Joint Condensed Matter
and
Center for Soft Matter and Biological Physics
Seminar

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Mechanics at the nanoscale: Local stress calculations in Biomolecular systems

Monday, April 30, 2018

4:00pm – 5:00pm

304 Robeson Hall

The microscopic or local stress field provides a unique connection between molecular simulations and mechanics of materials at the nanoscale. Lateral stress profiles are routinely used to understand the mechanical behavior of liquid interfaces such as lipid membranes from molecular dynamics (MD) simulations. However, the 1-dimensional stress profiles are not adequate to understand the multidimensional mechanical state in complex asymmetrical systems such as membrane proteins or other macromolecular structures. Furthermore, the fact that the microscopic stress from MD simulations is not uniquely defined is a theoretical consideration that is most often ignored, which has acute practical consequences when atomistic models are considered. I will present our recent work on the development of objective 3D local stress calculations by way of expressions that satisfy balance of linear and angular momentum for force-fields with arbitrarily high many-body interactions. I will show how some definitions of the microscopic stress violate mechanical equilibrium through various examples including defective graphene, lipid membranes, and fibrous proteins. I will also demonstrate the use of the traction vector, computed from the microscopic stress, as a powerful tool to visualize the local balance of forces at an interface. Focusing on the bacterial mechanosensitive channel MscL, I will show how the traction vector allows identification of a unique association pattern of lipids at specific sites on the MscL surface that may mediate gating of the bacterial channel by membrane tension or other stimuli.