1108-92-474Anastasios Matzavinos* (matzavinos@brown.edu), Brown University, 182 George Street,
Providence, RI 02912. Dissipative particle dynamics simulations of polymer networks.

Networks of entangled or cross-linked polymers, such as the actin cytoskeleton, are ubiquitous in phenomena pertaining to cellular and molecular biology. In many cases, the structure of these networks is dynamically altered by the mechanical feedback of biological lipid membranes and cytoplasmic flows. However, current modeling and computational approaches neglect such mechanical feedback for the sake of computational tractability.

In this talk, we present a dissipative particle dynamics approach to simulating the meso-scale dynamics of polymer networks. Our simulations explicitly include mechanical interactions with other meso-scale structures (e.g., lipid membranes) and cytoplasmic flows. We compare the results of our approach to those of Brownian dynamics simulations. We also discuss ongoing work on stochastic homogenization, bridging the gap between the meso-scale description and macroscopic models of bulk mechanical properties. (Received January 19, 2015)