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

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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]:

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

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

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

where $F(\phi)=0.25(\phi^2-1)^2$, ϵ is the gradient energy coefficient, $\Omega=\prod_{i=1}^d(0,L_i)$, $d=1,2,3$, and $\mathbf{n}$ 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

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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:

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

That is,

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

where $\delta\mathcal{E}(\phi)/\delta\phi=F'(\phi)-\epsilon^2\Delta\phi$ 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]:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t}=-\left[\text{grad}\mathcal{E}_c(\phi^{n+1})-\text{grad}\mathcal{E}_e(\phi^n)\right], \tag{1.6}$$

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

$$\begin{aligned}\frac{\phi^{n+1}-\phi^n}{\Delta t}&=-\text{grad}\mathcal{E}_c(\phi^{n+1})+\text{grad}\mathcal{E}_e(\phi^{n+1})-\text{grad}\mathcal{E}_e(\phi^{n+1})+\text{grad}\mathcal{E}_e(\phi^n)\\&=-\text{grad}\mathcal{E}(\phi^{n+1})-\text{grad}\mathcal{E}_e(\phi^{n+1})+\text{grad}\mathcal{E}_e(\phi^n)\\&=-\text{grad}\mathcal{E}(\phi^{n+1})+\Delta(\phi^{n+1}-\phi^n).\end{aligned} \tag{1.7}$$

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

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

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.