

Abstract Submitted  
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**Multi-scale Simulation of Receptor-Ligand-Mediated Adhesion of Two (PMN) Leukocytes** VIJAY GUPTA, UMBC, KOSTAS KONSTANTOPOULOS, The Johns Hopkins University, CHARLES EGGLETON, UMBC — Leukocytes are recruited from the bloodstream to the site of inflammation through interactions between cell surface receptors and complementary ligands expressed on the surface of the endothelium. PMNs rolling on activated endothelium can mediate secondary capture of PMNs flowing in the free stream through homotypic interactions. This interaction is mediated by L-selectin binding to PSGL-1 between the free-stream and adherent PMNs. Both L-selectin and PSGL-1 molecules are concentrated on the tips of PMN microvilli. It has been demonstrated that steady application of a threshold level of shear rate is necessary to support PMN homotypic aggregation in bulk suspension. A reduction of shear rate below a threshold value diminishes the probability of cell adhesion. Cell aggregation is a complex phenomenon involving the interplay of bond kinetics and hydrodynamics. We simulate PSGL-1–L-selectin-mediated homotypic leukocyte adhesion-dissociation under an externally applied force field using the Immersed Boundary Method. We investigate the influence of membrane elasticity and kinetic parameters on contact area, bond dynamics, average number of bonds formed and their respective life time. A Hookean spring model is used to characterize receptor-ligand bonds and their stochastic nature is simulated using the Monte Carlo technique.

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