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# Linear, second order and unconditionally energy stable schemes for the viscous Cahn–Hilliard equation with hyperbolic relaxation using the invariant energy quadratization method

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ABSTRACT

In this paper, we consider numerical approximations for the viscous Cahn–Hilliard equation with hyperbolic relaxation. This type of equations processes energy-dissipative structure. The main challenge in solving such a diffusive system numerically is how to develop high order temporal discretization for the hyperbolic and nonlinear terms, allowing large time-marching step, while preserving the energy stability, i.e. the energy dissipative structure at the time-discrete level. We resolve this issue by developing two second-order time-marching schemes using the recently developed "Invariant Energy Quadratization" approach where all nonlinear terms are discretized semi-explicitly. In each time step, one only needs to solve a symmetric positive definite (SPD) linear system. All the proposed schemes are rigorously proven to be unconditionally energy stable, and the second-order convergence in time has been verified by time step refinement tests numerically. Various 2D and 3D numerical simulations are presented to demonstrate the stability, accuracy, and efficiency of the proposed schemes.



## 1. Introduction

The classical Cahn–Hilliard (CH) equation dates back to 1958 in Cahn and Hillard's seminal paper [1]. In the past decades, it has been well studied and broadly used to investigate the coarsening dynamics of two immersible fluids. Recently, researchers have devoted tremendous attention on the relaxed CH system, i.e. the viscous Cahn–Hilliard (VCH) system and its perturbed form with the hyperbolic relaxation (HR) effect (referred to as the perturbed viscous Cahn–Hilliard equation). Both VCH and VCH-HR have been well-studied theoretically where the topics are mainly focused on the well-posedness, sharp interface limit or global attractor, etc., see [2–12] and the references therein. Formally, the governing equation of the VCH-HR system is slightly different from the CH equation by incorporating two extra terms, including a strong damping (or called "viscosity") term and a hyperbolic relaxation term (or called "inertia"). The viscous effect is first proposed by Novick-Cohen [2] in order to introduce an additional regularity and some parabolic smoothing effects, can be viewed as a singular limit of the phase field equations for phase transitions [13]. The hyperbolic relaxation term was proposed by Galenko et al.

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in [10], in order to describe strongly non-equilibrium decomposition generated by rapid solidification under supercooling into the spinodal region occurring in certain materials (e.g., glasses). Since the VCH-HR system combines the hyperbolic relaxation and the viscosity together, it is mathematically more tractable comparing to the CH or VCH systems [9,12,14].

Before developing efficient numerical schemes to solve the VCH-HR system, we remark that its reduced version, the classical CH equation, is now widely applied to model the interfacial dynamics in various scientific fields (cf. [1,15–18] and the references therein). The CH equation and its analogous counterpart model, the Allen–Cahn equation, are both categorized as representative equations of phase field type models. From the numerical point of view, when solving phase field models, it is desirable to establish efficient numerical schemes that can verify the so-called "energy stable" property at the discrete level irrespectively of the coarseness of the discretization. In what follows, those algorithms will be called *unconditionally energy stable* or *thermodynamically consistent*. Schemes with this property are especially preferred since it is not only critical for the numerical scheme to capture the correct long-time dynamics of the system, but also provides sufficient flexibility for dealing with the stiffness issue. In spite of this, we have to point out a basic fact that larger time step will definitely induce larger computational errors. In other words, the schemes with unconditional energy stability can allow arbitrary large time step only for the sake of the stability concern. In practice, the controllable accuracy is one of the most important factors to measure whether a scheme is reliable or not. Therefore, if one attempts to use the time step as large as possible while maintaining the desirable accuracy, the only possible choice is to develop more accurate schemes, e.g., the unconditionally energy stable second order schemes, which is the main focus of this paper.

It is remarkable that, despite a great deal of work done for the numerical solution of the classical CH system, almost all research related to the VCH or VCH-HR system had been focused on the theoretical PDE analysis with very few numerical analysis or algorithm design. To the best of the authors' knowledge, no schemes can be claimed to possess the following three properties, namely, easy-to-implement, unconditionally energy stability and second-order accuracy for the VCH-HR model since there exist a large number of the numerical difficulties, including the proper discretization for the viscous term and the hyperbolic inertia, as well as the regular stiffness issue induced by the nonlinear double well potential. At the very least, even for the reduced version, i.e. the CH system, the algorithm design is still challenging. It can be seen clearly from the following fact that some severe stability restrictions on the time step will occur if the nonlinear term is discretized in some normal ways like fully explicit type approach. Such a time step constraint can cause very high computational cost in practice [19,20]. Many efforts (primarily for CH system) had been done in order to remove this constraint and two commonly used techniques were developed, namely, the nonlinear convex splitting approach [4,21–23], and the linear stabilized approach [20,24–39]. The convex splitting approach is unconditionally energy stable, but it produces nonlinear schemes, thus the implementation is complicated and the computational cost might be high. The linear stabilized approach is linear so it is efficient and very easy to implement. But, its stability requests a special property (generalized maximum principle) satisfied by the classical PDE solution or the numerical solution, which is not trivial to prove. Moreover, it is difficult to extend to second-order while preserving unconditional energy stability (cf. [20]).

Therefore, in order to develop some more efficient and accurate time marching schemes for solving the VCH-HR equation, we use the *Invariant Energy Quadratization* (IEQ) approach, which has been successfully applied to solve a variety of phase field type models, see [40–52]). Its idea is very simple but quite different from those traditional methods like implicit, explicit, nonlinear splitting, or other various tricky Taylor expansions to discretize the nonlinear potentials. The essential strategy of IEQ is to make the free energy *quadratic*. To be more specific, the free energy potential is transformed into the quadratic form forcefully via the change of variables. Then, upon a simple reformulation, all nonlinear terms are treated by the semi-explicit way, which in turn yields a linear system. We develop two second-order schemes, in which, one is based on the the Crank–Nicolson scheme, and the other is based on the Adam-Bashforth scheme (BDF2). The schemes are *second order accurate*, *easy-to-implement* (linear system), and *unconditionally energy stable* (with a discrete energy dissipation law). Moreover, we show that the linear operators of all schemes are *symmetric positive definite*, so that one can solve it using the well-developed fast matrix solvers efficiently (CG or other Krylov subspace methods). Through various 2D and 3D numerical simulations, we demonstrate stability and accuracy of the proposed schemes.

The rest of the paper is organized as follows. In Section 2, we present the whole system and show the energy law in the continuous level. In Section 3, we develop the numerical schemes and prove their unconditional energy stabilities. In Section 4, we present various 2D and 3D numerical experiments to validate the accuracy and efficiency of the proposed numerical schemes. Finally, some concluding remarks are presented in Section 5.

## 2. Model equations

First of all, we give a brief description for the model equations. We consider a binary alloy in a bounded domain $\Omega \in \mathbb{R}^d$, $d = 2, 3$ with $\partial\Omega$ Lipschitz continuous. For any $g_1, g_2 \in L^2(\Omega)$, we denote the inner product and $L^2$ norm as

$$(g_1, g_2) = \int_\Omega g_1 g_2 d\boldsymbol{x}, \quad \|g_1\| = \int_\Omega |g_1|^2 d\boldsymbol{x}. \tag{2.1}$$

We define $\phi(\boldsymbol{x}, t)$ as volume fraction of one material component, and $\boldsymbol{J}$ the diffusion flux, then the balance law for volume fraction gives

$$\phi_t + \nabla \cdot \boldsymbol{J} = 0. \tag{2.2}$$