Modeling sickle cells

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Sickle cell disease is a genetically inherited condition, in which a single amino acid change causes hemoglobin proteins to aggregate into stiff rods inside the red blood cells. Under certain conditions, regulated by oxigen concentration, these rods become very long, reach and deform the cell membrane, and the normally disk shaped red blood cells eventually become very distorted with protrusions. The fluid dynamic flow properties of the distorted cells significantly differ from the healthy ones, and can cause small blood vessels to jam. The resulting oxigen depletion increases the rate of hemoglobin aggregation, which causes very painful crises in patients.

The aim of this miniproject is to develop a numerical model of the formation of the deformed cells. One possibility is to use the MultiParticle Collision Method (MPC) to model the fluid both inside and outside the cell membrane, use deformable lattice for the cell membrane, and develop some model for the aggregation of hemoglobin into relatively stiff (but still elastic) rods. Expected results include numerical determination of the deformed shapes, and possibly an early investigation of the flow properties. The project has in principle prospects to develop into a PhD project, with focus on flow properties and faithful representation of the actual biological system.

The work is numerically oriented and involves significant amount of programming. A code for 3d MPC (without the membrane) will be provided, but work can also start from freely available MD codes if preferred.



Normal as well as sickle-shaped red blood cells [wikipedia].