

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**A Molecular Dynamics-Decorated Finite Element Method (MDeFEM) Framework for Simulating the Gating of Mechanosensitive Channels** XI CHEN, YUYE TANG, GUOXIN CAO, JEJOONG YOO, ARUN YETHIRAJ, QIANG CUI, Columbia University — The gating pathways of mechanosensitive channels of large conductance (MscL) are studied using the finite element method. The phenomenological model treats transmembrane helices as elastic rods and the lipid membrane as an elastic sheet of finite thickness. The interactions between various continuum components are derived from atomistic energy calculations. The structural variations along the gating pathway are consistent with previous analyses based on structural models and biased molecular-dynamics simulations. Upon membrane bending, there is notable and nonmonotonic variation in the pore radius. This emphasizes that the gating behavior of MscL depends critically on the form of the mechanical perturbation. Compared to popular all-atom simulations, the MDeFEM framework offers a unique alternative to bridge detailed intermolecular interactions and biological processes occurring at large spatial and timescales. It is envisioned that such a hierarchical multiscale framework will find great value in the study of a variety of biological processes involving complex mechanical deformations such as muscle contraction and mechanotransduction.

Xi Chen

Date submitted: 21 Nov 2006

Electronic form version 1.4