THE FOURTH ORDER RUNGE-KUTTA EXPONENTIAL TIME DIFFERENCE METHOD FOR THE ALLEN-CAHN EQUATION

T. B. Tilavova
Jizzakh State Pedagogical University
https://doi.org/10.5281/zenodo.10279279

Abstract. *In this paper we present a numerical method for solving the Allen-Cahn equation with a corresponding boundary condition. The Allen-Cahn equation is discretized by the Chebyshev spectral method in space. We use the Fourth Order Runge-Kutta Exponential Time Difference method with Fourier's transformation for its diagonalization in time. The numerical results of solution of the Allen-Cahn equation are obtained by using Matlab code.*
Keywords: *Allen-Cahn equation, ETDRK4, Chebyshev spectral methods, exponential time difference, Runge-Kutta method.*

Introduction

The nonlinear partial differential equations are very important in a variety of scientific fields, especially in fluid mechanics, solid state physics, plasma physics, capillary-gravity waves and chemical physics. Most of the laws of physics, electrical and heat engineering and other sciences are described by ordinary differential equations or partial differential equations with the corresponding initial and boundary conditions. The Allen-Cahn equation is a nonlinear parabolic reaction-diffusion equation which describes various physical, biological and chemical objects. It is used as mathematical model of phase separation processes, the problem of mass and heat transfer, chemical kinetics. On the other hand, the Allen-Cahn equation or its natural modifications are used to modeling nonlinear evolutionary processes in a various field of mathematical and quantum physics. This equation was originally introduced by John W. Cahn and Sam M. Allen in 1979 [1] to describe the phase transition of a thermodynamic system from one phase to another. The equation has also been widely used in many complexes moving interface problems in materials science and fluid dynamics, such as the motion of mean curvature flows, image analysis, crystal growth, membrane fluidity, nucleation of solids, and mixture of two incompressible fluids [1–3].

The Allen-Cahn equation

It is well known that the exact solution of the Allen-Cahn equation is very complex problem due to its non-linearity [1]. Applications of numerical methods play an important role to get an exact or approximate solution of the equation [1-3]. One of such methods to resolve the problem is the exponential time difference (ETD) scheme. This method was first introduced in [4] and developed by Kassam and Trefethen [5]. The idea of the ETD scheme is the exactly integrate the linear part of equation and approximate the non-linear terms by a polynomial [6]. So, the linear part of obtained differential equation can be solved exactly [7]. The main advantage of spectral methods is that they can be applied directly to various types of nonlinear differential equations, significantly reducing the size of calculations, while maintaining high accuracy of the numerical solution. A good general introduction to the spectral methods and the exponential time differencing scheme ETDRK4 is given in detail by Cox and Matthews [4].

The object of study of this work is numerical modeling of the Allen-Cahn equation. We applied the exponential time differencing fourth-order Runge-Kutta (ETDRK4) method to diagonalize the Allen-Cahn equation, with a corresponding boundary and initial conditions. The numerical implementation of the scheme was carried out in Matlab computer algebra system.

The Allen-Cahn equation is a well-known equation in the field of reaction-diffusion systems [1]

$$u_t = \varepsilon u_{xx} + u - u^3, \qquad x \in [-1,1], \quad (t \geq 0), \tag{1}$$

Here ε is a constant. One of the interesting features of this equation is that its solution regions close to ±1 is flat, and the interface between such regions may remain the same for a very long time before suddenly changing. Usually, the equation (1) is considered together with boundary conditions that are natural for applications, and in most cases, periodic boundary conditions were chosen as boundary conditions. We present the initial and boundary conditions in the following form

$$u(x,0)=0.53x+0.47\sin\left(-1.5\pi x\right), \tag{2}$$

$$u(-1,\ t) = -1,\ \ u(1,\ t) = 1. \tag{3}$$

Research methodology. The idea of the ETD methods is similar to the method of the integrating factor (see for example [8] or [9]): we multiply both sides of a differential equation by some integrating factor, then we make a change of variable that allows us to solve the linear part exactly and, finally, we use a numerical method of our choice to solve the transformed nonlinear part. When a time-dependent partial differential equation in the form

$$\frac{du}{dt} = Lu + N(u,t), \tag{4}$$

where L and N are the linear and nonlinear operators respectively. For most of our discussion, initial boundary value problems with either periodic or homogeneous Dirichlet boundary conditions are considered for the equation (1). Discretizing the partial differential equation (1) in the spatial variables, for instance, by spectral approximations or by finite element approximations, a system of ordinary differential equations is often obtained

$$\frac{du}{dt} = \mathbf{L}u + \mathbf{N}(u,t). \tag{5}$$

The exponential time differencing (ETD) methods can be described in the context of solving the equation (5). Integrating the equation over a single time step from $t = t_n$ to $t_{n+1} = t_n + h$, we get

$$u(t_{n+1}) = e^{\mathbf{L}h}u(t_n) + e^{\mathbf{L}h}\int_0^h e^{-\mathbf{L}s}\mathbf{N}(u(t_n+s), t_n+s)ds. \tag{6}$$

Denote the numerical approximation to $u(t_n)$ by u_n, the first order scheme ETD1 is given by

$$u_{n+1} = e^{\mathbf{L}h}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h} - \mathbf{I})\mathbf{N}(u_n, t_n). \tag{7}$$

Higher order ETD schemes, for instance, the second, third and fourth order ETD Runge-Kutta schemes can also be found in [5, 10]. For completeness, we give below the formulae for a fourth–order scheme (ETD4RK)

$$a_n = e^{\mathbf{L}h/2}u_n + L^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})N\left(u_n, t_n\right),$$

$$b_n = e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}\left(a_n, t_n + \frac{h}{2}\right),$$

$$c_n = e^{\mathbf{L}h/2}a_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\left[2\mathbf{N}\left(b_n, t_n + \frac{h}{2}\right) - \mathbf{N}(u_n, t_n)\right],$$

$$u_{n+1} = e^{\mathbf{L}h/2}u_n + h^{-2}\mathbf{L}^{-3}\left[-4\mathbf{I} - h\mathbf{L} + e^{\mathbf{L}h/2}(4\mathbf{I} - 3h\mathbf{L} + (h\mathbf{L})^2\right]\mathbf{N}(u_n, t_n)$$

$$+2\left[2\mathbf{I} + h\mathbf{L} + e^{\mathbf{L}h}(-2\mathbf{I} + h\mathbf{L})\right]\left(\mathbf{N}\left(a_n, t_n + \frac{h}{2}\right) + \mathbf{N}\left(b_n, t_n + \frac{h}{2}\right)\right).$$

$$\left[-4\mathbf{I} - 3h\mathbf{L} - (h\mathbf{L})^2 + e^{\mathbf{L}h/2}(4\mathbf{I} - h\mathbf{L})\right]\mathbf{N}(c_n, t_n + h)$$

More detailed derivations of the ETD schemes with Runge-Kutta time stepping can be found in [4]. We will write the discretization of Allen-Cahn equation in standard form [6]

$$L = \varepsilon D^2, \tag{8}$$

$$N(u, t) = u - u^3. \tag{9}$$

where D is the Chebyshev differentiation matrix, L is a complete matrix [6]. The part of the solution (8) is approximated on a set of discrete grid points, (where j = 1, ...,N) via differentiation matrices (see Refs. [5-7]). In order to deal with the boundary conditions, one defines u = w + x and works with the variable w which has homogeneous boundary values. The default parameter values are N = 120 and $\varepsilon = 0.01$.

The results and discussions. Sample Matlab code to solve this problem using an explicit ETDRK4 scheme for the time-derivative and a Chebyshev pseudospectral differentiation matrix for the spatial derivative is listed on page 141 of [5]. We solve the problem in Fourier space and use ETDRK4 scheme for the time step up to t = 200. Numerical experiments of the Allen-Cahn equation are performed over the interval [-1, 1] using h = ¼ time step and M = 32 number of points. The time evolution for the Allen-Cahn equation is shown in Figs.1 and 2.

Fig.1. Time evolution for the Allen-Kahn equation N=120 and ε = 0.01. The x-axis runs from x=-1 to x=1 and the t-axis runs from t=0 to t=150 s.

In the next step we use ETDRK4 for the time step and solve up to t = 200 s with ε = 0.01. Time evolution for the Allen-Cahn equation is presented in Fig.2.

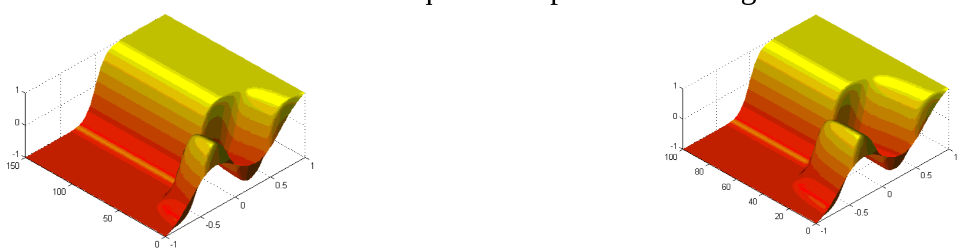

Fig.2. Time evolution for the Allen-Kahn equation N=120 and ε = 0.01. The x-axis runs from x=-1 to x=1 and the t-axis runs from t=150 to t=200 s.

According to the results presented in these figures, the present method offers high accuracy for the numerical solutions of the nonlinear Allen-Cahn equation. On the other hand, the results obtained by the exponential time differencing fourth-order Runge-Kutta (ETDRK4) method have better than results obtained from the other numerical schemes.

Conclusion

We applied the exponential time differencing fourth-order Runge-Kutta (ETDRK4) method to diagonalize the Allen-Cahn equation, with a corresponding boundary and initial conditions. The Allen-Cahn equation is discretized by the Chebyshev spectral method in space. The numerical results have been implemented by Matlab software. The present method is a very reliable, simple, small computation costs, flexible, and convenient alternative method. The proposed scheme can be used in a wide class of nonlinear parabolic reaction-diffusion equations, which describe various physical, biological and the problem of mass and heat transfer, chemical kinetics.

REFERENCES

1. S.M. Allen, J.W. Cahn. A microscopic theory for antiphase boundary motion and its application to antipahse domain coarsening. Acta Metall. 1979, 27, 1085–1095.
2. J.W. Choi, H.G. Lee, D. Jenog, J. Kim. An unconditionally gradient stable numerical method for solving the Allen–Cahn equation. Physica A 2009, 388, 1791–1803.
3. J. Zhang, Q. Du. Numerical studies of discrete approximations to the Allen–Cahn equation in the sharp interface limit. SIAM J. Sci. Comput. 2009, 31, 3042–3063.
4. S.M. Cox, P.C. Matthews. Exponential Time Differencing for Stiff Systems, J. Comput. Phys. 2002, 176, 430–455.
5. A. Kassam, L.N. Trefethen. Fourth-Order Time Stepping for Stiff PDEs, SIAM J. Sci. Comput. 2005, 26, 1214–1233.
6. J. D. Lawson, Generalized Runge-Kutta Processes for Stable Systems with Large Lipschitz Constants, SIAM J. Numer Anal, 1967, 4, 372-380.
7. A. K. Kassam, High Order Time stepping for Stiff Semi-Linear Partial Differential Equations, PhD thesis, Oxford University, 2004.
8. J.P. Boyd, Chebyshev and Fourier Spectral Methods. Second Edition (Revised), Dover, 2001.
9. L.N. Trefethen, Spectral Methods in MATLAB, SIAM, 2000.
10. B. Fornberg, A Practical Guide to Pseudospectral Methods, Cambridge University Press, 1998.