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High Accuracy Benchmark Problems for Allen-Cahn and Cahn-Hilliard Dynamics

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Abstract. There is a large literature of numerical methods for phase field models from materials science. The prototype models are the Allen-Cahn and Cahn-Hilliard equations. We present four benchmark problems for these equations, with numerical results validated using several computational methods with different spatial and temporal discretizations. Our goal is to provide the scientific community with a reliable reference point for assessing the accuracy and reliability of future software for this important class of problem.

AMS subject classifications: 65M06, 65M70

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1 Introduction

Many material science problems require an understanding of the microstructure that develops in a mixture of two of more materials or phases over time. One model of such

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phenomenon is the Cahn-Hilliard (CH) [10] equation that describes phase separation of a binary alloy during annealing. The problem is described by a scalar function u of space $\mathbf{x}$ and time t that takes values $u=+1$ in one phase and $u=-1$ in the other.

$$u_t = -\epsilon^2 \Delta\Delta u + \Delta(W'(u)), \tag{1.1}$$

where $W(u)=\frac{1}{4}(u^2-1)^2$ and Δ is the Laplacian operator. The parameter ϵ in the model is a length scale – the width of the layers between the regions of different phases. Such regions form quickly and subsequently they evolve on longer time scales, generically $\mathcal{O}(e^{C/\epsilon})$ for 1D Cahn-Hilliard [32]. In higher space dimensions formal analysis has shown that the Cahn-Hilliard model forms phase separated regions that evolve according to a Stefan problem on $\mathcal{O}(1)$ time scale and according to a Mullins-Sekerka flow on the longer $\mathcal{O}(\epsilon^{-1})$ time scales [31]. This analysis has been made rigorous for the Cahn-Hilliard equation with Neumann boundary conditions, [1], for periodic patterns, [2], and for patterns attached to the boundary, [3]. The study of equilibrium of the Cahn-Hilliard equation, equivalently the minimizers of the Cahn-Hilliard free energy

$$\mathcal{E}(u) := \int_\Omega \frac{1}{2}\epsilon|\nabla u^2| + \epsilon^{-1} W(u)\, dx, \tag{1.2}$$

has an even longer history. The key result, [30], established the $\epsilon \to 0$ limit of the Cahn-Hilliard free energy as the surface area of the interface. This result was generalized by many authors, in particular [35], see the excellent review article [33].

The Cahn-Hilliard model is in a larger family of phase field models. A review of the extensive use of such models in material science applications can be found in [11]. There are several interesting generalizations of the Cahn-Hilliard equation. Fourth order phase field models of increasing complexity are used to describe some aspects of cancerous tumour growth [44]. Sixth order models also arise in the study of network formation in functionalized polymers [20]. Because of the ubiquity and physical importance of these models, many numerical approaches have been developed to solve them, with a small sample given in the following references: [13, 16–18, 34, 38, 43]. Until now, there has been no way to evaluate the raw accuracy or the relative performance (accuracy for similar computational costs) of this array of numerical approaches. There is a set of benchmark problems described in [27]. However, these problems lack concrete numerical targets to assess accuracy. Another set of benchmark problems in [26] with radial symmetry is posed in an infinite domain, not suitable for comparison with many approaches in the literature. In this work, we propose four benchmark problems, three for Cahn-Hilliard and one for the second order Allen-Cahn equation. The problems are posed in periodic domains to allow the largest set of applicable techniques. We do not include any three dimensional (3D) problems since there is no extra structure to the dynamics in higher dimensions. The simplest form of the energy well (the canonical quartic) is considered, again to allow the largest set of computational approaches. Several methods with different spatial and temporal discretizations are applied to the benchmark problems to give