A new multi-component model to simulate the single red blood cell behaviour

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Abstract

We present a new mathematical/computational formulation for a multicomponent model to study normal and pathological behaviour of red blood cells in slow transient processes. We take into account (i) the lipid bilayer behaviour, (ii) the cytoskeleton dynamics, (iii) the interaction activity between them, and (iv) the internal cytoplasm flow.

The formulation considers the cytoskeleton as a discrete non-linear elastic structure. The first novelty is to couple it with continuum models of the lipid membrane and of the cytoplasm, instead of the usual discrete/particle models [1 - 5]. The second novelty is that the interaction of the cytoskeleton with the membrane is through adhesion forces adapted from efficient solid-solid adhesion algorithms.

The model is tested with virtual experiments such as relaxation towards equilibrium and stretching by optical tweezers.



Figure 1 Snapshot of the RBC system after the relaxation process. The lipid bilayer is visualized in red scale according to the curvature magnitude. A section of the internal fluid is displayed in sky-blue, according its pressure value. Indeed, the cytoskeleton network is plotted. The spectrin colors are referred to the edge tension.



Figure 2 Visualization of lipid bilayer velocity field and cytosol pressure field during the stretching process, performed by our model with and without cytosol. The transparency allows to see the cytoskeleton in the upper figures.

References

1. Li, X., Peng, Z., Lei, H., Dao, M., & Karniadakis, G. E. (2014). Probing red blood cell mechanics, rheology and dynamics with a two-component multi-scale model. *Phil. Trans. R. Soc. A*, 372(2021), 20130389.

2. Chang, H. Y., Li, X., Li, H., & Karniadakis, G. E. (2016). MD/DPD multiscale framework for predicting morphology and stresses of red blood cells in health and disease. *PLoS computational biology*, 12(10), e1005173.

3. Fu, S. P., Peng, Z., Yuan, H., Kfoury, R., & Young, Y. N. (2017). Lennard-Jones type pair-potential method for coarse-grained lipid bilayer membrane simulations in LAMMPS. *Computer Physics Communications*, 210, 193-203. 4. Rodrigues, D. S., Ausas, R. F., Mut, F., & Buscaglia, G. C. (2015). A semiimplicit finite element method for viscous lipid membranes. *Journal of Computational Physics*, 298, 565-584.

5. Tang, Y. H., Lu, L., Li, H., Evangelinos, C., Grinberg, L., Sachdeva, V., & Karniadakis, G. E. (2017). OpenRBC: a fast simulator of red blood cells at protein resolution. *Biophysical journal*, 112(10), 2030-2037.