Mechanical Behavior of Carbon Nanotube Turf

Stephen Mitchell[1], Harish Radhakrishnan[2], Sinisa Dj. Mesarovic[2]

[1]College of Engineering, Valparaiso University, Valparaiso IN 46383

[2]School of Mechanical and Materials Engineering, Washington State University, Pullman WA 99164

Introduction

Carbon nanotubes grown on a substrate form a turf – a complex structure of intertwined, mostly nominally vertical tubes, cross-linked by adhesive contact and few bracing tubes. The turfs are compliant and good thermal and electrical conductors. In this work we seek to gain an understanding of the mechanical behavior of the turf. We develop a discrete model of the turf using finite element analysis. The developed model is capable of representing large turfs and with longer time scales when compared with existing molecular dynamic simulations.

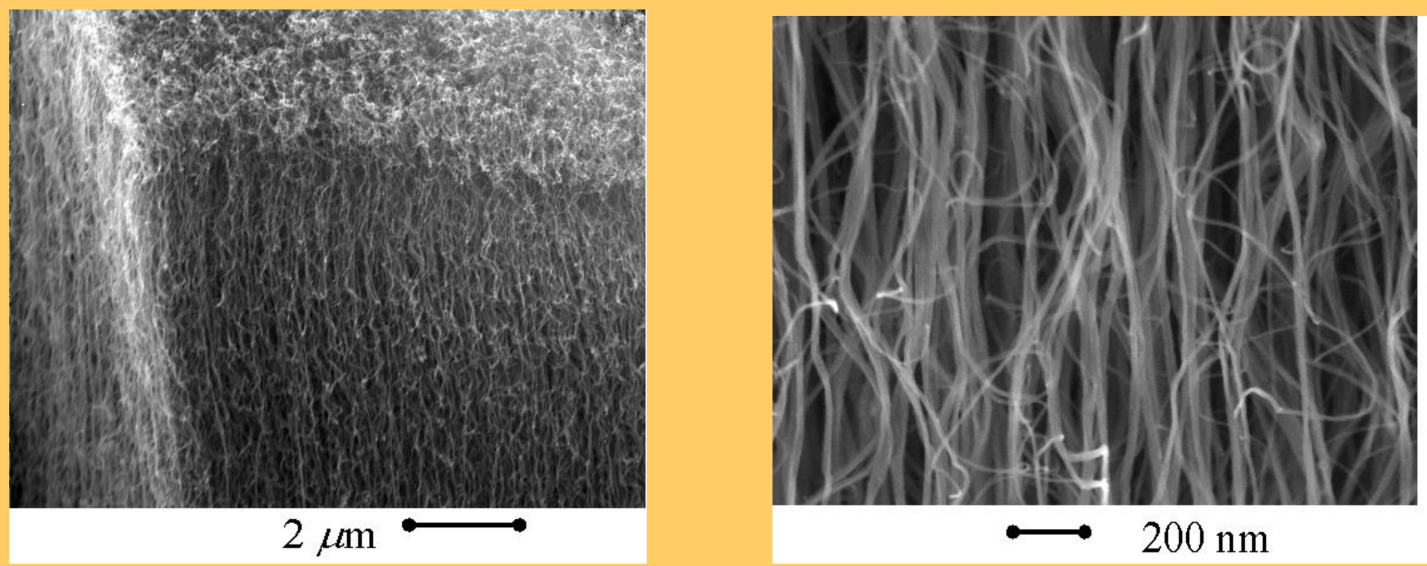

Figure: SEM images [Mesarovic et al., *Scripta Mat.* 2007]

Discrete Model of the Turf

- The turf is generated using a controlled random walk method.
- Parameters α, l and d control the tortuousity and density.
- The random walk points are fit using a cubic hermite polynomial.
- The turf is discretised using elastica finite elements and assumed to be singe walled tubes with (5,5) configuration

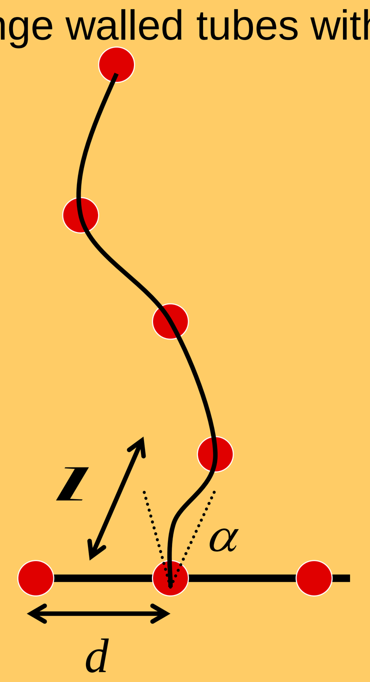

Figure: Controlled random walk

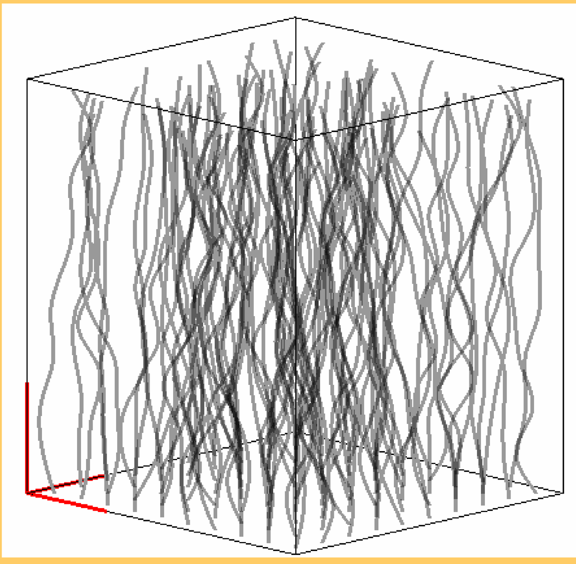

Figure: A 10 x 10 turf sample. Each tube has 10 random walk points

Elastica Element

- Inextensible: $r' \cdot \dot{r}' = 0$
- Stress Couple: $M = B\kappa\hat{b} + H\hat{t}$
- Cross-section remains undistorted.
- Equations of motion:

$$H' + m \cdot \hat{t} = 0$$

$$-\left(Br''\right)'' + \left(\lambda r'\right)' + \left[H\left(r' \times r''\right)\right]' + \left(r' \times m\right)' + q = m\ddot{r}$$

- Interpolation:

Positions – cubic interpolation
Twist angle – linear interpolation
Lagrange multiplier – quadratic interpolation

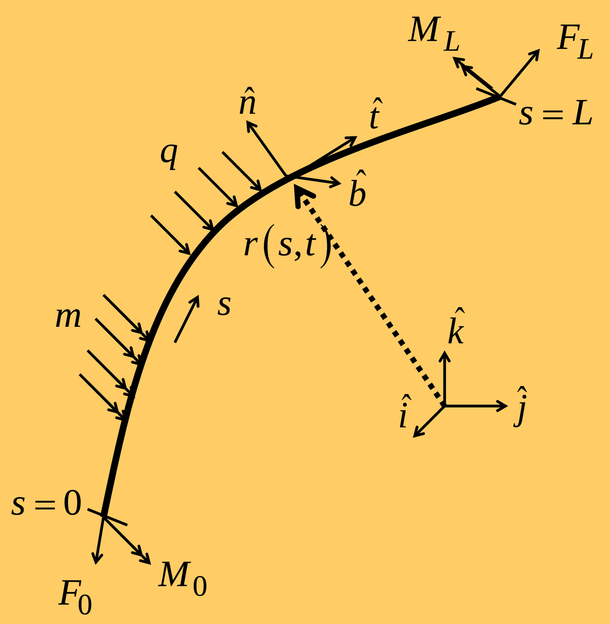

Figure: An elastica subjected to external loads.

Interaction Model

- Lennard-Jones type – non-bonded, pair wise interaction model

$$\phi = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- Parameters are chosen from MD simulations

Material Parameters

- Based on a (5,5) configuration single walled carbon nanotube
- Bending modulus: $EI =$ 6.65 x 10^{-26} Nm^2
- Density : 1953.23 amu/nm

Time Integration

- Equations of motion are solved using half-step leapfrog Verlet technique
- Velocities are calculated at half-step intervals

$$\dot{r}\left(t + \frac{\Delta t}{2}\right) = \dot{r}\left(t - \frac{\Delta t}{2}\right) + \ddot{r} \cdot \Delta t$$

- Positions are calculated at Δt intervals

$$r\left(t + \Delta t\right) = r\left(t\right) + \dot{r}\left(t + \frac{\Delta t}{2}\right) \cdot \Delta t$$

- Damping forces are calculated as a function of velocity. Damping coefficient C_{damp} is based on a damping ratio of 0.1

$$F_{damp} = -C_{damp} \cdot \dot{r}\left(t\right)$$

$$\dot{r}\left(t\right) = \dot{r}\left(t + \frac{\Delta t}{2}\right) + \frac{\ddot{r}\left(t\right)}{2} \cdot \Delta t$$

Results

- Analysis involves generation of the turf structure, relaxation and flat punch indentation
- Nanotubes are discretized using 100 elastic elements of approximately 12 nm in length
- Tubes are spaced apart at 12nm

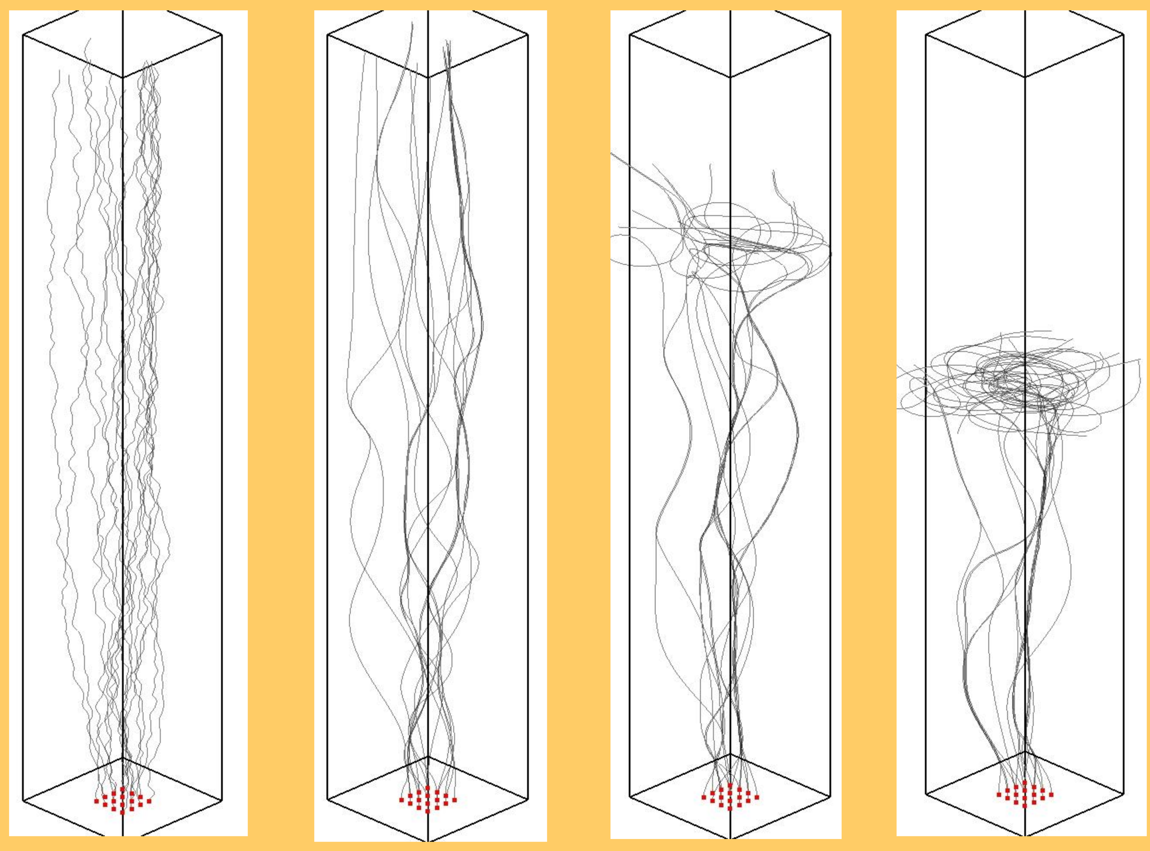

Figure: Turf simulation of 4 x 4 structure.

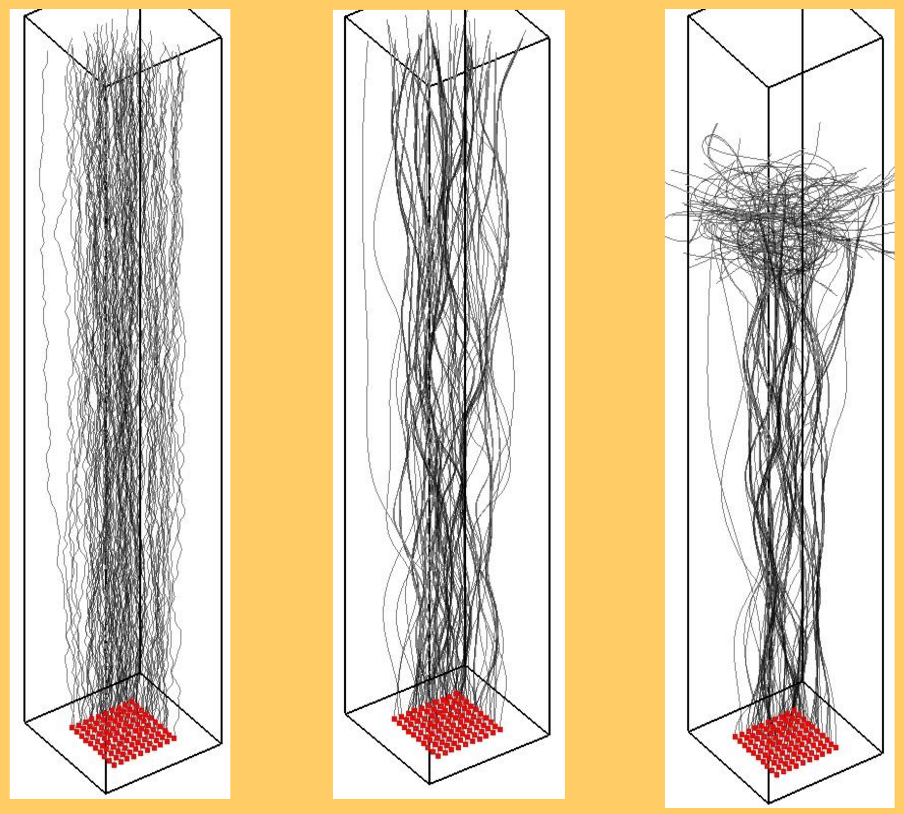

Figure: Turf simulation of 10 x 10 structure.

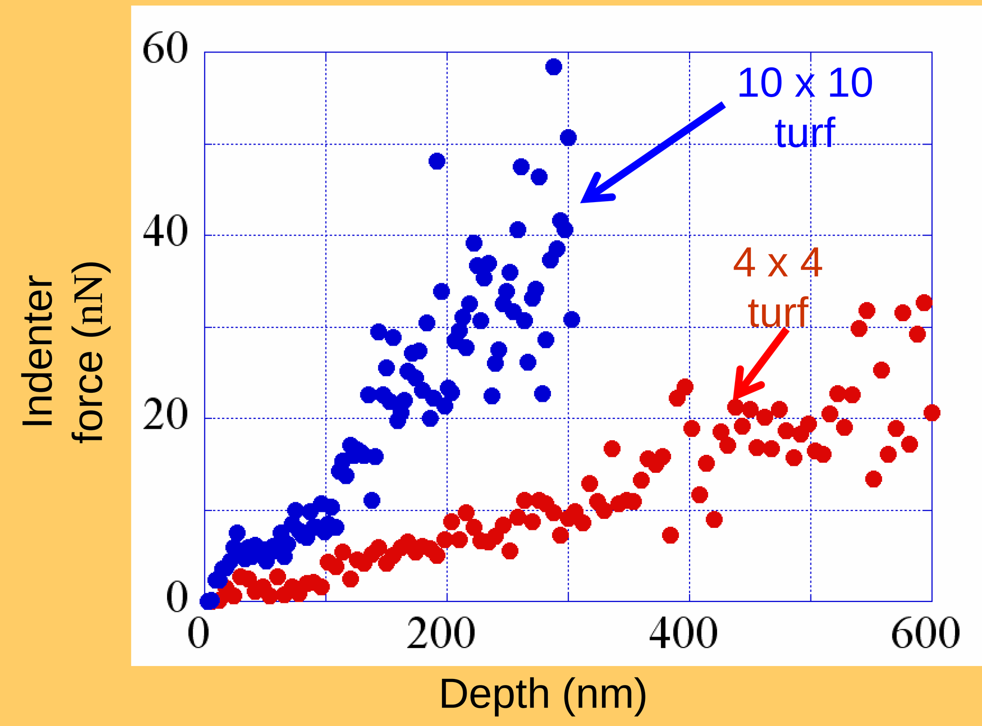

Figure: Load – depth curves

Conclusions

- The developed finite element model is capable of representing large turfs with longer time scales
- The results confirm that the adhesive contact between adjacent tubes remain unbroken with deformation.

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