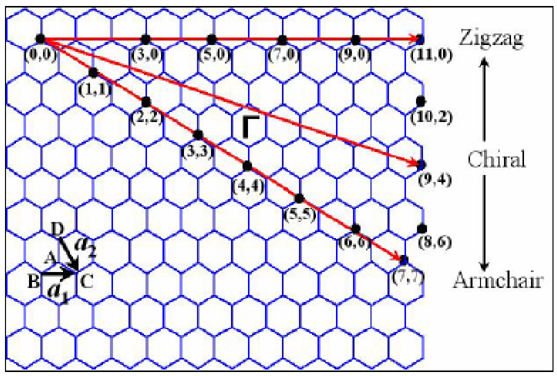
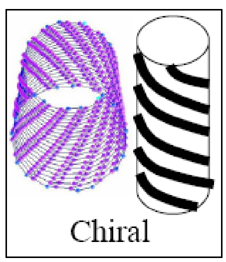
1D and 2D atomistic-continuum models for deformations of single-walled carbon nanotubes

Karthick Chandraseker
Department of Theoretical and Applied Mechanics, Cornell University

Carbon nanotubes possess remarkable electrical, thermal and mechanical properties, and their potential applications include such diverse areas as conductive and high strength composites, energy storage and conversion devices, sensors, field emission displays and radiation sources, hydrogen storage media, and nanometer sized semiconductor devices, probes and interconnects. This talk reports on our ongoing work in modeling mechanical deformations of single-walled carbon nanotubes (SWNTs) using enriched continuum models which incorporate atomistic detail into a continuum analysis.



Planar Graphene Sheet



The talk focuses on two elastic continuum models of SWNTs – a two-dimensional membrane model, and a one-dimensional rod model – in which the continuum strain energies are determined from analytic interatomic potentials and all-atom simulations respectively. The membrane model has been employed in the past to predict localized effects such as buckling modes of the effective continuum. We motivate and propose modifications to the existing membrane model, and employ it to study coupled extension-twist deformations of SWNTs. The rod model is a recent effort motivated by the need to model global behavior of long SWNTs. Numerical results on the elastic moduli for different deformation modes of SWNTs like extension, twist, bending and shear using these models, will be presented. It will be demonstrated that phenomena such as extension-twist coupling and bending-shear coupling that isotropic, linearly elastic models are unable to quantify, can be captured by such atomistic-continuum models in a unified manner.