Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Numerical Computation of Diffusion Properties in Molecular Systems on a Topology-Conforming Grid[1] IVAN TEO, KLAUS SCHULTEN, Department of Physics, University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science and Technology — Multiscale problems involving diffusion in molecular systems are a mainstay of computational biophysics. Given a molecular system, the local diffusion coefficient $D(\mathbf{r})$ as well as the equilibrium distribution function $P(\mathbf{r})$ that characterizes the local free energy are computed to describe the kinetics of diffusing particles at each point in space through the Smoluchowski equation (SE). An irregular grid of space-varying fineness conforming to $P(\mathbf{r})$ is generated via the method of topology-representing networks and a subsequent Voronoi tessellation. The discretized SE produces a rate matrix which describes the probabilities of particles hopping from point to point on the grid. We demonstrate the calculation of the rate matrix for ions diffusing through the balloon-like structure of the mechanosensitive channel of small conductance (MscS) and thence the determination of mean first-passage times that characterize conduction of ions through balloon and channel.

[1]Supported by NIH grants P41-RR005969 and R01-GM067887 and NSF grant PHYS0822613. XSEDE supercomputer time provided by NSF grant MCA93S028. High performance computing resources provided by Texas Advanced Computing Center, University of Texas at Austin.

Ivan Teo
Department of Physics, University of Illinois at Urbana-Champaign,
Beckman Institute for Advanced Science and Technology

Date submitted: 13 Dec 2011 Electronic form version 1.4