A Coarse-Grain model for Red Blood Cell membrane

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Abstract

We present a novel coarse-grained model with high computational efficiency for simulating the membrane of human red blood cells comprising a fluid lipid bilayer coupled to a spectrin network. The model for the lipid bilayer is solvent-free and the inter-grain interaction potential is anisotropic. The model also allows free diffusion of membrane agents. By simultaneously invoking these three characteristics, the proposed method facilitates simulations that span much larger length-scales (~ μm) and time-scales (~ ms) than currently possible with other methods based on classical molecular dynamics models or other coarse-grain approaches. The spectrin cortex is represented by a six-fold symmetric network whose elements follow the Worm-Like Chain model with adjustable connectivity. This model naturally facilitates comprehensive simulations of a wide spectrum of biophysical responses of human red blood cells that strongly influence a variety of human disease states.

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