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Benchmark Computations of the Phase Field Crystal and Functionalized Cahn-Hilliard Equations via Fully Implicit, Nesterov Accelerated Schemes

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Abstract. We introduce a fast solver for the phase field crystal (PFC) and functionalized Cahn-Hilliard (FCH) equations with periodic boundary conditions on a rectangular domain that features the preconditioned Nesterov's accelerated gradient descent (PAGD) method. We discretize these problems with a Fourier collocation method in space, and employ various second-order schemes in time. We observe a significant speedup with this solver when compared to the preconditioned gradient descent (PGD) method. With the PAGD solver, fully implicit, second-order-in-time schemes are not only feasible to solve the PFC and FCH equations, but also do so more efficiently than some semi-implicit schemes in some cases where accuracy issues are taken into account. Benchmark computations of four different schemes for the PFC and FCH equations are conducted and the results indicate that, for the FCH experiments, the fully implicit schemes (midpoint rule and BDF2 equipped with the PAGD as a nonlinear time marching solver) perform better than their IMEX versions in terms of computational cost needed to achieve a certain precision. For the PFC, the results are not as conclusive as in the FCH experiments, which, we believe, is due to the fact that the nonlinearity in the PFC is milder nature compared to the FCH equation. We also discuss some practical matters in applying the PAGD. We introduce an *averaged Newton preconditioner* and a *sweeping-friction* strategy as heuristic ways to choose good preconditioner parameters. The sweeping-friction strategy exhibits almost as good a performance as the case of the best manually tuned parameters.

AMS subject classifications: 74A50, 65M22, 65F08, 65B99

Key words: Phase field crystal, functionalized Cahn-Hilliard, preconditioning, Nesterov acceleration, nonlinear solver.

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1 Introduction

We are interested in fast and accurate numerical solvers for initial value problems (IVPs) for nonlinear parabolic partial differential equations of the form

$$\partial_t u = M\Delta\frac{\delta\mathcal{E}}{\delta u}(u), \quad t>0, \quad u|_{t=0}=u_0, \tag{1.1}$$

supplemented with periodic boundary conditions. Here, $\frac{\delta\mathcal{E}}{\delta u}$ denotes the variational derivative of the energy

$$\mathcal{E}(u)=\int_\Omega f(u,\nabla u,\Delta u)\mathrm{d}x.$$

The spatial domain is Ω, which is assumed to be rectangular throughout this paper, and $M:\mathbb{R}\to\mathbb{R}$ is the so-called *mobility constant*. While the mobility may depend on the unknown u in general, we confine ourselves to the case of constant mobility $M\equiv 1$ in this work. Two real world applications, the *phase field crystal* (PFC) and *functionalized Cahn-Hilliard* (FCH) equations (see Section 2 for more details) take this form and are of our main interest.

Our focus is on the numerical solvers. Nevertheless, for completeness, let us briefly mention existing works about the phenomena that the PFC and FCH equations model and their PDE analyses. These two equations are important models in materials science. The PFC equation describes crystal formation in a liquid bath, crack propagations in a crystal layer, and elastic and plastic deformations of a crystal lattice, to name a few. The FCH equations, on the other hand, describes network formation in a binary mixture and is a useful tool for modeling bilayer membrane formation and polymer electrolyte membrane evolution. The reader interested in applications is referred to [1,15–17] for the PFC, and [22,23,30] for the FCH model, respectively. There is some limited amount of work about these equations at the PDE level. For the PFC equation see [11,34]; whereas for the FCH see [6,12].

Both the PFC and FCH are nonlinear, sixth-order 'parabolic' equations. As such, they share common numerical difficulties, such as accuracy and stability, and there have been efforts to overcome them; see, for example, [7,24,26,35,39] for the PFC, and [20,27,37,38] for the FCH, respectively. If one wishes to have a long time evolution of the equations, explicit discretization schemes in time must typically be excluded due to their stringent restriction on the time step size, ($\mathrm{d}t\approx\mathrm{d}x^6$), for stability. On the other hand implicit schemes, which are more robust in terms of stability and accuracy, as a rule lead to a large, highly nonlinear system that must be solved at every time step. A substantial amount of work has been dedicated to developing schemes that mitigate the numerical difficulties or instabilities of either of these extreme approaches, fully explicit schemes, on one hand, and fully implicit schemes, on the other. Examples of this are the convex splitting technique [7, 24, 26, 27, 35, 37, 38], and the SAV technique [5, 8, 28], to name a few. Both of these approaches, however, are known to create larger local truncation errors than implicit schemes [36, 38]. If a reliable, robust, and efficient iterative solver is