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3D vesicle dynamics simulations with a linearly triangulated surface

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ABSTRACT

Simulations of biomembranes have gained an increasing interest in the past years. Specificities of these membranes propose new challenges for the numerics. In particular, vesicle dynamics are governed by bending forces as well as a surface incompressibility constraint. A method to compute the bending force density resultant onto piecewise linearly triangulated surface meshes is described. This method is coupled with a boundary element method solver for inner and outer fluids, to compute vesicle dynamics under external flows. The surface incompressibility constraint is satisfied by the construction of a projection operator.

1. Introduction

Simulation of moving interfaces into fluid flows is a long standing issue for Computational Fluid Dynamics (CFD). Many innovative methods such as Volume of Fluids (VOF), Immersed Boundaries (IBM), Front Tracking (FT), Phase Field (PF), Level Set (LS), Lattice Boltzmann (LB), were developed to handle simulation of multiphase flows. These methods have been widely used for the analysis of numerous problems where interfacial dynamics play a prominent role (solid–liquid and liquid–gas phase change, immiscible multifluid flows). With this background, attention is nowadays put towards behavior of biomimetic interfaces such as vesicles and capsules in different experimental environments, under stresses of various nature: mechanical [1], hydrodynamical [2,3], chemical [4,5], electrostatic [6]. Understanding and control of these microsystems are big challenges and have a lot of implications in biology or healthcare. Applications are as various as comprehending living systems at the cell scale, drug delivery vectorization, or exploiting those biomimetic systems for species carrier or microreactors in microfluidic processes.

Numerical simulations of these systems are simpler than multiphase flows simulations in some aspects since flows are most often limited to the Stokes regime. Moreover, phenomena involving topological changes (breaking, merging) are less crucial because of the nature of vesicle and capsule membranes, even if they are not absent for vesicles (exocytosis, fusion). Indeed, contrary to the separating surface between two fluids, these interfaces are made of a material which is different from the surrounding fluids and has structural mechanical properties (bending and membrane elasticity). It is this particular aspect which is challenging for CFD: the problem is very similar to a fluid–structure interaction problem, the structure being a very thin membrane (thickness is a few nm for a vesicle, to compare with a typical radius of 50 μm). At the system global

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scale, this membrane can be modeled as an interface, but has a much more rich behavior than a simple contact surface between two phases.

Vesicles and capsules can both be roughly described as bags enclosing a liquid (different or not from the suspending solution). Nevertheless, there is a big difference between vesicle and capsule membranes. The latter is composed of polymers forming a thin solid structure and its mechanical behavior is thus dominated by membrane elasticity. Hence, bending is often neglected in models although it has a crucial role for buckling. On the contrary, vesicle membrane is made of a lipid double layer, amphiphilic molecules being oriented with their hydrophilic head towards ambient fluid [7]. This organization, closely related to liquid crystals, gives vesicle membrane the properties of a two-dimensional incompressible fluid. It is thus bending rigidity that governs vesicle shapes, under the constraint of surface incompressibility.

Probably due to its importance in cellular biology, vesicle is the system which has been the most studied experimentally, theoretically as well as numerically. For numerical simulations, a distinction must be made between two levels of description: molecular scale modeling, typically used to study problems like the fusion of two small vesicles [8,9], and continuous scale modeling, to study problems involving more larger space and time scales like the deformation of a giant vesicle under shear flow [10,11] (and references therein). The numerical methods used are different as well. Molecular scale modeling is based on particle-dynamics, going from all atoms models (molecular dynamics simulations) to coarse-grained simulations [9,8]. In this kind of approach the macroscopic mechanical behavior (in the sense of continuous media) does not need to be introduced ab initio since it results from particles interactions. Given the actual capacity of computers, this level of description is not appropriate for the fluid–structure interactions that are looked at in CFD, even if many situations would require to combine descriptions at both scales.

The fluid–structure interaction problem for biomembranes involves two different numerical schemes: one to compute flows with boundary forces density imposed by the membrane, and the other to compute resultant force in the membrane due to its deformation by the flows. For the former, the flows considered being usually in the Stokes regime, it is possible to restrict the flows computations on the surface by a boundary integral method (BIM) and this is indeed the most used method for vesicle [12–18] and capsule [19–24] studies. For the latter, the membrane must be treated as a continuous material surface embedded in the euclidian 3D space, with mechanical properties encoding its molecular organization [25]. A vesicle or capsule membrane may then be considered as a thin shell, really thin and soft, especially for vesicles, with thickness being of the order of 4 nm and bending modulus of about $10k_BT$ (the membrane is sensitive to thermal fluctuations when it is not in a tensed state), where k_B is the Boltzmann constant and T the temperature. In this continuous media spirit, mechanical properties of vesicles and capsules may be separated into membrane effects (in-plane elasticity) and bending. Studies on capsules generally ignore the later [21,24,26–30], thanks to a thin shell hypothesis. As explained before, the situation for vesicles is somehow different, because of the prominent role of bending. Yet, several studies showed that bending for a capsule should be considered too [22,24,31–33]. Hence, modeling the flexural behavior is an issue for both kinds of system, although we will consider only the case of vesicles in the present study. Two issues are thus computationally challenging: bending computations and surface incompressibility.

Bending computation requires some computational efforts because the bending stresses are closely related to the geometry evolution. However, usual geometrical approximations cannot preserve every geometric properties of a real surface. On this specific point, one must set apart approaches where the interface is not explicitly represented in the model, such as PF and LS. The surface position is represented by an isovalue of a phase indicator function. Phase-field has been used for simulation of equilibrium shapes of vesicles [34–36], pearling phenomena [37], as well as vesicle behavior in external flows [38–40] or under electrical fields [41]. Relations between PF and LS, when applied to vesicle studies, have been underlined in [40]. To our knowledge, no studies of capsules with these methods have been attempted, probably because the history of membrane deformations is not easily accessible in these purely Eulerian approaches. On the other hand, such methods handle more easily topological changes like splitting or merging. Methods such as Immersed Boundary Methods may be classified as diffuse interface methods too. Indeed, ambient fluid flows are determined on a spatial mesh not conformal to the evolutive position of the interface. The forces the interface exert on fluids are then taken into account by diffusing them on the closest spatial mesh nodes. However, contrary to the PF or LS methods, they often use an explicit discrete representation of the interface to compute the forces, at least when they are applied to study vesicles or capsules [26,42,28,29]. The model developed by Noguchi and Gompper [43] must be cited aside. It is closely related to coarse-grained methods cited previously, but uses as well a triangulation of the interface for the computation of curvatures and bending forces.

Thus the most used strategy to take into account bending (and surface elasticity in general) is to introduce an explicit discrete representation of the interface and use this representation to compute the relevant geometrical quantities. This mesh can be either structured, either triangulated. Depending on the type of mesh, several numerical methods can be used. Structured meshes permit a global parametrization, and thus spectral methods can be used onto those [33]. A thin shell finite element approach can deal with structured as well as unstructured meshes. However, thin shell elements are not free of difficulties (shear blocking, membrane blocking etc.) [44], and the fluid nature of the lipid membrane (especially the fact that there is no in-plane stress other than an isotropic tension related to incompressibility) may introduce additional difficulties. Moreover, these elements have been developed such that displacements are computed for known imposed external forces. Here, one wants to compute resultant forces for imposed displacements. To our knowledge, no approach of this type has been attempted for vesicles, let alone with a coupling with a fluid solver.

We propose a method to compute bending forces onto a triangulated surface with C^0 regularity. Several simulations of vesicles have been performed with such meshes, however the computation of bending forces was based on a numerical