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A parallel overset-curvilinear-immersed boundary framework for simulating complex 3D incompressible flows

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ABSTRACT

We develop an overset-curvilinear immersed boundary (overset-CURVIB) method in a general non-inertial frame of reference to simulate a wide range of challenging biological flow problems. The method incorporates overset-curvilinear grids to efficiently handle multi-connected geometries and increase the resolution locally near immersed boundaries. Complex bodies undergoing arbitrarily large deformations may be embedded within the overset-curvilinear background grid and treated as sharp interfaces using the curvilinear immersed boundary (CURVIB) method (Ge and Sotiropoulos, J Comput Phys, 2007). The incompressible flow equations are formulated in a general non-inertial frame of reference to enhance the overall versatility and efficiency of the numerical approach. Efficient search algorithms to identify areas requiring blanking, donor cells, and interpolation coefficients for constructing the boundary conditions at grid interfaces of the overset grid are developed and implemented using efficient parallel computing communication strategies to transfer information among sub-domains. The governing equations are discretized using a second-order accurate finite-volume approach and integrated in time via an efficient fractional-step method. Various strategies for ensuring globally conservative interpolation at grid interfaces suitable for incompressible flow fractional step methods are implemented and evaluated. The method is verified and validated against experimental data, and its capabilities are demonstrated by simulating the flow past multiple aquatic swimmers and the systolic flow in an anatomic left ventricle with a mechanical heart valve implanted in the aortic position.

1. Introduction

Handling arbitrarily complex geometries and/or moving boundaries is a major challenge in simulations of real-life biological flows, which requires creative approaches for mesh generation and boundary condition implementation. Many methods, including Chimera overset grid [1,2], immersed boundary methods [3,4], level set methods [5,6], vortex methods [7,8], and penalization methods [9–11] have been developed and successfully applied to specifically address this challenge. In particular, major advances in immersed boundary methods, which are of interest in this work, have made it possible to efficiently study flow problems that are far more complicated than those that traditional computational fluid dynamics (CFD) methods (simple structured or unstructured grids) could handle in the past. Recent successful applications of immersed boundary methods include, among others, simulations of prosthetic heart valves [3,12–14], biofilming processes [15], flexible fibers [16], flapping filaments [17], aquatic swimming [18–20], vortex-induced vibrations [21], etc.

The most attractive feature of immersed boundary methods is the inherent separation of grid generation from the underlying geometry. The computational domain, which contains both the fluid and embedded solid regions, is discretized with a single, fixed, non-boundary conforming mesh system, most commonly a Cartesian grid. The effect of immersed boundaries is accounted for by adding forcing terms, either explicitly or implicitly, to the governing equations of fluid motion such that the presence of the appropriate boundary conditions at the location of the immersed boundaries are satisfied [3,4]. Depending on the specific approach employed to enforce the boundary conditions at immersed bodies, immersed boundary methods are typically classified as diffused [3,17,22] or sharp-interface methods [18,23–25]—see [4] for a recent review of various approaches. Despite many attractive features of the immersed boundary methods, a number of important limitations makes their application rather challenging for certain types of flows.

The first such limitation arises when applying an immersed boundary method to a flow problem involving moving bodies

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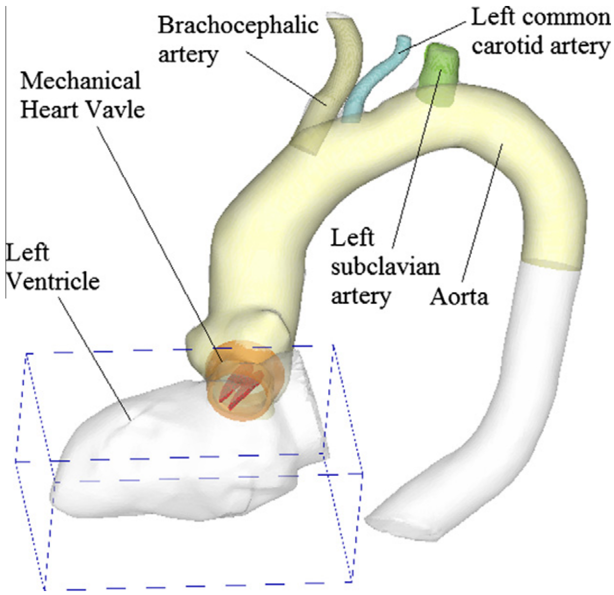

Fig. 1. Anatomical geometry of the left heart system consisting of multiple branching and large moving boundaries.

undergoing large displacements and/or complex multi-connected geometries. For example, when the immersed body is displaced within the background grid over large distances, such as in the case of a falling sphere or a swimming fish, the entire background grid region within which the body is displaced should be discretized with high numerical resolution, which could increase the computational costs considerably. This problem can be solved either by adaptively refining the grid following the motion of the swimmer [22,26–28], or, when appropriate, by choosing a non-inertial frame of reference with respect to which the displacement of the body is reduced or completely eliminated [29–31]. Immersed boundary methods in conjunction with the non-inertial reference frame formulation have indeed been used to reduce the computational cost in simulations of such problems [32,29,30]. Note that, however, it is obviously not possible to apply the non-inertial formulation to problems involving multiple moving bodies. Nevertheless, for problems involving a single moving body the non-inertial frame formulation is preferred over the adaptive grid method because of its overall simplicity and lower computational costs. Furthermore, efficient parallelization of an adaptive grid solver is not straight forward and continues to be the subject to active research [27]. The standard non-inertial frame formulation of the Navier–Stokes equations contains source terms for the translational, Coriolis, and centrifugal accelerations. Such source terms reduce the stability of the numerical algorithm. For that a conservative formulation has been proposed, which does not have source terms and has improved stability properties [31,33]. This formulation, however, has thus far been applied in conjunction with immersed boundary methods only on Cartesian grids [30].

The second limitation arises when the Cartesian-grid based immersed boundary methods are applied to internal flow problems, especially multi-branching configurations typically encountered in cardiovascular anatomies, pulmonary airways, etc. (Fig. 1). Although in such problems one could use the brute-force approach, namely discretizing the entire computational domain with a single structured background grid and embedding the entire complex geometry of the solid walls as an immersed body, such treatment results in a large number of wasted computational nodes located outside the regions of interest and is thus very impractical [34]. To overcome such difficulties different strategies have been proposed. One approach is to discretize the multi-connected domain using body-fitted unstructured grids [35,36] while another is to recast the structured Cartesian formulation into an unstructured Cartesian grid layout [34]. These methods, however, change the structured layout of the grid making it difficult to use efficient parallel structured solvers. A more versatile modeling paradigm, which we propose in this work, is to integrate the overset grid approach with structured curvilinear grids, and a sharp-interface immersed boundary method. For example, with reference to Fig. 1, the left ventricle, which undergoes large deformation during the cardiac cycle, is embedded in a background curvilinear grid and treated as an immersed boundary, the aorta may be discretized with a separate boundary-fitted curvilinear grid or also treated as an immersed boundary in a background curvilinear domain approximating the shape of the aorta, and the mechanical valve prosthesis or any other native or prosthetic aortic valve, which typically undergoes large displacement and/or deformation, is also treated as an immersed boundary. The background left ventricle and aorta grids overlap in the left-ventricle outflow track region and the solutions in these two sub-domains communicate using the overset grid approach. Such hybrid approach could be extended to include other blood vessels in the simulations, such as the subclavian and carotid arteries shown in Fig. 1, and used to model efficiently a broad range of complex internal flows with embedded immersed boundaries undergoing large displacement and/or deformation. It is the main objective of this paper to develop the computational infrastructure required to achieve such general and versatile modeling paradigm.

In traditional overset grid formulations, pioneered by [37–40,1], a complex flow domain is decomposed into a set of simpler, overlapping subdomains such that it can be discretized easily with a set of simple, boundary conforming, curvilinear coordinates [41]. The governing equations are solved independently on each subdomain and information from one subdomain is transferred to another subdomain by specifying the boundary conditions at their interfaces [42,41]. Our method only requires the mass (or volume) flux at the boundaries, i.e., only the mass flux is exchanged at the boundaries and it is corrected to satisfy the conservation of mass on each subdomain. This is similar to the flux-exchange method [43–46] (not the state-exchange method based on domain decomposition [47–49]) employed in coupling continuum and molecular dynamics domains in multi-scale simulations [50]. More specifically, the flux-exchange method is based on the direct exchange of flux information in the overlap domain between the particle region and the continuum region, and relies on the matching of fluxes of mass, momentum and energy [48]. In the state-exchange method the state information between the particle simulation and the Navier–Stokes equations is transferred through an overlap region where the particles' dynamics is constrained; the constrained dynamics is often imposed via a dynamic relaxation technique [48].

The simplest approach to specify the boundary conditions at the interface is to interpolate all the variables from one subdomain to the other [1,51,2,52]. Such interpolation, however, does not necessarily satisfy global conservation, and for that a critical aspect of the overset grid method is the development of conservative interpolation schemes [41,42,53–56]. However, if a fractional step method is used to advance the incompressible flow governing equations in time the intermediate velocities are not conservative quantities—do not satisfy mass conservation. Therefore, any type of conservative interpolation from such non-conservative velocities cannot satisfy global mass conservation. Consequently, an explicit mass-imbalance correction needs to be added to the interpolated velocity field to ensure global mass conservation on each overlapping grid. Zang and Street [57] add such an explicit correction, which is proportional to the local flux at each cell, and Burton and Eaton [58] add an explicit correction, which is proportional to the local area