In-silico modelling of accurate blood transport characteristics

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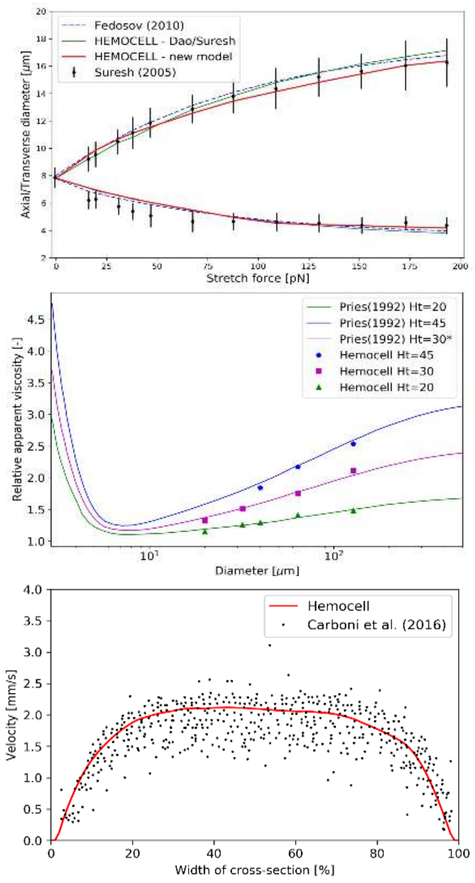
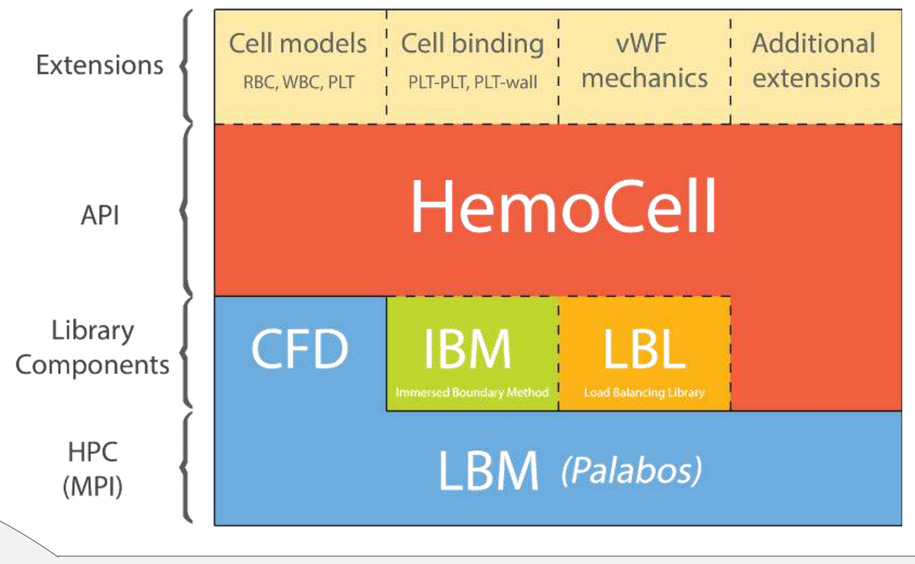
Validation of cell mechanics



- We introduced a new mechanical model for the RBCs. It extends on the ideas of previous models: we assume that the cytoskeleton has a role in every large enough deformation of the membrane. This cell mechanical model, detailed in [1], was validated against optical tweezer experiments (top figure) and shear flow measurements.
- The emerging transport properties reproduced the apparent viscosity in straight tubes accurately at various hematocrit levels (middle figure). They also reproduced the expected cell-free layer and the margination of platelets.
- Finally, the velocity profile in a rectangular channel was matched against the results of recent video microscopy measurements (bottom figure).

Structure and extensibility

The software framework is called *HemoCell* and it is targetted at dense cellular flow simulations. The plasma is represented as a continuous fluid simulated with the lattice Boltzmann method (using Palabos, an open source LBM library), while the cells are represented as discrete element method (DEM) membranes coupled to the fluid flow by the immersed boundary method (IBM). The framework is designed to be easily extendable with additional cell types and biochemical fields interacting with the blood flow.

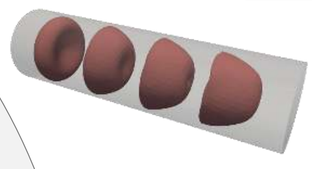


Application for medical devices

The framework can be applied to compute transport mechanics in micro-medical devices, such as flow diverters (in top figure) or lab-on-a-chip type microfluidic systems. It can provide insight on bulk flow properties such as viscosity, or on specific cell trajectories.

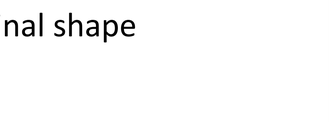
https://www.hemocell.eu

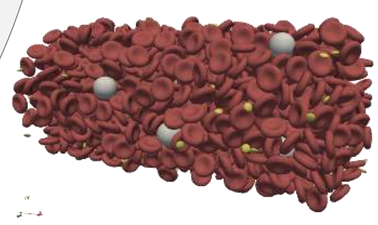
Single-cell mechanics



In small capillaries, the RBCs take up a “parachute” shape as they traverse the channel.

RBC cytoplasm has a five times higher viscosity compared to the surrounding plasma. It affects fast collisions and the characteristic time to regain the original shape after collision.

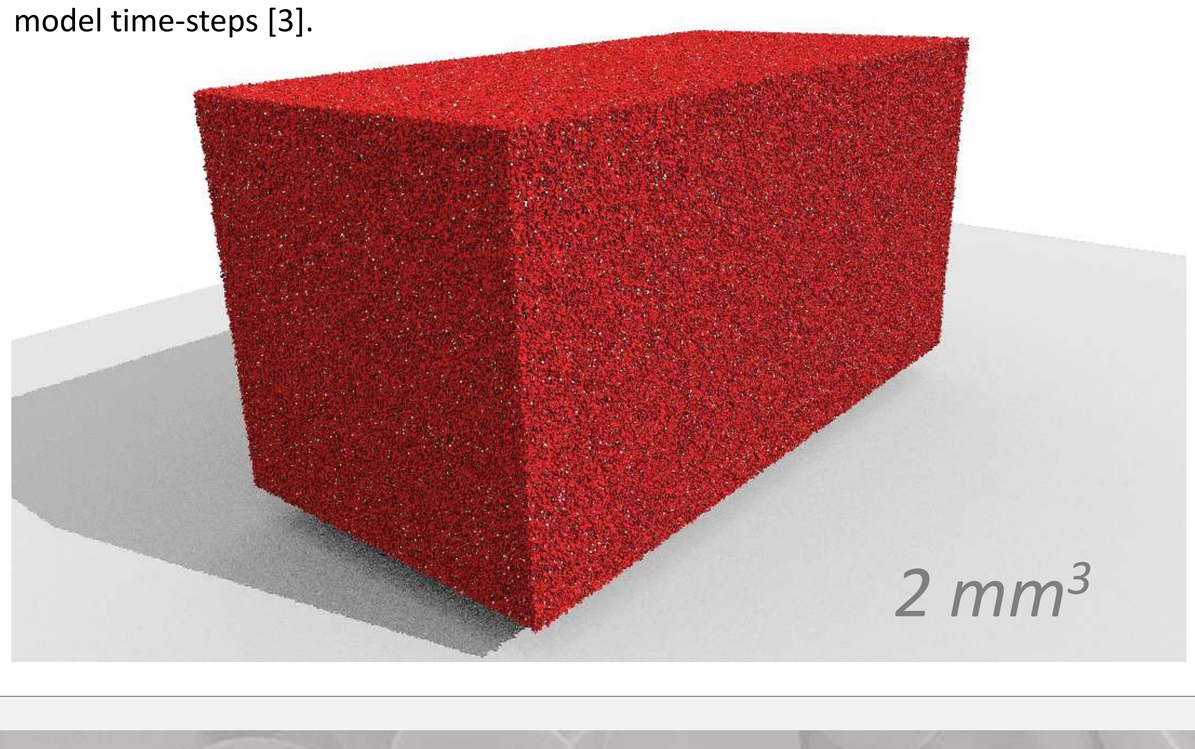




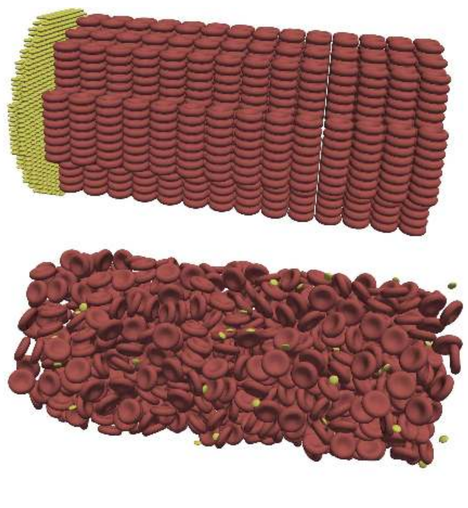
Additional cell types are also available, such as white blood cells with distinct material models.

Performance and scaling

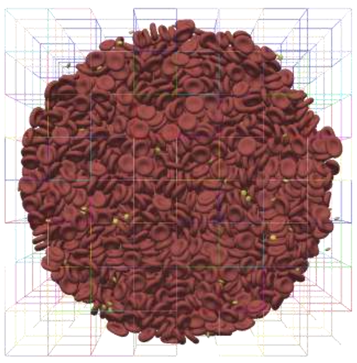
HemoCell exhibits excellent scaling properties over thousands of cores [2].
It is possible to scale the simulated system up to millions of cells (in the figure: over 8 million cells filling a 2 mm^3 volume). The high performance was achieved through rigorous code optimisations and the adaptivity of the constitutive model time-steps [3].



Initialisation and load-balancing



HemoCell uses a kinetic simulation of hard ellipsoids (enclosing the cells) to generate randomised, well mixed initial positions for the cells [3]. This can substantially reduce the simulation costs by shortening the ”warm-up” phase. In our typical simulations, this shaves off ~30% of the total computational time.



During the simulation, the local hematocrit is not constant due to geometry and varying shear and cell deformations. As a consequence, a significant load difference can arise between the subdomains during the computation. *HemoCell* dynamically checks for this imbalance and redistributes the subdomains to reduce computational time.

[1] Závodszky, G. et al. Cellular level in-silico modeling of blood rheology with an improved material model for red blood cells. *Frontiers in Physiology, 2017.*
[2] Mountrakis, L. et al. Parallel performance of an IB-LBM suspension simulation framework. *Journal of Computational Science, 2015.*
[3] Závodszky, G. et al. Hemocell: a high-performance microscopic cellular library. *Procedia Computer Science, 2017.*

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