Mechanical behaviour of interlinked carbon nanotubes for nanocomposites

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Abstract

This proposal is a follow-on to a Class C project in which we have benchmarked the simulations required for the work proposed here. The proposed work involves using molecular dynamics (MD) simulations to investigate the mechanical behaviour of bundles of interlinked carbon nanotubes (CNTs) for use in nanocomposites. A custom version of the public-domain code LAMMPS will be used. The objective is to model carbon atom irradiation of bundles of multi-walled CNTs (MWCNTs), in order to induce controlled levels of inter-tube and inter-wall bonding. A side-effect of irradiation will be some intra-wall defects. The resulting cross-linked CNT bundles will then be tested for two mechanical properties: tensile strength and shear stress under pullout of individual tubes or tube walls from the bundle. These are critical quantities in determining the strength and toughness of CNT-based nanocomposites. Simulating *bundles* of CNTs using MD is highly computationally expensive due to the large number of atoms involved. Therefore, individual simulations can take days or even weeks to solve on our computer cluster within the Materials and Surface Science Institute (MSSI) at the University of Limerick (UL). Parameter studies like the one proposed here can therefore only be done using the Irish Centre for High End Computing (ICHEC) facilities. We would also like to request some time on the Blue Gene (BG /L) system to assess our LAMMPS models on that system, since we are advised by the ICHEC staff that LAMMPS is likely to scale very well for massively-parallel simulation.