**Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures**

Noah Trebesch and Emad Tajkhorshid

University of Illinois

[trebesc2@illinois.edu](mailto:trebesc2@illinois.edu)

**Abstract**

Membranes are fundamental to the function and structure of cells, and molecular dynamics (MD) simulations have the potential to reveal deep insights about the basic physics and biochemistry that produce their behavior. However, MD simulations of cellular membranes have been extremely limited up to this point due to the geometric complexity and sheer size of such membranes. To overcome these limitations, we have developed xMAS (Experimentally-Derived Membranes of Arbitrary Shape) Builder, software designed to turn low-resolution 3D meshes derived from experimental techniques into atomistic membrane models that can be simulated using MD. In the first application of this software, we have used an experimentally-derived 3D mesh and lipid composition to develop a realistic atomistic model of a Terasaki ramp, a helicoidal membrane structure found in the endoplasmic reticulum. The model measures approximately 1.97μm by 1.59μm by 0.61μm and is composed of ~36.6 million lipids (~4.5 billion atoms), making it one of the largest atomistic biological models to ever be built. Building this model with xMAS Builder involves several methodologically innovative steps, including using MD to simulate ~36.6 million Lennard-Jones particles while attracted to grid-based potentials to optimize the packing of the membrane lipids and running billion atom MD simulations to fix ring piercings and other complex lipid clashes using a newly developed energy minimization technique. Simulations of the cellular membrane models built using xMAS Builder will allow us to computationally probe the complex interactions that give rise to function at an unprecedented atomistic level of resolution, and they will allow us to build better coarse models of the systems for simulation of longer timescale phenomena.