Small scale mechanics from atomistic models: accessing large space-scales in carbon nanostructures and long time-scales in biomolecules

Direct atomistic simulations accessing the relevant length- and time-scales are extremely challenging in many applications. This can be due to the very large number of atoms involved in representative material samples, or to the extremely long simulation times required for conformational changes in proteins relative to the fast atomic vibrations. In this talk, I will provide general background on multiscale modeling and simulation, and present two examples addressing the space and time issue respectively: (1) the mechanics of carbon nanostructures at mesoscopic levels from atomistic models, and (2) the acceleration of molecular dynamics (MD) simulations of biomolecules. Regarding (1), experimentally tested carbon nanotube or graphene systems easily reach 10^8 atoms, yet their mechanics are dictated by bonded and non-bonded inter-atomic interactions. I will show how continuum models of different nature, incorporating the net effect of atomistic interactions, can efficiently capture the nonlinear mechanics of such systems and access the engineering scales. As for (2), I will present ideas on how to feasibly compute effective models for complex biomolecules, which bridge the gap between MD and thermodynamic observables.