



KOÇ UNIVERSITY

Math-Science Seminar

Speaker: Pemra Doruker (Chemical Engineering Department, Bogazici University)

Title: Coarse-Grained Modeling and Simulation of Macromolecules

Date and Time: Thursday, March 29, 4:45 pm.*

Place: Room Z42, Science Building, Koç University, Rumelifeneri Yolu, Sariyer 80910 Istanbul, Turkey.

Abstract: A coarse-grained simulation technique that increases the time and length scales accessible in the simulation of synthetic polymers will be described. This method reversibly bridges the gap between simulations of coarse-grained (on-lattice) and fully atomistic (in continuous space) models of specific polymers. Using this technique, it is possible to elucidate important interfacial properties of amorphous thin films and nanofibers, such as the density profiles, the orientation of bonds and chains and the segregation of chain ends at the free surfaces. Moreover, the dynamic properties (mobility and diffusion) that require efficient equilibration of the system are determined for polyethylene thin films. Another coarse-grained model that has proven effective for extracting the functionally relevant, collective motions of proteins will be demonstrated using a viral membrane protein as the specific example. In this analytical approach, the folded protein structure is viewed as an elastic network, the nodes of which are the α -carbons and the springs connect the sufficiently close residue pairs. The largest scale collective motions can still be extracted after further coarse-graining of the protein structure along the backbone. Thus, the dynamics of large protein complexes are now accessible by this approach. In summary, both of the techniques described above are effective tools for the analysis of macromolecular systems with large dimensions, which are far beyond the reach of atomistic modeling and simulation.

*Refreshments to be served in Science Building, Room Z40 at 4:30 pm.