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Modelling Protein-induced Membrane Deformation using Monte Carlo and Langevin Dynamics Simulations[1] R. RADHAKRISHNAN, N. AGRAWAL, University of Pennsylvania, N. RAMAKRISHNAN, P.B. SUNIL KUMAR, Indian Institute of Technology Madras, J. LIU, University of Pennsylvania — In eukaryotic cells, internalization of extracellular cargo via the cellular process of endocytosis is orchestrated by a variety of proteins, many of which are implicated in membrane deformation/bending. We model the energetics of deformations membranes by using the Helfrich Hamiltonian using two different formalisms: (i) Cartesian or Monge Gauge using Langevin dynamics; (ii) Curvilinear coordinate system using Monte Carlo (MC). Monge gauge approach which has been extensively studied is limited to small deformations of the membrane and cannot describe extreme deformations. Curvilinear coordinate approach can handle large deformation limits as well as finite-temperature membrane fluctuations; here we employ an unstructured triangular mesh to compute the local curvature tensor, and we evolve the membrane surface using a MC method. In our application, we compare the two approaches (i and ii above) to study how the spatial assembly of curvature inducing proteins leads to vesicle budding from a planar membrane. We also quantify how the curvature field of the membrane impacts the spatial segregation of proteins.

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