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Isogeometric boundary integral analysis of drops and inextensible membranes in isoviscous flow

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ABSTRACT

The Boundary Integral Method (BIM) is applied to investigate the dynamics of a single drop and an inextensible membrane in isoviscous shear flow. The novelty of this work resides in the application of Isogeometric Analysis (IGA) to define the interface of the deformable objects. The employed B-spline basis functions facilitate the direct evaluation of surface normal vectors and curvatures, as required by the BIM. Collocation and L^2-projection methods are implemented to approximate the velocity of the B-spline control points. In particular, a comparison between these two methods for the case of the drop is reported and shows that the collocation method provides faster and more stable results. The collocation method is also applied for the determination of the surface tension in an inextensible membrane. A series of simulations is conducted to verify the isogeometric approach, and various computational aspects are studied.

1. Introduction

Deformable objects such as drops, vesicles and red blood cells have received considerable research interest due to their industrial applications and biomedical relevance. For instance, to understand the properties of polymer blends intended for fiber-, film- or bulk-plastic production, formation of emulsions or water-in-water biopolymer mixtures, it is important to study the dynamics and deformation of drops in a continuous phase. As such, the research on drop deformation in multiphase systems has been studied extensively and remains a topic of active research. Single drop deformation studies provide valuable insights into the behavior of systems with multiple drops. The research on inextensible membranes, vesicles and red blood cells is motivated by the need for getting a better understanding of *e.g.* thrombus formation, diabetes and thalassemia. Increasing the understanding of the motion of such deformable objects is key to the development of more effective treatment strategies.

Numerical studies on the motion of deformable objects are primarily concerned with the simulation of the dynamic behavior of the interfaces. As a consequence of the low Reynolds numbers encountered in the applications in this contribution, the motion of the objects can be described by the steady Stokes equations. The availability of fundamental solutions for these problems, known as Stokeslets, makes it possible to simulate the motion of an interface using the Boundary Integral Method (BIM) [1,2]. The fundamental advantage of the BIM is that a volumetric multiphase flow formulation can be cast into a formulation that involves the interface between the various fluids only. In fact, over the past decades, the BIM has been found to provide an accurate and reliable way of dealing with interfacial flow problems, which has made this method widely applied in this field. For example, the BIM has been used for the simulation of drop deformation and break-up [3,4], drop coalescence [5,6], drop sliding on an inclined plane [7], drop-drop interaction [8], drop deformation in confined geometries [9], inextensible capsule deformation [10], vesicle migration in Poiseuille flow [11], and many other multiphase flow phenomena.

We note that the boundary integral formulation relies on the transformation of a linear partial differential equation where a reduction in dimension is achieved: the resulting equation is solved on a surface instead of the volume. This directly implies that non-linearities due to inertia or non-linear rheology are out of the scope of the method. On the other hand, by modifying the kernels one has quite some freedom to study drop/membrane interaction close to a wall or in confinement. For shear, elongation and Poisseuille flow, there is no restriction to use the method.

An essential ingredient of the BIM for the simulation of deformable objects suspended in Stokes flow is the evaluation of the stress jump across an interface. In general, this stress jump is a function of the geometry of the interface through quantities such as the surface normal vector, curvature, and, in the case of a vesicle or red blood cell, surface gradients of these geometric quantities. It is self-evident that successful application of the BIM to such problems

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requires the evaluation of these surface stress jumps to be accurate and efficient. The evaluation of the stress jumps is non-trivial when using non-smooth continuous surface meshes, as is common in boundary integral methods [1,2]. On such meshes, the curvature is not defined along the element boundaries. Proper numerical treatment of the associated difficulties is required to obtain a robust boundary integral formulation for the simulation of the motion of deformable objects.

The goal of this work is to study the applicability and performance of isogeometric analysis for the simulation of drops and inextensible membranes using the boundary integral formulation. Isogeometric Analysis (IGA) was introduced by Hughes et al. in 2005 [12] as a novel analysis paradigm to integrate computer aided design (CAD) and finite element analyses. The fundamental idea of IGA is to employ the spline basis functions used in CAD directly in the analysis, thereby eliminating geometry clean-up and meshing operations. An additional advantage of using splines in the analysis comes from the smoothness of these basis functions. The distinct properties of the spline basis functions have been shown to be advantageous for a wide range of problems [13].

The smoothness of the spline basis functions used in IGA allows for a unique definition of curvatures over element boundaries, which gives IGA the potential to be a robust and accurate analysis tool for the simulation of deformable objects. Recent studies on the combination of IGA and BIM, referred to as IGA-BIM, have demonstrated the potential advantages of this method compared to traditional boundary element and boundary integral formulations. IGA-BIM has been applied for example to solve potential-flow problems [14], Laplace's equation [15], elastostatics problems [16], Stokes flow problems [17] and shape optimization problems [18].

1.1. The droplet

The pioneering work on single drop behavior was carried out by Taylor [19,20]. He introduced small deformation theory to express that the mechanism behind drop deformation depends purely on the capillary number and viscosity ratio between internal and external fluids. Taylor theory is still being used in many studies to find the interfacial tension [21–24] and has been verified experimentally [25,26]. Small deformation theory is only applicable when the drop remains practically spherical, which is generally the case if the capillary number is much smaller than unity [27]. A few theoretical analyzes limited to the small capillary number and near-sphere shape of the drop are reported by [28,29]. For larger capillary numbers the drop deviates from the spherical shape and becomes slender, and the drop may eventually break-up in multiple drops. Slender-body theories, which can be regarded as extensions of the small deformation theory, have been introduced for such cases [30–33,9]. Some complex phenomena, such as drop-break up and drop-drop interaction, have also been studied both theoretically and experimentally [34].

To study arbitrary deformations of single and multiple drop systems and phenomena such as drop break-up and drop coalescence, numerical analysis is indispensable. For instance, agreement between numerical simulations and experimental observations in drop break-up in three-dimensional viscous flows has been reported by Cristini et al. [3]. They have also studied the deformation and break-up of the drops in isotropic turbulent flow using the boundary integral method (BIM) [35]. The same method has been used to investigate the interaction between deformable drops in Stokes flow with large deformations [36]. In addition, Janssen and Anderson [9,37] used the boundary integral method to solve the governing Stokes equations on drops in confined geometries. In general, in traditional boundary integral formulations, the surface of a drop is parameterized by the definition of piece-wise polynomials over elements. Efficient methods have been developed to overcome the difficulties in traditional BIM that arise from the non-unique definition of surface gradients on the element boundaries and vertices, see *e.g.* [8,9,37].

1.2. The inextensible membrane

There are numerous computational and analytical studies on the inextensible membrane model of a red blood cell, mostly in shear flow. Kholeif and Weymann [38] conducted a theoretical study on a two-dimensional model of a membrane with a biconcave shape (which resembles the cross section of an undeformed red blood cell). Depending on the viscosity ratio and the shear rate, the membrane was found to either rotate as a rigid particle or to show tank-treading behavior (*i.e.* the shape-preserving rotation of the membrane around the interior of the cell). The obtained results were found to be in a good agreement with experimental observations reported by Stone [39], Schmid-Schönbein and Wells [40] and Goldsmith [41], confirming that the inextensible membrane is (to some extend) a representative model of a red blood cell. Sugihara and Niimi [42] and Niimi and Sugihara [43] considered an ellipse as the initial shape of a two-dimensional membrane and investigated the flow fields inside and outside of the membrane using the finite element method to discretize the Stokes equations. They computed the tension in the membrane and measured the time until membrane break-up. They also theoretically showed that the membrane undergoes an unsteady cyclic loading as a consequence of its tangential rotation around the interior. Zahalak et al. [44] considered a two-dimensional membrane with a circular initial shape and presented a fifth-order perturbation series solution of the resulting free boundary-value problem. They studied the tension distribution in the membrane for small and moderate deformations.

The inextensible membrane has also been studied in three dimensions. Keller and Skalak [45] developed an analytical solution by considering a cell with an ellipsoidal shape in a shear flow for which the surface area was conserved only globally. Sutera et al. [46] used the same model to estimate the membrane's effective viscous and elastic properties. Zhou and Pozrikidis [10] used the boundary integral method to present both two- and three-dimensional simulations of an inextensible membrane in shear flow. In two dimensions, they extended the work by Zahalak et al. [44] by the prediction of the membrane behavior for large deformations. They studied the tension distribution in the membrane in the case of a highly elongated initial shape. In addition, they presented a three-dimensional initial ellipsoidal membrane in shear flow and observed a relation between the distribution of the tension and the mean curvature of the surface. They numerically observed that the equilibrium shape of a membrane is independent of the initial inclination angle by simulating three ellipsoids with three different initial orientations.

Though Zhou and Pozrikidis [10] successfully simulated three-dimensional inextensible membranes in shear flow for a limited range of initial shapes, they also found that sawtooth instabilities associated with their boundary integral formulation negatively influence the robustness of the method [47]. In the two-dimensional case, this instability manifested itself by minor oscillations in the approximated shape of the cell. In three dimensions, however, the numerical results were found to diverge. To eliminate this instability they applied the five-point smoothing formula of Longuet-Higgins and Cokelet [48]. This technique practically eliminated the sawtooth instability problem in two dimensions, but it did not overcome these stability problems in three-dimensional simulations. As an alternative stabilization method they also considered a spectral projection method. In two dimensions, this stabilization method was found to be very effective. In three dimensions, the application of this stabilization strategy permitted the simulation of a limited range of initial shapes.