Effective Time Step Analysis of a Nonlinear Convex Splitting Scheme for the Cahn–Hilliard Equation

Seunggyu Lee$^1$ and Junseok Kim$^2, *$

$^1$National Institute for Mathematical Sciences, Dajeon 34047, Republic of Korea.
$^2$Department of Mathematics, Korea University, Seoul 02841, Republic of Korea.

Received 21 December 2017; Accepted (in revised version) 3 January 2018

Abstract. We analyze the effective time step size of a nonlinear convex splitting scheme for the Cahn–Hilliard (CH) equation. The convex splitting scheme is unconditionally stable, which implies we can use arbitrary large time-steps and get stable numerical solutions. However, if we use a too large time-step, then we have not only discretization error but also time-step rescaling problem. In this paper, we show the time-step rescaling problem from the convex splitting scheme by comparing with a fully implicit scheme for the CH equation. We perform various test problems. The computation results confirm the time-step rescaling problem and suggest that we need to use small enough time-step sizes for the accurate computational results.

AMS subject classifications: 37M05, 65M22, 65T50

Key words: Cahn–Hilliard equation, convex splitting, effective time step, Fourier analysis.

1 Introduction

We consider the effective time step size of a nonlinear convex splitting scheme for the following Cahn–Hilliard (CH) equation [1]:

$$\phi_t(x,t) = \Delta [F'(\phi(x,t)) - \epsilon^2 \Delta \phi(x,t)], \quad x \in \Omega, \quad t > 0, \quad (1.1)$$

$$n \cdot \nabla \phi(x,t) = n \cdot \nabla \mu(x,t) = 0, \quad x \in \partial \Omega, \quad (1.2)$$

$$\phi(x,0) = \phi_0(x), \quad x \in \Omega, \quad t > 0, \quad (1.3)$$

where $F(\phi) = 0.25(\phi^2 - 1)^2$, $\epsilon$ is the gradient energy coefficient, $\Omega = \prod_{i=1}^d (0, L_i)$, $d = 1,2,3$, and $n$ is the outer normal vector. The CH equation is a phenomenological model of the process of a phase separation in a binary mixture [1]. Its physical applications have been extended to many scientific fields such as image inpainting, spinodal tumor growth

*Corresponding author. Email addresses: sglee@nims.re.kr (S. Lee), cfdkim@korea.ac.kr (J. Kim)
simulation, decomposition, topology optimization, diblock copolymer, microstructures with elastic inhomogeneity, and multiphase fluid flows, see a recent review paper [15] for the relevant references. The CH equation can be derived by a gradient flow with the following total energy functional:

$$E(\phi) = \int_\Omega \left( F(\phi) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x}. \quad (1.4)$$

That is,

$$\phi_t = -\text{grad}E(\phi) = -\Delta \left( \frac{\delta E(\phi)}{\delta \phi} \right), \quad (1.5)$$

where $\delta E(\phi)/\delta \phi = F'(\phi) - \varepsilon^2 \Delta \phi$ is the variational derivative. For a review of the physical, mathematical, and numerical derivations of the CH equation, see a review paper [16]. Also, for the basic principles and practical applications of the CH Equation, see [15].

Because there has been no closed-form solution for the CH equation with arbitrary initial conditions, we need to resort to numerical approximations to solve the equation. The explicit Euler scheme has severe time-step restriction. Both the fully implicit and Crank–Nicolson schemes have also solvability time-step restriction. To overcome these time-step restrictions, Eyre proposed the following convex splitting method for the Cahn–Hilliard equation [9]:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\text{grad}E_c(\phi^{n+1}) - \text{grad}E_e(\phi^n), \quad (1.6)$$

where $\text{grad}E(\phi) = \text{grad}E_c(\phi) - \text{grad}E_e(\phi)$. For the nonlinear stabilized splitting scheme, we define $\text{grad}E_c(\phi) = -\Delta[(\phi^{n+1})^3 - \varepsilon^2 \Delta \phi^{n+1}]$ and $\text{grad}E_e(\phi^n) = -\Delta \phi^n$. Let us rewrite Eq. (1.6) in terms of the fully implicit Euler scheme:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\text{grad}E_c(\phi^{n+1}) + \text{grad}E_e(\phi^{n+1}) - \text{grad}E_e(\phi^{n+1}) + \text{grad}E_e(\phi^n)$$

$$= -\text{grad}E_c(\phi^{n+1}) - \text{grad}E_c(\phi^{n+1}) + \text{grad}E_c(\phi^n)$$

$$= -\text{grad}E_c(\phi^{n+1}) + \Delta(\phi^{n+1} - \phi^n). \quad (1.7)$$

Then, the scheme (1.6) can be written as follows:

$$(1 - \Delta t \Delta) \left( \frac{\phi^{n+1} - \phi^n}{\Delta t} \right) = -\text{grad}E(\phi^{n+1}). \quad (1.8)$$

The main purpose of this article is to investigate a mode-dependent effective time-step of a nonlinear convex splitting scheme for the CH equation using the fully implicit Euler algorithm. The convex splitting method is the most popular numerical schemes in the phase-field method to overcome the time-step restriction [6, 20]. Furthermore, in recent years, the convex splitting numerical schemes have been extensively studied for the Cahn–Hilliard model coupled with a certain fluid such as the Cahn–Hilliard–Hele–Shaw [23], Cahn–Hilliard–Brinkman [7], Cahn–Hilliard–Navier–Stokes [8, 11] equations.