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Benchmark Computation of Morphological Complexity in the Functionalized Cahn-Hilliard Gradient Flow

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Abstract. Reductions of the self-consistent mean field theory model of amphiphilic molecules in solvent can lead to a singular family of functionalized Cahn-Hilliard (FCH) energies. We modify these energies, mollifying the singularities to stabilize the computation of the gradient flows and develop a series of benchmark problems that emulate the "morphological complexity" observed in experiments. These benchmarks investigate the delicate balance between the rate of absorption of amphiphilic material onto an interface and a least energy mechanism to disperse the arriving mass. The result is a trichotomy of responses in which two-dimensional interfaces either lengthen by a regularized motion against curvature, undergo pearling bifurcations, or split directly into networks of interfaces. We evaluate a number of schemes that use second order backward differentiation formula (BDF2) type time stepping coupled with Fourier pseudo-spectral spatial discretization. The BDF2-type schemes are either based on a fully implicit time discretization with a preconditioned steepest descent (PSD) nonlinear solver or upon linearly implicit time discretization based on the standard implicit-explicit (IMEX) and the scalar auxiliary variable (SAV) approaches. We add an exponential time differencing (ETD) scheme for comparison purposes. All schemes use a fixed local truncation error target with adaptive time-stepping to achieve the error

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target. Each scheme requires proper "preconditioning" to achieve robust performance that can enhance efficiency by several orders of magnitude. The nonlinear PSD scheme achieves the smallest global discretization error at fixed local truncation error, however the IMEX and SAV schemes are the most computationally efficient as measured by the number of Fast Fourier Transform (FFT) calls required to achieve a desired global error. Indeed the performance of the SAV scheme directly mirrors that of IMEX, modulo a factor of 1.4 in FFT calls for the auxiliary variable system.

AMS subject classifications: 35K35, 65M06, 65M12, 65M50

Key words: Phase field model, benchmark computations, adaptive time stepping, functionalized Cahn-Hilliard.

1 Introduction

We present a series of physically motivated computational benchmark problems addressing the evolution of the functionalized Cahn-Hilliard (FCH) gradient flow. This system supports families of equilibria with rich morphological structure separated by slightly different energies. The faithful resolution of final end states requires significant computational accuracy. There has been considerable recent attention to the development of energy stable computational schemes for gradient descent flows [16, 18, 26, 37, 38, 46, 48, 49]. Gradient flows are defined by the dissipation of a free energy, and it is essential that numerical schemes preserve that property. Energy stable schemes have the desirable property that the energy, or a modified energy, decreases at every time-step irrespective of time-step size. We argue that where possible energy decay should be a consequence of accuracy. In some situations energy decay without accuracy can lead to plausible but incorrect computational outcomes. Conversely accuracy should be balanced against computational cost. This motivates a comparison of computational efficiency between schemes as measured by the minimal computational cost required to achieve a desired global discretization error.

Meaningful assessment of computational efficiency can be achieved from gradient flows that harbour strong nonlinear interactions that generate selection mechanisms between distinct outcomes with small energy differences. For motivation, we emulate the "morphological complexity" experiments presented in [30]. By strongly dispersing (stirring) amphiphilic diblock polymers in solvent, and then allowing the mixture to relax, the authors of that study observed the formation of a wide variety of structures whose evolution and end-state depend sensitively upon the polymer chain and mixture properties, see Fig. 1 and [1, 2]. Reductions of the self-consistent mean field theory models of amphiphilic molecules in solvent can lead to a singular family of FCH energies, [47]. We modify these energies, mollifying the singularities to produce a family of computationally tractable, but highly nonlinear, FCH gradient flows similar to those studied earlier, [14, 15, 21]. We present a series of benchmark problems that recover the onset of