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Validation of an immersed thick boundary method for simulating fluid-structure interactions of deformable membranes

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ABSTRACT

This paper constitutes an extension of the work of Mendez et al. (2014) [36], for three-dimensional simulations of deformable membranes under flow. An immersed thick boundary method is used, combining the immersed boundary method with a threedimensional modeling of the structural part. The immersed boundary method is adapted to unstructured grids for the fluid resolution, using the reproducing kernel particle method. An unstructured finite-volume flow solver for the incompressible Navier-Stokes equations is coupled with a finite-element solver for the structure. The validation process relying on a number of test cases proves the efficiency of the method, and its robustness is illustrated when computing the dynamics of a tri-leaflet aortic valve. The proposed immersed thick boundary method is able to tackle applications involving both thin and thick membranes/closed and open membranes, in significantly high Reynolds number flows and highly complex geometries.

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1. Introduction

Solving the fluid-structure interaction (FSI) problem involved when a membrane is deformed by a flow is a scientific challenge which has been tackled for several decades, due to its wide range of applications. When dealing with numerical simulation of flow-induced deformation of membranes, the state of the art is extremely varied. Different communities work on the topic, focusing on various applications. A large part of these applications are considering deformable particles such as capsules, vesicles or cells. All these systems are constituted by a liquid droplet enclosed by a very thin structure (its thickness is much smaller than the size of the object). This structure can be a polymer structure for capsules, a phospholipid bilayer for vesicles, or a more complex biological membrane in the case of red blood cells [1]. Due to their small size, computations of flows of these deformable particles are often based on boundary integral methods (BIM) [2]. This method can be used for low Reynolds number flows, when the flow is well described by the Stokes equations. The BIM is a very popular technique to compute flows of capsules [3–9], vesicles [10–14] and red blood cells [15–17], because of its precision and its relatively moderate computational cost (only the membranes and boundaries need to be discretized). When the flow is governed by the Navier-Stokes equations, methods with the fluid grid following the deformation of the interface, based on

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the Arbitrary Lagrangian–Eulerian (ALE) formalism are developed [18–20]. However, they are not the most popular, as they involve frequent remeshing. Authors generally prefer one-fluid formalisms, where the fluid equations are solved everywhere, over a fixed Eulerian grid. The membrane location is computed by advecting either a function as the level-set function or a second Lagrangian grid following the membrane displacement. One can cite the advected-field approach [21,22], level-set methods [23–26] and immersed boundary or immersed interface methods [27–34].

The immersed boundary method (IBM) was originally developed by Peskin et al. [35] and has since been extensively studied and applied to a wide variety of FSI problems. In a previous work, Mendez et al. [36] used the IBM to study fluid-structure interactions of deformable particles in flows at arbitrary Reynolds numbers, in the context of complex geometries often encountered when dealing with medical artificial devices. Since this work was only considering the 2D resolution, the main purpose of the present paper is to extend it to 3D. The IBM being originally developed to deal with zero volume structures, a membrane-like structure with an infinitely thin thickness can be considered, neglecting the bending stiffness of the membrane. Although suitable when modeling very thin capsules under flow [37,38], this approach reaches its limitations when considering membranes having a significant bending rigidity. To capture bending effects, an additional model based on the Helfrich energy [39] can be introduced (also used by Mendez et al. [36]), and has been notably used to model flowing capsules and red blood cells [40,41]. Another approach is the one introduced by Le and Tan [32], where the IBM is combined with a thin-shell model to simulate the deformation of liquid capsules under flow [32,42,33].

In the present paper, another approach to simulate flowing deformable membranes in the context of the IBM is proposed, the immersed thick boundary method (ITBM). This approach is inspired from the extended immersed boundary method (EIBM), introduced by Wang and Liu [29], and later adapted to the immersed finite element method (IFEM) [43,44]. Instead of the volumeless immersed boundary, a submerged solid which occupies a finite volume within the fluid domain is considered. This approach constitutes an alternative to the one consisting in combining the IBM with a thin shell model. Indeed, rather than representing implicitly the thickness of the membrane using a thin shell model (as Dupont et al. [45]), the thickness is represented in an explicit manner, modeling the membrane as a 3D continuum using the classical finite-element method. A full description of the ITBM is done in section 2. The use of a classical finite-element framework in the IBM is not generally employed for thin membranes. As a consequence, the present paper presents an extensive validation work in section 3, in order to thoroughly determine the real limitations of such an approach. The case of very thin membranes will be treated with particular attention. Note that the present approach is not limited to closed membranes. Both closed membranes and open membranes can be simulated using the ITBM, and an application to the flow through a tri-leaflet aortic valve is presented in section 4.

2. The immersed thick boundary method

In the IBM framework, two independent meshes are considered to discretize the solid domain Ω_s and the fluid domain Ω_f . The solid is discretized by a moving Lagrangian mesh, and the fluid is discretized by a fixed Eulerian mesh, which can be either structured or unstructured (Fig. 1). The different steps of the IBM are the following, as introduced by Peskin [27]:

- (1) Knowing the displacement $\overrightarrow{U_m}$ of each solid node *m*, the mechanical force $\overrightarrow{F_m}$ resulting from the membrane deformation is calculated,
- (2) The mechanical force $\overrightarrow{F_m}$ is regularized on the fluid mesh, resulting in a field of volumetric force $\overrightarrow{f_j}$, calculated on each fluid node *j*, which represents the forces exerted by the membrane on the fluid,
- (3) The Navier–Stokes equations (forced by the regularized mechanical forces) are solved on the fluid mesh, yielding the velocity of the fluid $\vec{v_j}$ on each fluid node *j*,
- (4) The velocity of the membrane $\overrightarrow{V_m}$ on each solid node *m* is interpolated from the $\overrightarrow{v_j}$ field, enabling to deduce the new position $\overrightarrow{X_m}$ from the position at the previous timestep $\overrightarrow{X_m}^{previous}$, such as $\overrightarrow{X_m} = \overrightarrow{X_m}^{previous} + \Delta t \overrightarrow{V_m}$. The displacement is then updated $\overrightarrow{U_m} = \overrightarrow{X_m} \overrightarrow{X_m^0}$, where $\overrightarrow{X_m^0}$ stands for the initial stress-free position, also referred to as the reference position.

In the present study, step (1) is performed by the LMGC90 solid mechanics solver [46], while steps (2)–(4) are performed by the YALES2BIO numerical tool [36,47,48] (http://www.math.univ-montp2.fr/~yales2bio/), based on a massively parallel unstructured finite volume flow solver for the incompressible Navier–Stokes equations [49]. Note however that steps (2) and (4) could be handled by a dedicated coupling program, in the case where modifications in the fluid solver cannot be easily performed. YALES2BIO being an in-house solver, this option was not considered further.

The main distinction between the IBM and the ITBM is that instead of having a cluster of solid nodes spread over a surface, the cluster defines a volume mesh (see Fig. 1). The different steps of the ITBM are detailed below.

2.1. Computation of the mechanical force

When considering immersed volumetric objects, as this is the case with the EIBM [29], the actual structural force to regularize is commonly composed of the internal mechanical force $\overrightarrow{F_m}$ resulting from the static deformation of the structure, and the inertial force $M\overrightarrow{U_m}$ resulting from the dynamics of the structure, the mass matrix M being written as:

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