MESOSCOPIC DISTINCT ELEMENT METHOD-ENABLED MULTISCALE COMPUTATIONAL DESIGN OF CARBON NANOTUBE-BASED COMPOSITE MATERIALS

TEAM

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RESEARCH OBJECTIVES

- Currently, a multiscale simulation capability, able to predict mechanical properties of polymer/Carbon nanotube (CNT) nancomposites, is missing
- We propose to develop an integrated multiscale simulation package able to simulate the strain to failure of thermoplastic and thermoset/CNT systems
- The concepts behind the modeling approaches are published. The methodology validation will enable computational-guided fabrication of CNT composites

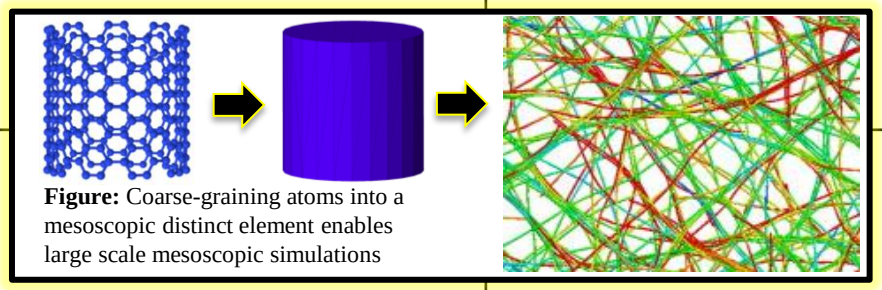

Figure: Coarse-graining atoms into a mesoscopic distinct element enables large scale mesoscopic simulations

APPROACH

- Couple mDEM for CNTs with LAMMPS to allow for mesoscopic simulations of CNT films with sizes up to 1 µm3
- Build a comprehensive mesoscopic contact models database, to accurately capture the load transfer in individual CNTs, CNT-CNT, and CNT-polymer interfaces
- Perform multiscale modeling and simulations on distributed-memory supercomputers
- Formulate strain to failure predictions for purified CNT films, and thermoplastic/CNT and thermoset/CNT composites

POTENTIAL IMPACT

- Thermoplastic/CNT and thermoset/CNT nanocomposites are of great interest for space applications. The proposed effort will accelerate progress by providing the ability to guide experimental design. There is potential for infusing NASA's CNT-composite research program, and other electronic and multifunctional materials programs
- The developed framework could additional strategies for enhancing the load transfer in CNT-based nanocomposites, such as by introducing cross-links via irradiation