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Phase Field Models Versus Parametric Front Tracking Methods: Are They Accurate and Computationally Efficient?

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Abstract. We critically compare the practicality and accuracy of numerical approximations of phase field models and sharp interface models of solidification. Here we focus on Stefan problems, and their quasi-static variants, with applications to crystal growth. New approaches with a high mesh quality for the parametric approximations of the resulting free boundary problems and new stable discretizations of the anisotropic phase field system are taken into account in a comparison involving benchmark problems based on exact solutions of the free boundary problem.

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1 Introduction

The solidification of a liquid or the melting of a solid lead to complex free boundary problems involving many different physical effects. For example, latent heat is set free at the interface and a competition between surface energy and diffusion leads to instabilities like the Mullins-Sekerka instability. The resulting model is a Stefan problem with boundary conditions taking surface energy effects and kinetic effects at the interface into account, see e.g. [37, 51]. Crystals forming in an undercooled melt lead to very complex

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patterns and, in particular, dendritic growth can be observed since the growth is typically diffusion limited, see [20].

The numerical simulation of time-dependent Stefan problems, or variants of it, is a formidable task since the evolving free boundary has to be computed. Hence, direct front tracking type numerical methods need to adequately capture the geometry of the interface and to evolve the interface approximation, often with a coupling to other physical fields. This coupling, in particular, represents a significant initial hurdle towards obtaining practical implementations, and thus numerical simulations for the problem at hand. Examples of the implementation of such direct methods can be found in e.g. [1,3,6,13,53,54,57,72–75,81,86].

A further drawback of direct front tracking methods has been the inability of most direct methods to deal with so-called mesh effects, or to prevent them altogether. When a discrete approximation of an interface, for example a polygonal curve in the plane, evolves in time, then in general it is possible for the approximation to deteriorate or to break down. Examples of such pathologies are self-crossings and vertex coalescence. While for simple isotropic problems in the plane these issues can be dealt with, for example by frequent remeshings or by using clever formulations that only allow equidistributed approximations, see e.g. [57, 81], until very recently there has been no remedy for fully anisotropic problems in two and three space dimensions.

However, building on their work for isotropic problems in [8, 9, 11], the present authors recently introduced stable parametric finite element schemes for the direct approximation of anisotropic geometric evolution equations in [10, 12], for which good mesh properties can be guaranteed. In particular, even for the simulation of interface evolutions in the presence of strong anisotropies, no remeshing or redistribution of vertices is needed in practice. These schemes, in which only the interface without a coupling to bulk quantities is modelled, have been extended to approximations of the Stefan problem with fully anisotropic Gibbs-Thomson law and kinetic undercooling in [13]. The novel method from [13] can be shown to be stable and to have good mesh properties. We remark that these approaches extend earlier ideas from [39, 73, 74]. Here we recall the pioneering work of Schmidt [73, 74], where the full Stefan problem in three dimensions was solved within a sharp interface framework for the first time.

Phase field methods are an alternative approach to solve solidification phenomena in the framework of continuum modelling. In phase field approaches a new non-conserved order parameter φ is introduced, which in the two phases is close to two different prescribed values and which smoothly changes its value across a small diffuse interfacial region. A parabolic partial differential equation for φ is then coupled to an energy balance, which results in a diffusion equation for the temperature taking latent heat effects into account. We refer to [27,36,59,70,83] and to the five review articles [25,33,62,77,79] for further details. In particular, it can be shown that solutions to the phase field equations converge to classical sharp interface problems, see e.g. [2, 28, 29, 78] and the references therein.

The popularity of phase field methods, often also called diffuse interface methods,