HPC Study to Quantify the Factors Affecting Conductive Percolation Analysis

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Motivation and Objective: The electrical conductivity of polymer composite materials is generally characterized by its dependence on the filler volume fraction. At low filler loadings, the conductivity of the composite is still very close to that of the pure polymer matrix. At some critical loading, called the percolation threshold, the conductivity increases several orders of magnitude with very little increase in the filler amount. After this region of drastic increase, the conductivity once again levels off and is close to that of the filler material. At percolation threshold where enough filler has been added it begins to form a continuous conductive network through the composite. Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical solutions. Efficient percolation algorithms integrated with Monte Carlo methods are needed for developing Representative Volume Element (RVE) based design and analysis tools with 3D network of fillers for electrical conductivity of nanocomposites. 3D network modeling of nanocomposites requires that the distance between each filler be calculated to prevent unphysical inter-penetration of fillers. Algorithms for filler-filler contact are currently being developed in our research group) and are demonstrated for high aspect ratio fiber nanocomposites. These algorithms are used to generate models without inter-filler penetration, check the spatial distribution among fibers in the model, and determine when the percolation is achieved in the 3D system. The primary objective of this work is to improve the computational efficiency of these algorithms implementing parallelization of the code using High Performance Computing (HPC) facilities at Georgia Tech.

Research Approach and Scope: In the percolation analysis the computation time increases with volume fraction. The most computationally intensive part of the current code is the contact algorithm. Selective segment comparison method is 15 times faster than approach 2 at 1% volume fraction and nearly 100 times faster than approach 1 at 1%. Though the selective segment comparison method has better running times, at higher volume fractions it still requires much time to run. To speedup of the algorithm, parallelization of the code is needed. By splitting the work among processors, the calculation of the distance can be done at the same time rather than serially. The current algorithm will be augmented with periodic boundary conditions for percolation analysis. For large RVE sizes with higher volume fraction of the filler HPC facilities at Georgia Tech will be used for reducing the computational burden.

Semester Progress

RVE models with material periodicity: For RVE of 2000 nm cube with 0.2% volume fraction of filler, various material periodic conditions are developed as shown in Figures 1 for various applications. In the 3D analysis for mechanical or electrical property characterization any combination of these conditions can be used as appropriate. For example, if the 3D RVE models are used for predicting the effective mechanical properties of polymer composite, the 2D faces in the loading direction (X) are subjected to translate boundary conditions and the filler are relocated inside the RVE in the X direction and periodic boundary conditions are applied in other to faces, Y and Z. This condition is denoted as 1-3-3 as shown in Figure 1. If the 3D RVE models are used for predicting percolation analysis and for predicting the effective electrical conductivity of CNT composite, the 2D faces in X direction, where the voltage is applied are subjected cut-off boundary conditions and periodic boundary conditions are applied in other to faces Y and Z. This condition is denoted as 2-3-3 as shown in Figure 1. If the RVE models are used for quantifying the electrical conductivity of composite

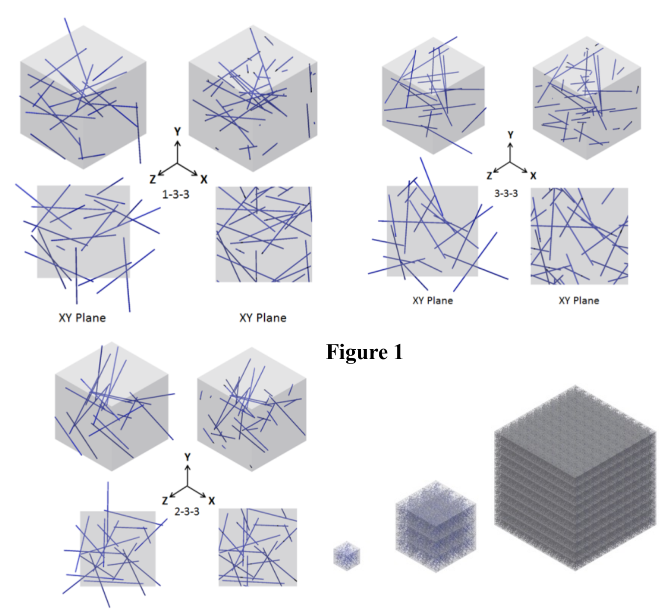
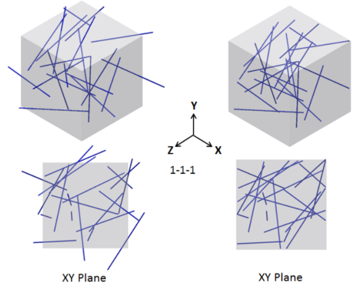


Figure 1

system using Resistor – Capacitor (R-C) approach periodic boundary conditions are applied on all three faces of RVE. This condition is denoted as 3-3-3 as shown in Figure 1. Figure 1 also illustrates material periodic boundary conditions, which involves placing the fillers that exceed the RVE into their respective position on the opposite face of RVE as if the RVE with 3-3-3 boundary conditions were part of a larger set of RVEs.



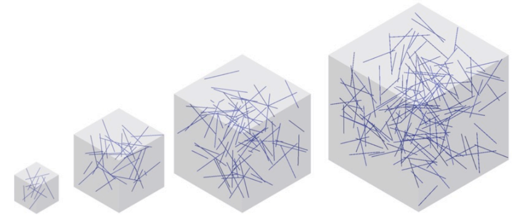
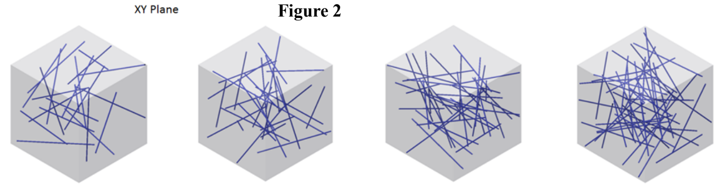
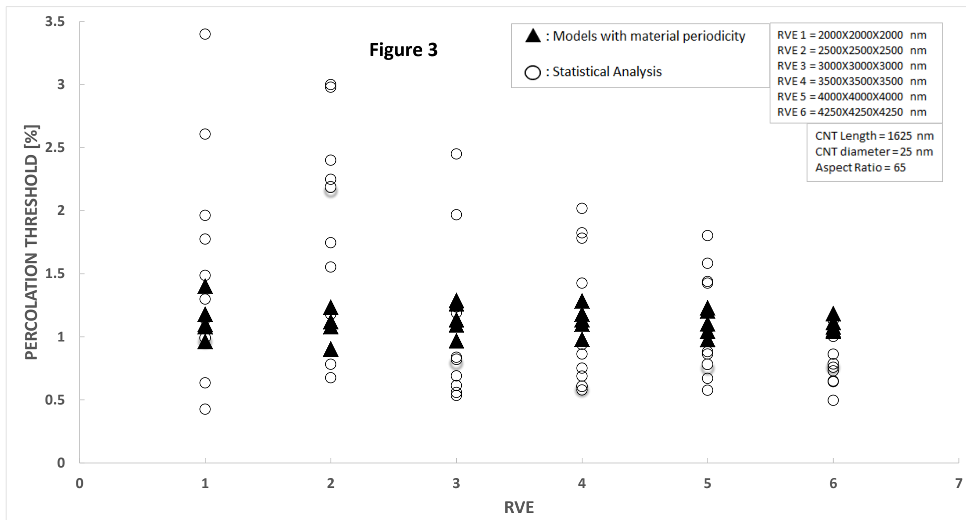


Figure 2



RVE Models for Statistical Analysis: RVE models with random distribution of CNT within polymer are developed for statistical analysis. In all statistical analysis models, translate boundary wall conditions are used by moving the fillers that exceed the RVE until they find a new spatial locations within RVE (1-1-1) as shown in Figure 2. To predict the critical RVE size, models with increased RVE sizes and increased volume fraction for each RVE size are developed as shown in Figure 2.

Computational homogenization models with material periodicity: The percolation analysis using statistical models using HPC with translation boundary conditions (1-1-1) indicates that the predicted percolation threshold values are dependent on RVE size (see Figure 3). It is also important to note that percolation analysis with statistical models requires large RVE size to arrive at more homogenized results and are thus computationally expensive. Percolation analysis is also performed using computational homogenization models with material periodic boundary conditions (see filled triangles in Figure 3) to study the effect of boundary conditions and RVE size. 2-3-3 material periodic boundary conditions are used and the analysis is repeated for each RVE studied. Figure 4 shows percolation threshold values for models with material periodicity for various RVE sizes. As can be seen from Figure 4, a homogenized value of percolation threshold is achieved independent of RVE size. The 3D RVE models with material periodicity presented in this work are attractive for homogeneous mechanical and electrical property estimation of CNT-polymer composite structures.



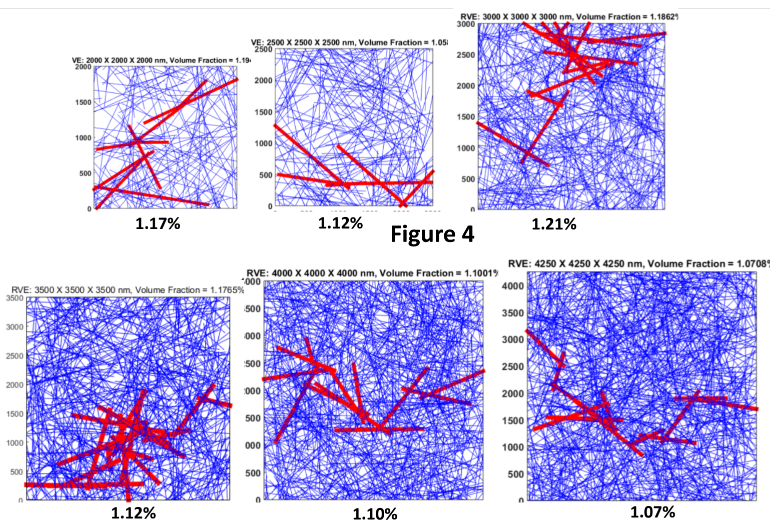


Figure 4

Based on this work following Manuscript is submitted to ***"Composite Structures"*** journal as a full-length paper.

Wonsup Song Vikram, Krishnaswamy and Raghuram V. Pucha, *Computational Homogenization in RVE Models with Material Periodic Conditions for CNT Polymer Composites*