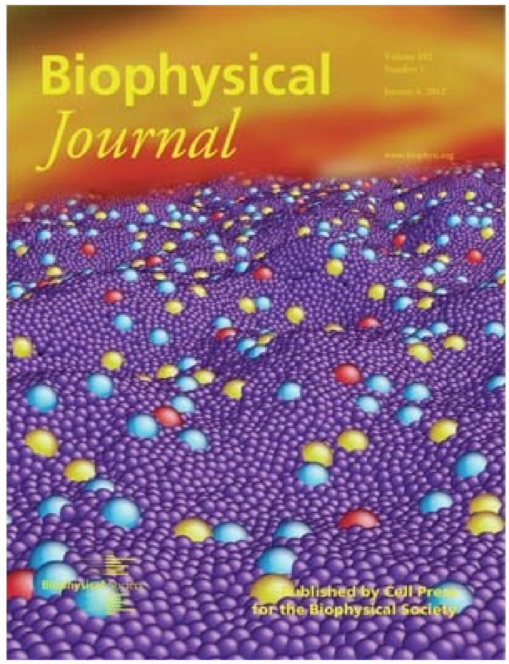
biophysicalsociety

Official blog of the Biophysical Society

Where Science Meets Art with BiophysJ Author George Lykotrafitis

Posted on January 3, 2012 by biophysicalsociety

Biophysical Journal *author George Lykotrafitis, Assistant Professor of Mechanical Engineering at the University of Connecticut, discusses the image he created for the cover of the latest issue of* BiophysJ.



In our lab, we develop computational models and perform experiments at the cellular level to study quantitatively how diseases affect the chemomechanical properties and structure of human cells. Our main focus is sickle cell disease, a hereditary blood disorder caused by a one point mutation in the gene that encodes adult hemoglobin. In the deoxygenated state, the defective hemoglobin (Hemoglobin S) polymerizes to form stiff hemoglobin fibers which interact with the erythrocyte membrane and alter its properties. As a result, the erythrocytes of patients with sickle cell disease are stiffer and more adherent than normal erythrocytes while they have an abnormal sickle shape in the deoxygenated state.

In this article, we present a solvent-free coarse-grain molecular dynamics model for the membrane of normal human erythrocytes. The model combines the lipid bilayer and the erythrocyte cytoskeleton, thus exhibiting both the fluidic behavior of the lipid bilayer and the elastic properties of the erythrocyte cytoskeleton. Three types of coarse-grained particles are introduced to represent clusters of lipid molecules, actin junctions and band-3 complexes. An in-house developed parallel molecular dynamics program is used for the work. The proposed model is part of a larger effort to simulate the biomechanical behavior of sickle red blood cells.

Visualization of molecular dynamics simulations is an essential part of the postprocessing of the numerical results. Here, we employ AtomEye as a visualization tool. The red particles represent actin junctions, the yellow particles represent band-3 complexes attached to the spectrin tetramer, and the light blue particles represent free band-3 complexes. The smaller particles correspond to the lipid bilayer. While the original file was created by using AtomEye, the image was enhanced by digital processing. The original length scales of the image were preserved. The artist Xiaohong (Lucia) Liao (PhD) helped us to create an artistically interesting composition.

All in the lab feel great pleasure that our image is selected for the cover of the *Biophysical Journal*. We believe that it will increase the visibility of this particular work and of our research in general. Please visit the website of the Cellular Mechanics Laboratory at the University of Connecticut for more information on our research and on our outreach activities.

Posted in BiophysicalJournal | Tagged AtomEye, BiophysicalJournal, CellularMechanicsLaboratory, hemoglobin, sicklecelldisease, UniversityofConnecticut comment