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Isogeometric Analysis of the Navier–Stokes–Cahn–Hilliard equations with application to incompressible two-phase flows

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ABSTRACT

In this work, we provide a unified and comparative description of the most prominent phase field based two-phase flow models and present our numerical results of the application of Galerkin-based Isogeometric Analysis (IGA) to incompressible Navier–Stokes–Cahn–Hilliard (NSCH) equations in velocity–pressure–phase field-chemical potential formulation. For the approximation of the velocity and pressure fields, LBB compatible non-uniform rational B-spline spaces are used which can be regarded as smooth generalizations of Taylor–Hood pairs of finite element spaces. The one-step θ-scheme is used for the discretization in time. The static and rising bubble, in addition to the nonlinear Rayleigh–Taylor instability flow problems, are considered in two dimensions as model problems in order to investigate the numerical properties of the scheme.

1. Introduction

Multiphase flows of immiscible fluids, that is, flow of fluids which are incapable of mixing, such as e.g. oil and water, are omnipresent in nature and industrial systems. By way of example we refer to the Deepwater Horizon oil spill in the gulf of Mexico and the respective industrial plant in charge with pumping an oil water mixture to the surface. In particular, in a multiphase flow context the dynamics of bubbles and droplets including their deformation, coalescence and breakup are intriguing processes which have gained a lot of attention in the scientific community, cf. [4,6,22,25,26]. In two-phase flows, being the most common multiphase flow configuration involving two distinct fluids, the fluids are segregated by a very thin interfacial region where surface tension effects and mass transfer due to chemical reactions may appear. The former is caused by molecular force imbalances in the vicinity of the fluid interface. The extension of the physical model to multiple fluids, with each fluid being allowed to have its own density and viscosity, comes at a cost of potentially sharp gradients of these quantities and pressure jumps across the phase separating interface. As for methodologies to address these issues, the sharp- and diffuse-interface methods are among the most widely used ones to model fluid interface dynamics. Traditionally, phase transition phenomena have been described with sharp interface models. This involves the tracking of the phase separating interface as it evolves over time. Among Eulerian interface tracking methods the volume-of-fluid [19] and the level-set [31] method constitute the most prominent sharp interface models and have been applied in a multitude

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of multiphase applications. However, especially in the realization of the latter method discontinuous functions are often regularized and artificially "smoothed" with regularized Heaviside or step functions. The regularization aids to circumvent problems with numerical integration when discontinuous coefficients and functions are involved. Henceforth, the level-set method can sometimes be regarded as a diffuse interface method as well, since it introduces a narrow transition region across which the regularization of discontinuous coefficients is realized.

In this work we use a phase field diffuse interface method based on the Cahn–Hilliard (CH) equation and apply Isogeometric Analysis for the discretization of the involved equations. Diffuse-interface models have been used in a wide spectrum of fields, ranging from material sciences to fracture mechanics. Moreover, in recent years they have been successfully used to describe the flow of two or more immiscible fluids for both numerical and theoretical studies. Particularly for two-phase flows, they have gained a lot of attention due to their ability to easily handle moving contact lines and topological transitions without any need for reinitialization or advective stabilization. On a general note, diffuse interface models allow the modeling of interfacial forces as continuum forces with the effect that delta-function forces and discontinuities at the interface are smoothed by smearing them over thin yet numerically resolvable layers. The phase field method – also known as the diffuse interface model – is based on models of fluid free energy and offers a systematic physical approach by describing the interface in a physical rather than in a numerical sense. One principal advantage of diffuse interface models is their ability to describe topological transitions like droplet coalescence or break-up in a natural way. In the phase field framework, the interface is modeled by a function $\varphi(x,t)$ which represents the concentration of the fluids. The function $\varphi(x,t)$, also referred to as the order parameter, or the phase field, attains a distinct constant value in each phase and rapidly, but smoothly, changes in the interface region between the phases. For a binary fluid, a usual assumption is that φ takes values between -1 and 1, or 0 and 1. The relaxation of the order parameter is driven by local minimization of the fluid free energy subject to the phase field conservation. As a result, complex interface dynamics such as coalescence or segregation can be captured without any special procedures [3,35].

The mathematical modeling of phase field-based two-phase incompressible flows dates at least back to the work of Gurtin et al. [17] and has originated a multitude of different models ever since. These models differ from each other by a group of quite diverse criteria, one of them being e.g. the treatment of the density, that is, considering it constant or variable. Moreover, not all models are based on a divergence-free velocity field and the modeling of extra contributions of additional forces to the stress tensor such as e.g. the surface tension induced capillary forces is quite varied across the models. While for some models no energy inequalities are known, others are shown to admit an energy law and to be thermodynamically consistent. For the latter to hold, some of the affected models are extended by additional terms. Each of these models has its own advantages and disadvantages in terms of suitability for particular flow scenarios, physical consistency and implementation simplicity. Following the agenda to assess Isogeometric Analysis-based approximations of various variable density two-phase flow problems with respect to reference "sharp interface"-based results, the identification of a reasonable model turned up to be a time consuming and tedious process. This is founded on the fact that there are quite a number of different models at one's disposal, each having a distinct set of traits determining its overall suitability. As an additional reason, we identify the lack of a consolidated inventory with emphasis on the most essential features and shortcomings of each model. In order to address this issue and to make this article self contained, we have decided to briefly present and screen the models in a dedicated section (see Section 2).

Using the numerical benchmark setups of Hysing et al. [22] for two-dimensional bubble dynamics, Aland et al. [2] compared three different phase field-based incompressible two-phase flow models utilizing a classical finite element discretization. More specifically, the results computed with the models of Ding, Boyer and Abels (see Section 2) are compared to both each other and to those of Hysing being based on a level-set sharp interface model. The performed numerical analysis indicates a good result-wise agreement among all three phase field models and in particular exhibits rather small differences between the models of Ding and Abels. Using this finding, we identify the model proposed by Ding as suitable for our purposes and apply Isogeometric Analysis to the above mentioned two-phase flow benchmark problems. To our best knowledge this is the first work aiming to recover Hysing's sharp interface based variable density and variable viscosity two-phase flow benchmark results applying Isogeometric Analysis to a NSCH model. Besides, the robustness of the Isogeometric discretization of the NSCH system is further underpinned by its application to other challenging two-phase flow scenarios such as for instance the "Rayleigh–Taylor instability".

We consider the combination of Isogeometric Analysis and the NSCH system for the numerical treatment of multiphase flow problems as very powerful. This is attributed on the one hand to the above mentioned benefits of phase field methods, and on the other hand to the ability to perform finite element type numerical analysis on complex geometries without the necessity to discretize it with straight line segments or flat faces. This has proven in a row of different context to yield gains in accuracy compared to alternative numerical methods [8]. Moreover, the Cahn–Hilliard equation in its primal formulation involves fourth order spatial derivatives requiring $\mathcal{C}^1$ continuous discrete approximation spaces which can easily be spanned with high regularity basis functions in Isogeometric Analysis.

As of writing of this article there are in all conscience two other works combining Isogeometric Analysis with the advective Cahn–Hilliard phase field model and fluid flow. The first article [29] uses the advective Cahn–Hilliard equation and presents an Isogeometric Analysis-based numerical study of spinodal decomposition of a binary fluid undergoing shear flow. In contrast to this work, however, they use a passive and externally provided velocity field and in particular do not solve a coupled NSCH system. The second work [12] on the other hand, aims to analyze the dynamics of liquid droplets in a liquid continuum. It does involve a NSCH system and utilizes divergence-free B-spline spaces to obtain a discrete pointwise