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Numerical simulation of a compound capsule in a constricted microchannel

John Gounley[1], Erik W. Draeger[2], and Amanda Randles[1]

[1] Department of Biomedical Engineering, Duke University, Durham, NC
john.gounley@duke.edu, amanda.randles@duke.edu

[2] Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA
draeger1@llnl.gov

Abstract

Simulations of the passage of eukaryotic cells through a constricted channel aid in studying the properties of cancer cells and their transport in the bloodstream. Compound capsules, which explicitly model the outer cell membrane and nuclear lamina, have the potential to improve computational model fidelity. However, general simulations of compound capsules transiting a constricted microchannel have not been conducted and the influence of the compound capsule model on computational performance is not well known. In this study, we extend a parallel hemodynamics application to simulate the fluid-structure interaction between compound capsules and fluid. With this framework, we compare the deformation of simple and compound capsules in constricted microchannels, and explore how deformation depends on the capillary number and on the volume fraction of the inner membrane. The computational framework's parallel performance in this setting is evaluated and future development lessons are discussed.

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1 Introduction

The passage of eukaryotic cells flowing through a constriction has several applications, including the study of cancer cells. Microfluidic devices with constricted channels are used to study how single or clustered cancer cells pass through narrow capillaries in blood flow [1]. Similar microfluidic devices are used to study the properties of cancer cells themselves [2]. Finally, the process by which cancer cells extravisate from the blood stream includes passage through narrow intercellular openings in the endothelial layer [28]. Numerical simulations of all three applications have the potential to complement and extend *in vitro* studies, by clarifying the role of a single physical parameter in a complex process or exploring regions of the parameter space that are otherwise difficult to access.

Computational studies of cell deformation have generally focused on red blood cells and other non-eukaryotic models. A common paradigm, developed for red blood cells, has modeled

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cells as fluid-filled capsules surround by a single zero-thickness [13, 7] or finite thickness [6] membrane. Simulations of red blood cells passing through a constricted microchannel have been validated [20] and extensively studied (e.g., [14]). However, the discoidal shape, lack of a nucleus, and high membrane incompressibility of red blood cells may preclude the direct extension of their behaviour in constricted microchannels to eukaryotic cells.

Single membrane models have also been used to model eukaryotic cells [18, 12]. Recent studies have sought to improve model fidelity for eukaryotes by explicitly including the nucleus with a compound capsule model. In a compound capsule, the outer cell membrane and nuclear lamina are modeled with two separate membranes. As opposed to the simple (single) capsule used for red blood cells, the two membranes are uncoupled and may be modeled with different physical properties. Luo *et al* used a front-tracking method to simulate the deformation of an elastic compound capsule in shear flow [16]. These results were extended from initially spherical to ellipsoidal compound capsules, the dynamics of which were investigated in depth [15]. Similar compound models have been developed for vesicles [26, 11] and droplets [25, 29].

Initial applications have used compound capsules to simulate the passage of a eukaryote through a constricted microchannel. Using dissipative particle dynamics, Xiao *et al.* showed that a stiff inner membrane can preclude the passage of a compound capsule through a constriction [28]. Casquero *et al.* performed a two-dimensional simulation and observed deformation of the inner membrane to be highest at the exit of the narrowed region [3]. However, only a single, proof-of-concept compound capsule simulation was conducted in these studies.

Further, it is not well understood how the addition of a second membrane representing the nucleus alters the computational cost or parallel performance of the fluid-structure interaction (FSI) simulation, as previous performance studies have focused on red blood cells (e.g., [5, 23, 17]). Intuitively, the addition of a second membrane may increase FSI- and capsule-related computation by as much as 100%. Further, compound capsules seem to require higher fluid grid resolutions than simple capsules, even in shear flow [16]. These potential increases in computational expense underscore the importance of efficient parallel codes for FSI.

HARVEY is a massively parallel computational fluid dynamics solver, focused on hemodynamics and based on the lattice Boltzmann method [21, 22]. In this paper, we integrate HARVEY with FSI-functionality, using the immersed boundary method to couple a finite element model for deformable capsules to the fluid model. We discuss how the parallelization strategy for the FSI framework builds on existing HARVEY parallelism. The code is used to simulate passage of simple and compound capsules through a constricted microchannel, comparing results from simulations with and without an inner membrane to quantify the influence of the 'nucleus' on capsule deformation during transit of the constriction. We study the dependence of compound capsule deformation on the capillary number and on the inner capsule's volume fraction. Finally, we evaluate the parallel performance of the FSI solver in this setting.

2 Methodology

2.1 Lattice Boltzmann

The lattice Boltzmann method (LBM) is a deterministic, mesoscopic approach to numerically solve the Navier-Stokes equations [4]. The fluid is represented as a particle distribution function $f_i(\mathbf{x}, t)$, which denotes the number of particles at grid point $\mathbf{x}$ at time t with discrete velocity $\mathbf{c}_i$. The evolution of distribution f is governed by the lattice Boltzmann equation,

$$f_i(\mathbf{x} + \mathbf{c}_i\delta t, t + \delta t) = f_i(\mathbf{x}, t) - \Omega\Big(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\Big) + \delta t F_i(\mathbf{x}, t). \tag{1}$$