods with non-periodic boundary conditions. In space the equation is discretized by Chebyshev spectral method, while in time the exponential time differencing fourth-order Runge-Kutta (ETDRK4) and implicit-explicit scheme is used. For comparison we also use the finite difference scheme in both space and time.

Keywords: Allen-Cahn equation; non-periodic boundary conditions; different time stepping methods; Chebyshev spectral method.

1 Introduction

Consider the initial-boundary value problem of the form

\[
\begin{aligned}
  u_t & = \varepsilon u_{xx} + u - u^3, \quad x \in [-1, 1], \quad t \geq 0, \\
  u(x, 0) & = \sin(5\pi x/2), \\
  u_x(\pm 1, t) & = 0, \quad t > 0,
\end{aligned}
\]

where \(u\) indicates the phase state at each point in spaces and time and \(\varepsilon\) is a small parameter whose value is always positive constant known as the interaction length, which describe the thickness of the phase boundary.

Eq. (1) is a special type of nonlinear partial differential equation called Allen-Cahn equation (A-C), which arises as diffusion-convection equations in computational fluid dynamics or reaction-diffusion problem in material science. These equations are originally used to solve the phase transition problems, transformation of a thermodynamic system from one phase to another due to an abrupt change in one or more physical properties. These equations describe the evolution of a diffuse phase boundary, concentrated in a small region of size \(\varepsilon\). It also arising from phase transition in materials science.

Allen-Cahn equation, which has its origin in the modeling of phase transition or the equation which arises in the study of stationary waves for the nonlinear Schrödinger equation have been a subject of extensive research for many years. It provides a well-established framework for the mathematical description to free boundary problems for phase transitions. Unlike sharp interface models, it postulates a diffuse interface with a small thickness \(\varepsilon > 0\). The physical applications of the Allen-Cahn system are numerous, see for example [1], due to which a lot of interest has been shown in numerical as well as analytical solutions of Allen-Cahn equation.

Since the analytical solution of Allen-Cahn equation with non-periodic boundary conditions (BCs) is difficult to obtain, therefore a significant research interest in the numerical solutions of Allen-Cahn equation has been shown, see e.g. [2–4] and the references therein. When epsilon tends to zero the transition between phases in the Allen-Cahn equation becomes sharper. Solving this type of reaction-diffusion systems that exhibit sharp interfaces in their solutions with a Chebyshev pseudospectral method, it is worth to use an implicit method in time. Also when \(N\) (number of collocation points) gets bigger, the quadratic clustering of points close to the boundary in the Chebyshev grid severely constrains...
the admissible range of time steps if you solve the partial differential equations in time using an explicit method. To overcome this problem one can use operator splitting in combination with exponential integration. In Allen-Cahn equation the solution tends to exhibit flat areas close to the values separated by interfaces that might vanish on a long time scale, a phenomenon known as metastability [3]. A more comprehensive list of references about the Allen-Cahn equation and its applications in engineering can be found in [5].

In this paper an alternative approach by using different time stepping methods and space discretization method is proposed to provide an efficient numerical solution for Allen-Cahn equation (1), with non-periodic boundary conditions. In section 2 describes the finite difference scheme for the initial-boundary value problem (1), which is then followed by the spectral collocation method in section 3. Section 4 provide the numerical experiments. Section 5 is used to illustrate the concluding remarks.

2 Finite difference scheme

The finite difference discretization of the partial differential Eq. (1) is given by
\[
\frac{u_i^{n+1} - u_i^n}{\frac{\varepsilon}{\kappa}} = \frac{\varepsilon}{2\kappa^2} \left[ (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + (u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) \right] + u_i^n - (u_i^n)^3, \tag{2}
\]
where in space discretization we use the Crank-Nicolson scheme with \( \theta = 1/2 \). \( i \) and \( n \) are the indices which shows the discretization in space and time respectively. Eq. (2) can be written as
\[
\left( \frac{1}{\kappa} + \frac{\varepsilon}{h^2} \right)u_i^{n+1} - \frac{\varepsilon}{h^2} u_{i+1}^{n+1} + \frac{\varepsilon}{h^2} u_{i-1}^{n+1} = \frac{\varepsilon}{h^2} u_i^n + \frac{\varepsilon}{h^2} u_{i-1}^n + u_i^n - (u_i^n)^3. \tag{3}
\]
In matrix notation Eq. (3) is given by
\[
A_\Delta u^{n+1} = B_\Delta u^n, \tag{4}
\]
where
\[
A_\Delta = \begin{pmatrix}
\left( \frac{1}{\kappa} + \frac{\varepsilon}{h^2} \right) & -\frac{\varepsilon}{h^2} & 0 & \cdots & 0 \\
-\frac{\varepsilon}{h^2} & \left( \frac{1}{\kappa} + \frac{\varepsilon}{h^2} \right) & -\frac{\varepsilon}{h^2} & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & -\frac{\varepsilon}{h^2} & \left( \frac{1}{\kappa} + \frac{\varepsilon}{h^2} \right) & \cdots & \vdots \\
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
\vdots \\
u_m \\
\end{pmatrix}, \tag{5}
\]
and
\[
B_\Delta = \begin{pmatrix}
\frac{\varepsilon}{h^2} & \frac{\varepsilon}{h^2} & 0 & \cdots & 0 \\
\frac{\varepsilon}{h^2} & \frac{\varepsilon}{h^2} & \frac{\varepsilon}{h^2} & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & \frac{\varepsilon}{h^2} & \frac{\varepsilon}{h^2} & \left( \frac{1}{\kappa} - \frac{\varepsilon}{h^2} \right) \\
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
\vdots \\
u_m \\
\end{pmatrix}. \tag{6}
\]

3 Chebyshev spectral method

Spectral and pseudo-spectral methods are well known for their higher accuracy and applications to partial differential equations (PDEs) [6–9]. To approximate solution of the PDEs by spectral methods the unknown is replace by the set of smooth and global basis functions \( \Phi_i \ (i = 1, ..., N) \), (e.g) polynomials or trigonometric functions, to represent the unknown functions:
\[
u_i^n(x) \approx \sum_{i=1}^{N} a_i \Phi_i(x). \tag{7}
\]
To solve Eq. (1) by spectral method, we first consider the spatial part of the solution, which is approximated on a set of discrete grid points \( x_j \), \( j = 1, ..., N \) via so-called differentiation matrices which is one of many ways to implement spectral methods. To find a differential matrix \( D \), such that at the grid points \( x_j \), we have
\[
\frac{du}{dx} = Du. \tag{8}
\]
We use Chebyshev polynomail as a basis function, where the grid points are corresponding Chebyshev points, where the entries of the differentiation matrix are explicitly known. To obtain \( D \), we use Chebyshev spectral method of [6]. To
incorporate the Neumann boundary conditions in matrix $D$, we use the same idea as presented in [10]. To deal with the temporal part of Eq. (1), the linear part is integrated by Crank-Nicolson scheme and the non-linear by 2nd order Adams-Bashforth like [3], but we didn’t use the specialized fast algorithms described in [3] for spectral derivative operator to avoid the high stability restrictions. For comparison we also use for time discretization, the exponential time differencing fourth-order Runge-Kutta [2, 11].

4 Numerical experiments

In our numerical experiments we check all of our proposed numerical schemes for different values of thickness of the boundary $\varepsilon$ and the number of collocation points $N$. Due to small value of $\varepsilon = 0.01$, the diffusion process is low, therefore solution needs longer time to reach steady state as compared to large value $\varepsilon = 2.0$, in which the diffusion process is more dominant. Initially, the solution behaves like sinusoidal, however after certain time the periodic oscillation dampens and become flat, which is actually a steady state profile as shown in Fig. 1.

Due to the stability problem in time derivative, the finite difference scheme need small time step and is unstable for large time step see Fig. 2. Therefore using the finite different scheme is more costly in terms of CPU time.

In case of using the ETDRK4 for time stepping with Chebyshev spectral discretization in space, it is observed that this method encounter some problem shown in Fig. 3. This is may be because in this case our matrix $D$ is full and the problem occurs near eigenvalues equal to zero or close to zero in contrast to [2], where they use the same scheme, but with non-homogenous conditions. Fig. 4 and Fig. 5 shows that using the implicit-explicit scheme for nonlinear term with Chebyshev spectral discretization for time integration one can have a better results for large time step with more number of collocations points $N$.

![Figure 1: Initial condition and final ($t = 100$) state of Allen-Cahn equation using finite difference scheme in both space and time.](image1)

![Figure 2: Solution of Allen-Cahn equation using finite difference scheme with $\varepsilon = 0.01, 0.8$ respectively.](image2)
Figure 3: Solution of Allen-Cahn equation using Chebyshev spectral method in space and ETDRK4 in time with $\varepsilon = 0.01$ and $N = 5$.

Figure 4: Solution of Allen-Cahn equation with $\varepsilon = 2.0$, $N = 300$ and $N = 500$ respectively, using Chebyshev spectral method.
Figure 5: Solution of Allen-Cahn equation with $\varepsilon = 0.01$, $N = 300$ and $N = 500$ respectively, using Chebyshev spectral method.

5 Concluding remarks

In this article some efficient numerical methods for Allen-Cahn equation by using Chebyshev differentiation matrix in space with different time stepping method is applied. The use of implicit-explicit scheme allow us a large time-step as we know that an explicit method has less order of magnitude as compare to implicit-explicit method. In time-stepping the proposed ETDRK4 does not behaves well for this special kind of partial differential equation. This is may be due to the stiffness of a system caused by the linear term in general after discretization. After using the finite difference scheme in both space and time and making the comparison with all used method we found that by using the implicit-explicit scheme for nonlinear term with Chebyshev spectral discretization for time integration is the best.

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