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Chromodynamic Lattice Boltzmann Method for the Simulation of Drops, Erythrocytes, and other Vesicles

J. Spendlove[1,2], X. Xu[1,2], T. Schenkel[1,2], J. P. Gunn[3] and I. Halliday[3,*]

[1] *Department of Engineering and Mathematics, Sheffield Hallam University, Howard Street, S1 1WB, UK.*
[2] *Materials & Engineering Research Institute, Sheffield Hallam University, Howard Street, S1 1WB, UK.*
[3] *Department of Infection, Immunity and Cardiovascular Disease, The Medical School, Beech Hill Road, Sheffield, S10 2RX, UK.*

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Abstract. Recently, we have validated a three-dimensional, single framework multicomponent lattice Boltzmann method, modified to generate vesicles (rather than drops) ["Three-dimensional single framework multicomponent lattice Boltzmann equation method for vesicle hydrodynamics," Phys. Fluids 33, 077110 (2021)]. This approach implements an immersed boundary force distribution, characterised by bending rigidity, surface tension, preferred curvature and conserved membrane area, in which work we successfully validated isolated vesicle flows against other methodologies and experiment. Like most immersed boundary algorithms, our method relies on numerical computation of high-order spatial derivatives and an intricate body force density. The next step is to verify that it has sufficient numerical stability to address the anticipated application of high volume fraction flows of highly deformable objects in intimate interaction. It is this *in silico* verification – of both the class of fluid object attainable and the stability of the later in strong, straining and shearing flows which is at issue, here. We extend our method to simulate multiple variously deflated vesicles and multiple liquid droplets still within a single framework, from which our fluid objects emerge as particular parameterisations. We present data from simulations containing up to four vesicles (five immiscible fluid species), which threshold verifies that simulations containing unlimited fluid objects are possible ["Modeling the flow of dense suspensions of deformable particles in three dimensions," Phys. Rev. E 75, 066707 (2007)]. These

*Corresponding author. *Email addresses:* `i.halliday@sheffield.ac.uk` (I. Halliday), `James.Spendlove@student.shu.ac.uk` (J. Spendlove), `xu.xu@shu.ac.uk` (X. Xu), `T.Schenkel@shu.ac.uk` (T. Schenkel), `j.gunn@sheffield.ac.uk` (J. P. Gunn)

data also assure the ability of our immersed boundary forcing to preserve the character and integrity of fluid objects in interactions characterised by large local velocity gradients (intimate squeezing, shearing and elongational straining). Throughout, we take interfacial or membrane area, A, as a proxy for stability and physical veracity.

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1 Introduction

Advances in novel computational fluid dynamics (CFD) methodology hold-out the meaningful prospect of complex, three-dimensional time-dependent simulations of fluid objects, such as vesicles, cells and other suspended, neutrally buoyant entities, which deform when they advect, i.e., exhibit intimate coupling to any motion of the embedding, or background fluid. Of course, the complexity of what we designate fluid objects is variable, spanning for example:

– Deflated vesicles (i.e., erythrocytes), which have locally inextensible membranes, with bending rigidity, surface tension and, not least, a significant excess of conserved membrane area.

– Capsules, which contain in-plane shear elasticity (beyond the scope of the present work, but also have extensible interfaces with embedding fluid [1]).

– Drops, being the simplest fluid object, having an extensible interface governed only by interfacial tension.

A common feature of these objects is that all are filled with incompressible fluid, of a density similar to that of the embedding, background fluid. Furthermore, the interface or membrane is regarded as discontinuous (i.e., very narrow), when the fluid object is treated within the continuum regime of fluid mechanics [2].

The rheology of a wide range of complex fluids, defined as having emergent properties which rest upon their composition at the micron scale (which still lies within the continuum regime, of fluid dynamics, note) is of central importance in physiology, biomedicine, chemical engineering, food rheology, material science and bio-engineering applications *inter alia*. The simulation of liquid drops has high importance, e.g., in the emerging study of liquid drops' impact upon and wetting of the elastic surfaces of new materials [3]. Other fluid objects with small deflation and conserved membrane area widely serve as cell proxies and are frequently found in food processing and pharmacological flows [4]. Finally, the simulation of vesicles being of unquestionable importance