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A High Order Adaptive Time-Stepping Strategy and Local Discontinuous Galerkin Method for the Modified Phase Field Crystal Equation

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Abstract. In this paper, we will develop a first order and a second order convex splitting, and a first order linear energy stable fully discrete local discontinuous Galerkin (LDG) methods for the modified phase field crystal (MPFC) equation. In which, the first order linear scheme is based on the invariant energy quadratization approach. The MPFC equation is a damped wave equation, and to preserve an energy stability, it is necessary to introduce a pseudo energy, which all increase the difficulty of constructing numerical methods comparing with the phase field crystal (PFC) equation. Due to the severe time step restriction of explicit time marching methods, we introduce the first order and second order semi-implicit schemes, which are proved to be unconditionally energy stable. In order to improve the temporal accuracy, the semi-implicit spectral deferred correction (SDC) method combining with the first order convex splitting scheme is employed. Numerical simulations of the MPFC equation always need long time to reach steady state, and then adaptive time-stepping method is necessary and of paramount importance. The schemes at the implicit time level are linear or nonlinear and we solve them by multigrid solver. Numerical experiments of the accuracy and long time simulations are presented demonstrating the capability and efficiency of the proposed methods, and the effectiveness of the adaptive time-stepping strategy.

AMS subject classifications: 65M60, 35L75, 35G25

Key words: Adaptive time-stepping, local discontinuous Galerkin method, modified phase field crystal equation, convex splitting, pseudo energy, unconditionally energy stable, spectral deferred correction.

1 Introduction

In this paper, we consider local discontinuous Galerkin (LDG) spatial discretization and high order semi-implicit time marching methods in a bounded domain $\Omega \in \mathbb{R}^d (d \leq 2)$ for

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the modified phase field crystal (MPFC) equation:

$$\partial_{tt}\phi+\beta\partial_t\phi=\nabla\cdot(M(\phi)\nabla(\phi^3+(1-\epsilon)\phi+2\Delta\phi+\Delta^2\phi)), \tag{1.1}$$

where $M(\phi)\geq 0$ is a mobility, $\beta>0$ and $\epsilon\leq 1$.

In equation (1.1), when β=0, it is known as the phase field crystal (PFC) equation. The PFC model was recently proposed by Elder *et al.* [10,11] to study the nonequilibrium microstructure formation by introducing a free energy functional of the local-time-averaged density field. There have been many algorithms developed and simulations performed for the PFC equation recently, using finite difference methods [17,23,27], finite element methods [13] and local discontinuous Galerkin method [15]. The MPFC equation is an important extension of the PFC equation, and it was introduced in [20,21]. The MPFC equation (1.1) is a nonlinear damped wave equation, which models a viscoelastic response to perturbations to the density field. The PFC and MPFC equations have close relationship, and it is possible to apply numerical methods for the former equation to the latter one. However, one should keep in mind that the original energy of the MPFC equation may increase in time on some time intervals, so it is desirable to introduce a pseudo energy. Thus, we have to be very careful when designing energy stable convex splitting schemes for the MPFC equation.

There are a few numerical methods for the simulations of the MPFC equation. For example, Wang *et al.* [1,22] developed energy stable and convergent finite difference schemes for the MPFC equation. Baskaran *et al.* [2] provided a detailed convergence analysis for an unconditionally energy stable, second-order accurate convex splitting scheme for the MPFC equation. In which, the spatial discretization was central finite difference method, and only second order spatial accuracy was achieved. Grasselli and Pierre [14] proposed an energy stable and convergence finite element schemes for the MPFC equation. In this paper, an LDG spatial discretization method will be developed, obtaining arbitrary high order accuracy by choosing the local approximating basis. For temporal discretization, we will first construct the first order and second order convex splitting schemes, the first order linear scheme, and then employ the semi-implicit spectral deferred correction (SDC) method [24] to achieve high order temporal accuracy. To the best of our knowledge, the first order linear scheme and the second order convex splitting scheme are novel combined with the pseudo energy that we define.

The discontinuous Galerkin (DG) method is a class of finite element methods, using completely discontinuous, piecewise polynomials as the solution and the test spaces. It was first designed as a method for solving hyperbolic conservation laws containing only first order spatial derivatives, *e.g.* Reed and Hill [18] for solving linear equations, and later Cockburn *et al.* [5–8] for solving nonlinear equations.

It is not straightforward to apply the DG method directly to PDEs containing higher order spatial derivatives, therefore the LDG method was introduced. There are usually two steps to implement the LDG method: first rewriting the problem into a form which contains only first order derivatives, and then applying the DG method by choosing appropriate numerical fluxes to ensure stability. The first LDG method was constructed