Commun Nonlinear Sci Numer Simulat 61 (2018) 149–159

Contents lists available at ScienceDirect

Commun Nonlinear Sci Numer Simulat

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

Research paper

A benchmark problem for the two- and three-dimensional Cahn–Hilliard equations

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ARTICLE INFO

Article history:
Received 20 May 2017
Revised 21 December 2017
Accepted 6 February 2018
Available online 8 February 2018

Keywords:
Cahn–Hilliard equation
Finite difference method
Multigrid method
Benchmark problem

ABSTRACT

This paper proposes a benchmark problem for the two- and three-dimensional Cahn–Hilliard (CH) equations, which describe the process of phase separation. The CH equation is highly nonlinear and an analytical solution does not exist except trivial solutions. Therefore, we have to approximate the CH equation numerically. To test the accuracy of a numerical scheme, we have to resort to convergence tests, which consist of consecutive relative errors or a very fine solution from the numerical scheme. For a fair convergence test, we provide benchmark problems which are of the shrinking annulus and spherical shell type. We show numerical results by using the explicit Euler's scheme with a very fine time step size and also present a comparison test with Eyre's convex splitting schemes.

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1. Introduction

This paper proposes a benchmark problem for the two- and three-dimensional Cahn–Hilliard (CH) equations, which were originally introduced as a mathematical model of phase separation in a binary alloy [1,2]:

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = \Delta\mu(\phi(\mathbf{x},t)), \quad \mathbf{x}\in\Omega, \ 0<t\le T, \tag{1}$$

$$\mu(\phi(\mathbf{x},t)) = F'(\phi(\mathbf{x},t)) - \epsilon^2\Delta\phi(\mathbf{x},t), \tag{2}$$

where $\Omega\subset\mathbb{R}^d$ $(d=1,2,$ or $3)$ is a bounded domain, $F(\phi)=0.25(\phi^2-1)^2$, and ϵ is the gradient energy coefficient. The quantity $\phi(\mathbf{x}, t)$ is defined as the difference of molar fractions of two species.

The CH equation has been applied to model many scientific processes such as phase separation and coarsening phenomena [1,3], image inpainting (the process of reconstructing lost or deteriorated parts of images) [4], image segmentation [5], multiphase fluid flows [6–9], diblock copolymer (a polymer consisting of two types of monomers) [10–12], microstructures with elastic inhomogeneity [13,14], topology optimization for optimizing material shape within a given design space and a set of loads and boundary conditions [15,16], and tumor growth simulation [17–19]. Many efficient and accurate numerical methods have been proposed to solve the CH equation. For example, the methods are meshless method [20,21], dual reciprocity method [22], Galerkin method [23–25], Fourier spectral method [26–29], unconditionally stable scheme [30–32], multigrid [16], Crank–Nicholson method [33–35], and Runge–Kutta method [36].

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https://doi.org/10.1016/j.cnsns.2018.02.006
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However, the CH equation is highly nonlinear due to the term $F(\phi)$ and an analytical solution does not exist except trivial constant solutions. To test the accuracy of a numerical scheme for the CH equation, we have to resort to convergence tests, which consist of consecutive relative errors or a very fine solution from the numerical scheme. The growing phase field community has developed many numerical methods; however, the lack of benchmark problems to consistently evaluate the numerical performance of the developed code [37] has been an issue. Recently, a couple of research papers have been published that are related to benchmark problems. In [38], the author has derived analytical expressions for the solution of a surface Hele–Shaw model on the sphere, to serve numerical purposes, as a benchmark for the surface CH equation. In [37], the authors presented two benchmark problems for the numerical implementation of phase field equations that model solute diffusion along with second phase growth and coarsening.

The main purpose of this paper is to present benchmark problems for testing numerical schemes for the CH equations. The two benchmark problems are of the shrinking annulus and spherical shell type. These benchmark problems will help researchers in testing the accuracy of the developed computer codes for the CH equations. We give numerical results by using the explicit Euler's scheme with a very fine time step size and we also present a comparison test with Eyre's convex splitting schemes. This paper is organized as follows. In Section 2, we describe the numerical solution algorithm. The numerical results are presented in Section 3. Some concluding remarks are presented in Section 4.

2. Numerical solution

To obtain simple benchmark solutions, we consider the CH equation in radially (2D) as well as spherically (3D) symmetric forms:

$$\phi_t(r,t) = \frac{1}{r^{d-1}}[r^{d-1}\mu_r(r,t)]_r, \quad r \in \Omega, \ t > 0, \tag{3}$$

$$\mu(r,t) = F'(\phi(r,t)) - \frac{\epsilon^2}{r^{d-1}}[r^{d-1}\phi_r(r,t)]_r, \tag{4}$$

where d is the space dimension. Here, we use the homogeneous Neumann boundary conditions for both ϕ and μ. Note that Eqs. (3) and (4) represent the radially and spherically symmetric CH equations when $d=2$ and $d=3$, respectively. The derivation of Eqs. (3) and (4) is described below for more detail.

- The two-dimensional Cartesian coordinate can be represented by the polar coordinate as $(x,y) = (r\cos\theta, r\sin\theta)$. In the two-dimensional polar coordinate, Eqs. (1) and (2) become

$$\frac{\partial\phi(r,\theta,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\mu}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\mu}{\partial\theta^2},$$
$$\mu(r,\theta,t) = F'(\phi) - \frac{\epsilon^2}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) - \frac{\epsilon^2}{r^2}\frac{\partial^2\phi}{\partial\theta^2},$$

  where $r \ge 0, 0 \le \theta < 2\pi$, and $0 < t \le T$. If the solutions ϕ and μ are radially symmetric, that is, $\phi = \phi(r,t)$ and $\mu = \mu(r,t)$ are independent of θ, then $\frac{\partial^2\phi}{\partial\theta^2} = \frac{\partial^2\mu}{\partial\theta^2} = 0$. Therefore, we can obtain Eqs. (3) and (4) when $d=2$.
- In spherical polar coordinate, $(x,y,z) = (r\sin\theta\cos\psi, r\sin\theta\sin\psi, r\cos\theta)$, Eqs. (1) and (2) become

$$\frac{\partial\phi(r,\theta,\psi,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\mu}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\mu}{\partial\theta}\right) + \frac{\partial^2\mu}{\partial\psi^2}\right],$$
$$\mu(r,\theta,\psi,t) = F'(\phi) - \frac{\epsilon^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right)$$
$$-\frac{\epsilon^2}{r^2\sin^2\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\phi}{\partial\theta}\right) + \frac{\partial^2\phi}{\partial\psi^2}\right],$$

  where $r \ge 0, 0 \le \theta \le \pi$, $0 \le \psi < 2\pi$, and $0 < t \le T$. Likewise, if $\phi = \phi(r,t)$ and $\mu = \mu(r,t)$ are independent of θ and ψ, that is, spherically symmetric, then we have Eqs. (3) and (4) when $d=3$.

Now, we solve the CH Eqs. (3) and (4) in $\Omega = (0,1)$. Let N_r be a positive integer and $h = 1/N_r$ be the uniform grid size. Let ϕ_i^n and μ_i^n be approximations of $\phi(r_i, t^n)$ and $\mu(r_i, t^n)$, respectively. Here, $r_i = (i-0.5)h$ and $t^n = n\Delta t$. Then, we discretize Eqs. (3) and (4) in time, using the explicit Euler's method:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Delta_r\mu_i^n, \ \text{for } i = 1, \dots, N_r, \tag{5}$$

$$\mu_i^n = (\phi_i^n)^3 - \phi_i^n - \epsilon^2\Delta_r\phi_i^n. \tag{6}$$

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