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Accurate, robust and efficient multiphysics - methods for the simulation of three-dimensional complex problems with immersed boundaries from engineering as well as biophysics are a highly interesting and challenging research area. Within this context, our motivation was to develop a general framework to solve a variety of multiphysics problem classes such as fluid-structure interaction (FSI) [1] - [5] as well as multiphase-flow/combustion problems [6]. Special focus was put on a clear interface formulation on fixed grids, a highly accurate resolution of flow patterns around the interface, as well as the ability to impose arbitrary boundary conditions at the interface - features, which current Immersed Boundary Methods are still suffering from.

In this abstract we want to concentrate on the fluid-structure interaction approach with application to biophysical problems during the production process of novel spider silk materials. The described 2-field FSI approach allows the simulation of incompressible Navier-Stokes equations and does not pose any limitations to material and geometrical nonlinearities in the structure. The fluid field is described by an Eulerian formulation on a fixed fluid grid. A Lagrangian description is applied to the structure on a separate deformable mesh.

The structural surface introduces an explicitly given interface, which can arbitrarily deform and move through the fixed fluid background grid. This interface divides the fluid mesh into a physical and a fictitious domain. The latter does not require any fluid computations. We propose an accurate, robust and efficient algorithm for the localization of possibly curved interfaces [1]. In addition, the subtetrahedralization of an intersected fluid element, which is required for exact numerical integration, is explained. The EXtended Finite Element Method (XFEM) is applied here to model velocity and stress discontinuities within a fluid element, which is intersected by the structural interface.

In the regime of high Reynolds numbers, an additional deforming Arbitrary Lagrangian Eulerian (ALE) grid patch may be coupled to the structure in order to resolve moving boundary layers highly accurately [2, 3]. A further challenge poses the FSI-coupling due to non-matching meshes. We developed a novel Lagrange multiplier technique to embed Dirichlet conditions at the interface in the non-matching fluid mesh [5]. This formulation allows a full condensation of Lagrange multipliers at the element level and enables the application of fast iterative Algebraic Multigrid solver. The fluid discretization does not impose any restriction to the element size of the structural mesh. Different efficient fluid - structure coupling algorithms can be found in [7, 8].

All mentioned methods are implemented in our massively parallel research code ”Baci” developed at the Institute for Computational Mechanics at Technische Universität München.

Particular interest lies currently in the application of the FSI-approach to the simulation of mesoscopic biophysical problems such as suspensions [9]. The production of drug delivery systems made from spherical spider silk macromolecules in suspension, so-called hydrogels, are a highly active research area in experimental physics. Our work concentrates on providing a computational approach in order to optimize and refine the understanding of this process. To take the interaction and contact of mesoscopic structures into account, we combine a macroscopic contact formulation with a Finite Element formulation of interaction potentials (see Figure 1). Experimental validation of numerical results is performed by comparing them to the behaviour of hydrogel suspensions during the actual production of novel drug delivery systems. Further development will focus on an extension of the FSI-approach to include Brownian motion of mesoscopic structures.
Figure 1: Two parabolic inflow profiles on each side of the channel push both hydrogel structures together. The repulsive regime of an interaction potential prevents contact and causes deformation of the structures.

References


[8] Küttrler U., Wall W.A.; Fixed-point fluid-structure interaction solvers with dynamic relaxation; Computational Mechanics (Springer); 61-72; 2008