Atomistic Finite Element Method for Nanoscale Structures

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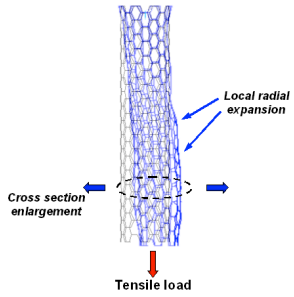
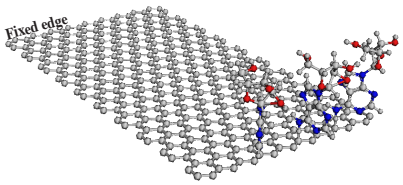
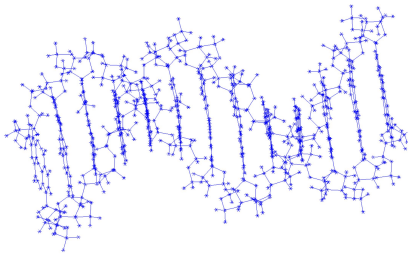
Abstract: Due to the recent developments in nano and biotechnology, research on nanoscale structures is rapidly expanding in many scientific and engineering disciplines. Such nanoscale structures include synthetic molecules such as carbon nanotube, boron nitride nanotube, zinc-oxide nanowire, graphene sheet and biological molecules such as DNA, RNA and protein. In this lecture we will discuss a unified finite element approach for mechanical analysis of such structures, where atomic bonds are equivalently modelled by "beam elements". An analytical formulation for the equivalent mechanical properties (Young's modulus, shear modulus and Poisson's ratio) of the C–C bond and other atomic bonds will be discussed. Using the proposed finite element approach, any molecule can be represented by truss-like structures with equivalent "element" properties. This approach will be illustrated for carbon nanotubes, boron-nitride sheets, graphene sheets, graphne based composites, DNA and nano-bio sensors.







Short Bio: Prof Adhikari is the chair of Aerospace Engineering in the College of Engineering of Swansea University. Currently he is a Wolfson Research Merit Award holder from the Royal Society. He received his PhD in 2001 from the University of Cambridge. During this time he was the Jawaharlal Nehru Memorial Trust scholar at the Trinity College. He was a lecturer at the Bristol University and a Junior Research Fellow in Fitzwilliam College, Cambridge. He was a visiting Professor at the Carleton University, University of Johannesburg and a visiting scientist at the Los Alamos National Laboratory.

His research areas are multidisciplinary in nature and include uncertainty quantification in computational mechanics, bio & nanomechanics (nanotubes, graphene, cell mechanics, nano-bio sensors), dynamics of complex systems, inverse problems for linear and non-linear dynamics and vibration energy harvesting. He has published about 150 journal papers and 100 conference papers in these areas. He was an Engineering and Physical Science Research Council (EPSRC) Advanced Research Fellow and winner of the Philip Leverhulme Prize (2007) in Engineering (given to an outstanding scholar under the age of 35).