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Hemocell: a high-performance microscopic cellular library

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Abstract

We present a high-performance computational framework (Hemocell) with validated cell-material models, which provides the necessary tool to target challenging biophysical questions in relation to blood flows, e.g. the influence of transport characteristics on platelet bonding and aggregation. The dynamics of blood plasma are resolved by using the lattice Boltzmann method (LBM), while the cellular membranes are implemented using a discrete element method (DEM) coupled to the fluid as immersed boundary method (IBM) surfaces. In the current work a selected set of viable technical solutions are introduced and discussed, whose application translates to significant performance benefits. These solutions extend the applicability of our framework to up to two orders of magnitude larger, physiologically relevant settings.

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1 Introduction

On the cellular level, blood is a complex suspension constituted of a continuous fluid phase (the plasma) and several types of suspended cells. The accurate modelling of the emerging transport phenomena of such a system is of utmost importance to progress our understanding of several in-vivo processes, e.g. thrombus formation, appearance of non-Newtonian viscosity, margination of platelets, the Fåhræus effect, appearance of a cell-free layer, or the scaling properties of shear-induced diffusion of red blood cells (RBCs) [1]. Such complex systems dealing with large amount of cells ($> 10^4 - 10^6$ cells) provide several computational challenges, such as the set up of the initial conditions for the cells or the storage of the resulting data, or simply the raw processing power required by the simulations. In Hemocell, the plasma is represented as a continuous fluid simulated with the use of Palabos [2], an open-source LBM solver. The cells are represented as surfaces modelled by DEM membranes coupled to the plasma flow through

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a tested in-house immersed-boundary implementation [3, 4], where we demonstrated that the simulation can be scaled up to 10^6 cells executing on 8192 cores without significant loss of parallel efficiency. The implementation itself is designed to be very flexible and applicable in various scenarios. In the following we discuss how we have further improved the computational performance of Hemocell by separating the time-scale of the material model integration from that of the fluid dynamics and by pre-computing a randomised dense packing of red blood cells to provide improved initial conditions.

2 Methods

Initial conditions for cellular flows are usually not trivial. An uniform packing of cells can be easily calculated using their bounding-boxes as a basis for packing space requirement. RBCs, however, have a unique biconcave shape that fills the bounding box with a low volume ratio. The usually applied term that describes the surface [5, 6] is as follows:

$$y = R\sqrt{1 - \frac{x^2+z^2}{R^2}}\left[c_0 + c_1\frac{x^2+z^2}{R^2} + c_2\frac{(x^2+z^2)^2}{R^4}\right],$$

where $(R, c_0, c_1, c_2) = (3.91\mu m, 0.1358, 1.001, -0.5614)$. If we aim to fill a rectangular domain with rectangular bounding boxes, in fortuitous cases the volume fill ratio (Φ_{BB}) might go up to a 100%. On the level of RBCs within the bounding boxes, this yields $\Phi_{RBC} \approx 32\%$ which might be far from the desired value since physiologic blood has a hematocrit (Φ_{RBC}) of approximately 45%. If non-rectangular domains are considered, e.g. in the case of flows in smaller vessels, this ratio might fall even lower. In our approach, we present a possible solution using a kinematic simulation of encompassing ellipsoids to effectively generate dense cell distributions with random positions and alignments. The diameters of the ellipsoid for the RBCs are $(D_x, D_y, D_x) = (2.5\mu m, 1.2\mu m, 2.5\mu m)$. The overlap of the RBC shape and the encompassing ellipsoid is shown in Fig. 1.

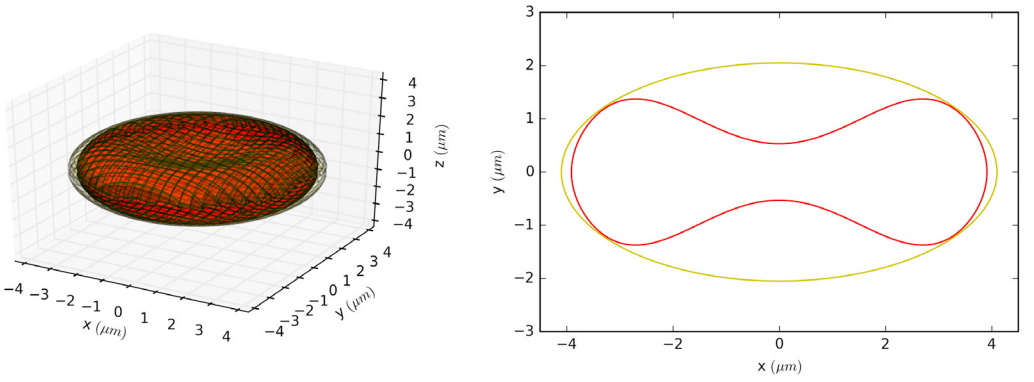

Figure 1: Left: 3D view of enclosing ellipsoid (yellow) overlayed on an RBC (red). Right: cut-plane visualising the volume fill ratios using the same colours for the contours.

Naturally, the enclosing ellipsoid has a larger volume than the RBC itself, therefore the above mentioned optimal rectangular bounding-box packing in case of $\Phi_{BB} = 100\%$ translates