Journal of Computational Physics 262 (2014) 153–171

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Accurate, efficient, and (iso)geometrically flexible collocation methods for phase-field models

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ARTICLE INFO

Article history:
Received 7 February 2013
Received in revised form 11 December 2013
Accepted 22 December 2013
Available online 9 January 2014

Keywords:
Collocation
Cahn–Hilliard equation
NURBS
Isogeometric analysis
Phase-field models

ABSTRACT

We propose new collocation methods for phase-field models. Our algorithms are based on isogeometric analysis, a new technology that makes use of functions from computational geometry, such as, for example, Non-Uniform Rational B-Splines (NURBS). NURBS exhibit excellent approximability and controllable global smoothness, and can represent exactly most geometries encapsulated in Computer Aided Design (CAD) models. These attributes permitted us to derive accurate, efficient, and geometrically flexible collocation methods for phase-field models. The performance of our method is demonstrated by several numerical examples of phase separation modeled by the Cahn–Hilliard equation. We feel that our method successfully combines the geometrical flexibility of finite elements with the accuracy and simplicity of pseudo-spectral collocation methods, and is a viable alternative to classical collocation methods.

1. Introduction

The Cahn–Hilliard equation is a central model in nonlinear interface dynamics [5] and pattern formation [66]. It was derived about fifty years ago as a model for phase separation of immiscible fluids [23,24]. Since then, it has been applied to a variety of physical problems, including planet formation [73], microstructure evolution of binary mixtures [2,3,26] and phase separation of polymer blends [27]. The Cahn–Hilliard equation is also one of the simplest equations that can model stable co-existence of two phases and, as such, is the basis for various multiphase flow theories [31,32,60,63]. Even more important is the fact that the ideas behind the Cahn–Hilliard equation have given rise to a new class of mathematical models termed phase-field models [40]. These models treat the interfaces as diffuse, track their dynamical evolution, and encode the interfacial physics at once. Phase-field models have had a significant impact on condensed matter physics [37,38], fluid mechanics [16,45,46], and solid mechanics [20,64,65]. Since the numerical challenges faced when dealing with phase-field equations are common to many different models, we feel that studying efficient and accurate algorithms for the Cahn–Hilliard equation is a significant goal in computational physics.

The Cahn–Hilliard model is a nonlinear partial differential equation that involves fourth-order derivatives in space. Typical solutions to the equation include thin layers that evolve dynamically through the computational domain. The length scale of these layers is given by a small parameter that multiplies the fourth-order derivative, making the problem singularly perturbed. All these features make the numerical approximation of the Cahn–Hilliard equation a significant challenge. Although, new finite element methods are being proposed to solve the Cahn–Hilliard equation [44,71,75], collocation methods continue to be the standard methodology for computational phase field modeling. The two most representative examples of

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.12.044

collocation methods for phase field models are the finite difference method [12,25,52,70] and spectral methods [12,33,54,69,72].

Most work on collocation methods for the Cahn–Hilliard equation has been focused on the development of algorithms to study the structure of the spatial patterns and free-energy evolution in extended systems, like in the spirit of the problem of isotropic turbulence decay in fluid mechanics. It is, however, becoming clear that technological applications will demand accurate and robust algorithms that can handle complicated geometries and boundary conditions (a significant example has been recently presented in [4]). This paper constitutes a first step in this direction. We propose a new collocation method for the Cahn–Hilliard equation that is fast, accurate, robust, geometrically flexible, and can handle a variety of different boundary conditions.

Our collocation scheme is based on IsoGeometric Analysis (IGA) [28,57]. IGA is a computational technology that uses functions from computational geometry to represent both the solution and the domain of a boundary-value problem. The most frequently utilized functions are Non-Uniform Rational B-Splines (NURBS) [29,57] and T-Splines [13] which are widely used in computational geometry and design. The first applications of IGA were within the framework of finite element discretizations in which NURBS replaced the standard piece-wise polynomials, giving rise to new and more accurate discretizations on a per-degree-of-freedom basis [10,14,15,21,22,30,35,39,50,58,59,61,62,67]. In fact, IGA is a generalization of finite elements because NURBS are a superset of piece-wise polynomials. However, IGA offers new possibilities not available in classical finite elements [56], such as, for example, the straightforward generation of basis functions of arbitrarily high global smoothness. Within the context of geometrically flexible methods, this seems to be a unique attribute of IGA with profound implications on the accuracy of the discretization [1,17,29,42]. Additionally, the possibility of generating arbitrarily smooth basis functions on complicated domains opens the door to geometrically flexible collocation methods [8], which have been already successfully applied in the fields of elastostatics and explicit elastodynamics [9], as well as for the development of innovative structural elements [11,18]. A detailed study on the advantages of isogeometric collocation over Galerkin approaches is provided by [68]. In that paper, the authors show the superior behavior, in terms of accuracy-to-computational-time ratio, attained by collocation with respect to Galerkin, in particular for higher order approximations. Although this study was performed for second-order partial-differential equations, we expect that similar advantages can be achieved also for higher-order equations, like those emanating from the phase-field theory.[1] Moreover, in the same paper, the authors introduce and analyze adaptive isogeometric collocation methods based on local hierarchical refinement of NURBS.

Here we use these ideas to derive new collocation methods for phase-field models. The numerical examples in this paper show that our algorithms are very efficient, and seem to be a successful combination of the geometrical flexibility of classical finite element methods and the accuracy, efficiency, and simplicity of pseudo-spectral collocation methods.

The outline of this paper is as follows: We introduce the Cahn–Hilliard equation in Section 2. Our numerical formulation is presented in Section 3. Section 4 illustrates, with several numerical examples, the efficiency, accuracy, and geometrical flexibility of our algorithm. We draw conclusion in Section 5.

2. The Cahn–Hilliard equation

We present the Cahn–Hilliard equation in the context of isotropic and isothermal phase separation of immiscible fluids. Within this simplified setting, the thermodynamic state of the mixture is defined by an order parameter u of the mass fraction. The assumption of an isothermal system indicates that the relevant thermodynamic potential is a free energy, which in the context of two-phase immiscible mixtures is called Ginzburg–Landau free energy.

2.1. Ginzburg–Landau free energy

Let V be an open subset of $\mathbb{R}^d$, where d is the spatial dimension. The Ginzburg–Landau free energy is defined as the functional $\mathcal{G} : H^1(V) \mapsto \mathbb{R}$ which takes the form

$$\mathcal{G}[u] = \int_V \left(F(u) + \frac{\varepsilon^2}{2} |\nabla u|^2 \right) \mathrm{d}V \tag{1}$$

where H^1 is the Sobolev space of square integrable functions with square integrable first derivatives. Following the interpretation of Cahn and Hilliard [23,24], F is the free energy of a homogeneous system and the gradient term accounts for the interfacial free energy. Among the various possibilities for the homogeneous free energy F, we take the simple form

$$F(u) = \frac{\alpha}{4} \left(u^2 - \frac{\beta}{\alpha} \right)^2 \tag{2}$$

This function is non-convex and presents a double well structure with two local minima located at $u = -\sqrt{\beta/\alpha}$ and $u = +\sqrt{\beta/\alpha}$, which are called the binodal points.

[1] A detailed study along these lines would be surely interesting, but it is beyond the scope of this paper and will be the subject of future research.