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Energy stable and efficient finite-difference nonlinear multigrid schemes for the modified phase field crystal equation

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ABSTRACT

In this paper we present two unconditionally energy stable finite difference schemes for the modified phase field crystal (MPFC) equation, a sixth-order nonlinear damped wave equation, of which the purely parabolic phase field crystal (PFC) model can be viewed as a special case. The first is a convex splitting scheme based on an appropriate decomposition of the discrete energy and is first order accurate in time and second order accurate in space. The second is a new, fully second-order scheme that also respects the convex splitting of the energy. Both schemes are nonlinear but may be formulated from the gradients of strictly convex, coercive functionals. Thus, both are uniquely solvable regardless of the time and space step sizes. The schemes are solved by efficient nonlinear multigrid methods. Numerical results are presented demonstrating the accuracy, energy stability, efficiency, and practical utility of the schemes. In particular, we show that our multigrid solvers enjoy optimal, or nearly optimal complexity in the solution of the nonlinear schemes.

1. Introduction

Crystalline materials are used in numerous engineering applications. In practice, most crystals have nanoscopic imperfections in the form of defects – such as vacancies, grain boundaries, and dislocations – and controlling, or at least predicting, the formation and evolution of such imperfections is a major challenge. Accurate modeling of crystal dynamics, especially defect dynamics, requires atomic-scale resolution. The phase field crystal (PFC) equation, a continuum model that has attracted significant attention in recent years, has shown promise in this regard [5,6,13]. In the PFC approach the crystal is described via a continuous phase field ϕ that approximates the number density of atoms. The field variable ϕ admits two qualitatively different solutions, a constant solution that represents the liquid phase and a periodic solution that represents the solid phase. The local extrema of the periodic solution lie on a near-perfect lattice, mimicking the atomic lattice of the crystal. The PFC equation is

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

where $\epsilon < 1$ and $M > 0$. This model, which is related to the dynamic density functional theory of freezing [5,11], has the important advantage over many atomistic models that the characteristic time is determined by the diffusion time scale and not by that of the atomic vibrations. This enables one to capture relatively long time processes, in contrast to atomistic models. The recent review by Provatas et al. [13] outlines a wide range of applications of the PFC modeling framework.

The major disadvantage of the PFC model is that it fails to distinguish between the elastic relaxation and diffusion time scales [5,14]. In [14,15], the authors introduced the modified phase field crystal (MPFC) model to overcome this difficulty. The MPFC equation is

$$\partial_{tt}\phi + \beta\partial_t \phi = M\Delta(\phi^3 + (1-\epsilon)\phi + 2\Delta\phi + \Delta^2\phi), \tag{1.2}$$

where $\beta > 0$. The MPFC equation (1.2) is a nonlinear damped wave equation modeling a viscoelastic response to perturbations to the density field. In this model, perturbations in the density field are transmitted by waves that travel essentially undamped up to a certain length scale determined by the parameters. When this length scale is of the order of the size of the system a separation of elastic relaxation and diffusion time scales may be practically observed [14].

The MPFC equation, like the PFC equation, is a sixth order evolutive nonlinear partial differential equation that cannot be solved analytically in practical circumstances. Efficient and accurate methods for approximating the solutions of the MPFC equation are therefore highly desirable. However, to date, very little research has been carried out in this direction.

Because of the close relationship between the MPFC and PFC models, methods for the latter equation can be adapted and applied to the former. See, for example, [1,3,5,8,12,20] for some recent approximation methods specifically for the PFC model. However, one must take care, as we show in the following pages, to adequately account for the wave-like nature of the MPFC solutions in the numerical method, especially in the design of provably energy stable schemes.

Methods specifically designed for the MPFC equation can be found in [10,15,17,18]. Stefanovic et al., [15] employed a semi-implicit finite difference discretization, with a multigrid algorithm for solving the algebraic equations. They provide no numerical analysis for their scheme, which is significantly different from schemes we propose and analyze. In particular, theirs is not expected to be unconditionally solvable or energy stable. The authors did, however, give some evidence of the efficiency of their multigrid solver. We will conduct a similar study for our multigrid solver in this paper. The MPFC scheme in [10] is more or less the same as the first-order convex-splitting that we devised earlier in [17,18]. The first-order convex splitting scheme in our work [17,18] has two fundamental properties. It is unconditionally energy stable and unconditionally uniquely solvable. We rigorously analyzed this convex splitting scheme in [17,18], but we did not provide a practical solution strategy. That gap is filled here.

In [8,20] we presented first and second-order accurate (in time) finite difference schemes for the purely parabolic PFC model, based on a convex splitting framework applied to the physical energy. The convexity splitting idea – in the context of first order (in time) convex splitting schemes – is generally credited to [7]. One of the main advances in [8] – and the more recent work in [22] – was the demonstration that the convex splitting framework can be extended to second-order (in time) methods as well, in a natural way. While the motivation in [8] was the application to the PFC model, the second-order convex splitting idea that we developed is, in fact, rather general.

The main goal of this paper is to apply the first and second-order convex splitting framework to the MPFC equation. The principal challenge in doing so is that the extension to damped wave dynamics appears, at first sight, not so straightforward. This obstacle was first surmounted in [17,18], as already mentioned, where we extended the first-order convexity splitting idea for the MPFC model. Specifically, we showed the existence of a pseudo energy (different from the physical energy), which is non-increasing in time for solutions of the MPFC model and to which the usual convexity splitting idea can be applied. As a side note, in [17] we used this energy stability approach to prove the existence and uniqueness of a global in time smooth solution for the MPFC partial differential equation.

Herein we present, for the first time, a new fully second-order convex splitting scheme for the MPFC model. The idea is general and can be applied to other damped wave equations. We also compare the first-order convex splitting scheme from [17,18] with the new second-order convex splitting scheme. We propose and test efficient (optimal complexity) nonlinear multigrid solvers for both. These two convex splitting schemes are shown to be unconditionally energy stable with respect to a pseudo energy, which is different from the physical energy, and mass conserving. Both schemes are nonlinear. But both are obtained via gradients of strictly convex, coercive functionals, facts which guarantee the unique solvability of the schemes, regardless of the time and space step sizes.

The paper is organized as follows. The MPFC model is recounted in Section 2. In Section 3 we present our first and second-order accurate (in time) convex splitting schemes and analyze their basic properties. We present some numerical results in Section 4 that give evidence of the convergence of the schemes and the efficiency of the multigrid solvers. In that section, we also show a couple of practical application of the model. The first is a problem of crystalization, the second, a problem of elastic relaxation in a strained crystal. We give some conclusions in Section 5. To keep the presentation short, we relegate some of the details of the schemes to two appendices. In Appendix A, we give the basics of our finite difference discretization of space, and we list some needed summation-by-parts formulae. In Appendix B, we give some details of the nonlinear multigrid solvers that we utilize to advance the nonlinear schemes in time.