1128-92-325 Prashanta Dutta\*, Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164, Deng Hua, Mechanical and Materials Engineering, Pullman, WA 99164, and Jin Liu, Mechanical and Materials Engineering, Pullman, WA 99164. Mesoscale stochastic modeling of receptor-mediated bioparticle transport.

Internalization of bioparticles, such as viruses and drug carriers, through receptor-mediated endocytosis (RME) plays essential roles in fundamental understanding of viral infections and targeted drug deliveries through blood brain barrier. RME of bioparticles is a highly complex process that may involve hundreds of proteins. The overall process is dictated by collective and cooperative interplay of many dynamic events, such as particle motion, membrane deformation, receptor diffusion, as well as molecular scale protein-protein and protein-lipid interactions. In this talk, we present a mesoscale stochastic computational model for the receptor-mediated endocytosis based on Metropolis Monte Carlo method. The model is a combination of a stochastic binding model with a mesoscopic membrane model based on the discretization of Helfrich Hamiltonian on a curvilinear space. Using our model, we will discuss two important biological processes involving RME: the entry of herpes simplex virus with the absence of clathrin and the internalization of trasferin-coated nanoparticles into endothelial cells with the existence of clathrin. Through these two examples, we investigate the key roles of particle size, ligand/receptor density and type, and the clathrin on RME. (Received February 28, 2017)