LUMPED MODELING OF CARBON NANOTUBES FOR M/NEMS SIMULATION

Richa Bansal[1], *Jason V. Clark*[1, 2]
Schools of [1]Mechanical Engineering, [2]Electrical and Computer Engineering
Purdue University, West Lafayette, Indiana, USA

ABSTRACT

This paper presents a lumped model of single walled carbon nanotube (CNT) using structural matrix mechanics. We implement a CNT model in SUGAR to facilitate the design, modeling, and simulation of combined micro- and nano-scale systems. That is, where users can explore the application of CNTs as components of an electromechanical system. Our lumped CNT model is able to represent the dynamic response of a zigzag or armchair chirality, with desired diameters, lengths, and distributed loading parameters. Our present dynamic CNT model is limited to small deflections and user-defined geometric properties. Our CNT modeling is accessible through the Web with remote computation on the nanoHUB.org.

Keywords: Carbon nanotubes, Micro/Nano-Electromechanical systems (M/NEMS), Reduced order modeling, Sugar, SugarCube.

1. INTRODUCTION

Due to their excellent electrical and mechanical properties, carbon nanotubes have been used for broad applications ranging from nano-composites to nano-electromechanical systems (NEMS). The extremely small size of CNT presents significant challenges in the evaluation of their mechanical properties. Design and analysis of CNT has been largely done with molecular dynamics tools, which limits access to molecular dynamics specialists and does not allow the exploration of CNTs as components of a system.

Many researchers have pursued the analysis of carbon nanotubes by theoretical modeling, generally classified into two categories: atomistic modeling and other techniques that include classical molecular dynamics, tight-binding molecular dynamics, and density function theory [1]. Structural mechanics based models of CNT have also been developed [1], [2]. An online tool available on the nanoHUB.org by Aluru et al. [3] simulates the pull-in behavior of carbon nanotube based NEMS for different applied voltages. However, this analysis is restricted to cantilever and fixed-fixed boundary conditions. Although a computer program called CoNTub 1.0 is available for construction of CNT [4], currently no application exists for the design and evaluation of the deformation behavior of NEMS under applied loading and for exploring their application as components of a system.

We present an addition to our SUGAR engineering tool for designing and dynamically simulating the response of CNTs. Our CNT model is an extension of a structural mechanics model developed by Wan and Delale in [2]. Our model simulates the dynamic response of CNTs with constant stiffness using an assemblage of our linear flexure model that we previously described in [5]. To achieve a lumped CNT model, we reduce the number of degrees without reducing accuracy by using the matrix condensation approach. The resulting lumped CNT model has six degrees of freedom at each end-node terminal (x, y, and z, and rotations about x, y, and z). This facilitates the connection of CNTs to other elements to generate complex system configurations. A benefit of our reduced order modeling is that it greatly reduces computation time and reduces the complexity of designing systems. We implement our CNT model in Sugar and SugarCube.

The rest of the paper is organized as follows: Section 2 describes the structural mechanics based CNT model and the matrix condensation based lumped model for CNT. Section 3 discusses the graphical model of the CNTs in Sugar and SugarCube. And Section 4 discusses the application of our lumped model in M/NEMS.

2. ALGORITHMS

2.1 Carbon Nanotubes

CNTs are allotropes of carbon with a cylindrical nanostructure. The structure of an ideal nanotube is formed by rolling up a graphite sheet into a cylinder and is defined by the vector linking the two equivalent carbon positions that are matched together after rolling, called the chiral vector C (see Figure 1).

$\vec{C} = n\overrightarrow{a_1} + m\overrightarrow{a_2}$.

According to the angle Q formed between the chiral vector and a_1, nanotubes are classified as armchair type (n=m) or zigzag type (m=0). These show symmetry in structure. All remaining nanotubes with no symmetry are known as chiral. The graphitic sheet is made up of hexagonal lattices with C-C bond length=1.415 Å. The diameter of a single-walled nanotube is given by $d = 0.0783(n^2 + m^2 + nm)^{\frac{1}{2}}$ nm.

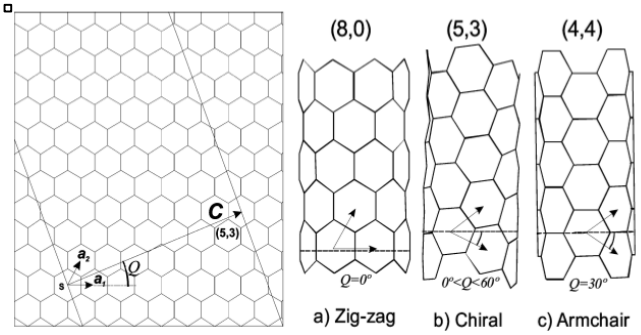

Figure 1: Nanotube geometry by means of graphitic plane rolling. Classification is according to the Chiral vector *C* and the chiral angle *Q*. (a) zigzag (*n*, 0); (b) chiral (*n,m*); (c) armchair (*n,n*) [4].

2.1 Structural Mechanics Model

We use a structural mechanics based model to develop the constant-stiffness model for a CNT. This model is based on the notion that the CNT carbon bonds may be represented as a geometrically-framed structure, where the primary bonds between two nearest-neighboring atoms act like load-bearing members. That is, the carbon-carbon bonds are treated as solid rectangular flexure elements. The model neglects non-bond interactions caused by van der Waals forces and electrostatic forces. The details of the structural mechanics model can be found in [3]. The table below summarizes the sectional properties that were used to develop the beam model in Sugar. Here, *b, h, l* represent width, height and length of the beam element, *E* is Young's modulus, *G* is Shear modulus and *v* is the Poisson's ratio.

Sectional properties of the modified beam model		
b = 0.127 nm	h = 0.086 nm	l = 0.1415 nm
G = 3260.32 GPa	E = 8476.84 GPa	ν = 0.3

The equation of motion for the CNT model is given by:

$$M\ddot{q} + D\dot{q} + Kq = \sum F$$

where *M, D*, and *K* represent the global mass, damping, and stiffness matrix respectively. The global mass matrix can be assembled from the elemental mass matrix by considering the mass of the carbon atom ($m_c = 1.9943\times10^{-26}$ kg) to be concentrated at the flexure joint. The elemental mass matrix $[M]^e$ is given by

$$[M]^e = diag\left[\frac{m_c}{3} \quad \frac{m_c}{3} \quad \frac{m_c}{3} \quad 0 \quad 0 \quad 0\right].$$

The global stiffness matrix is assembled from the elemental stiffness matrix $[K]^e$, which is given by

$$[K]^e = \begin{bmatrix} K_{ii} & K_{ij} \\ K_{ii}^T & K_{jj} \end{bmatrix}.$$

The detailed stiffness matrix can be found in [6]. Currently, our damping matrix (not shown) is proportional to the mass matrix.

2.2 Reduced Order Modeling

The CNT is often shown to be a web-like structure comprised of simple bond or flexure elements. However, larger the number of elements used, larger would be the size of the system stiffness and mass matrices. For example, a (4,4) armchair CNT model of length 10nm in Sugar has 1769 elements and 7212 x 7212 sized stiffness and mass matrix. Hence, the analysis of a large CNT structure, or a system of CNTs, can be computationally expensive.

Our model reduces the CNT structure of the given length, diameter, and chirality to an equivalent linear flexure structure, with 6 degree-of-freedom at each end-node (see Figure 2). All information of the interior nodes is hidden in the reduced system matrix. The equivalent stiffness and mass matrix for the reduced system is generated using the matrix condensation technique [6]. The first step is to partition the stiffness, displacement, and force matrices

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix},$$

such that F_1 contains all the applied forces, F_2 contains only zeros, and x_1 refers to all the displacements we wish to retain. For our model, these are the displacements of the first and the last node. Hence,

$$[K_{11,reduced}][x_1] = [F_1]$$

which yields,

$$K_{11,reduced} = K_{11} - K_{12}K_{22}^{-1}K_{21}.$$

The equivalent mass matrix M_c for the reduced degree-of-freedom system is given by

$$M_c = A_c^T M A_c, \text{ where } A_c = \begin{bmatrix} I \\ -K_{22}^{-1}K_{21} \end{bmatrix}.$$

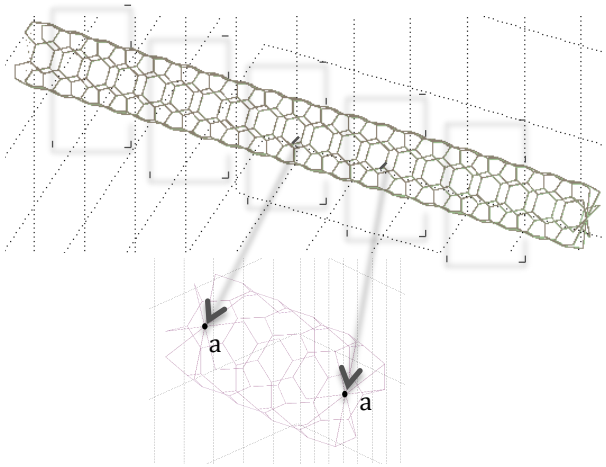

Figure 2: Lumped CNT Section of (4,4) armchair CNT modeled in Sugar. In the above figure, the complete length is obtained by a combination of 6 such reduced order sections, linked at their terminal, or nodes (a_1 and a_2). The forces and displacements at each node are related to the structure of the section. The interfacial links are massless and only provide moment and connectivity.

3. MODELING

3.1 Sugar Models

The CNT models of zigzag and armchair nanotubes are implemented in Sugar, a nodal analysis package for 3D MEMS simulation [5]. The user can simulate the structure and dynamic behavior of the CNT using either the original model or the reduced order model. The original model allows the user to analyze the deformation of geometry for the applied forces or moments. However, as was mentioned earlier, using this model for simulating the geometry of large CNTs can be computationally expensive and time consuming. For such geometries, the reduced-order models can be used, the details of which were given in Section 2.2. The display routine for this model first generates a flattened 2D image of the CNT with the given properties, and then

maps the 2D image onto a deformed 3D cylinder of required radius and length. The reduced-order model is much more computationally efficient, both structurally and graphically. For example: simulation of a zigzag (4,0) CNT of length 20nm takes only 54.24secs.

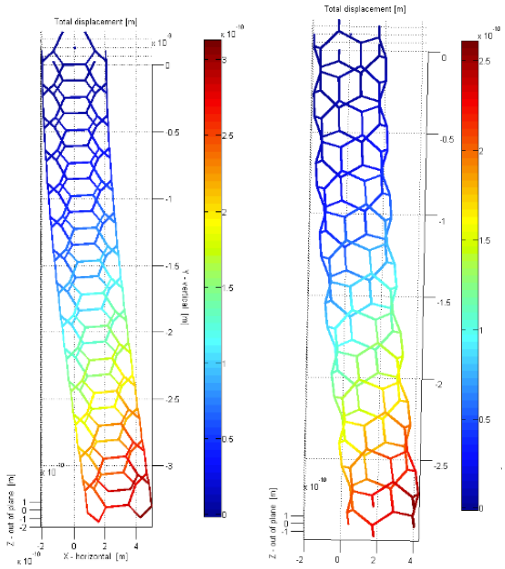

Figure 3: Sugar CNT model. Users can simulate CNTs of desired length and chirality in Sugar. Deflected CNT's are shown here. (a) Armchair (3,3) CNT and (b) Zigzag (5,0) CNT of length 3nm each.

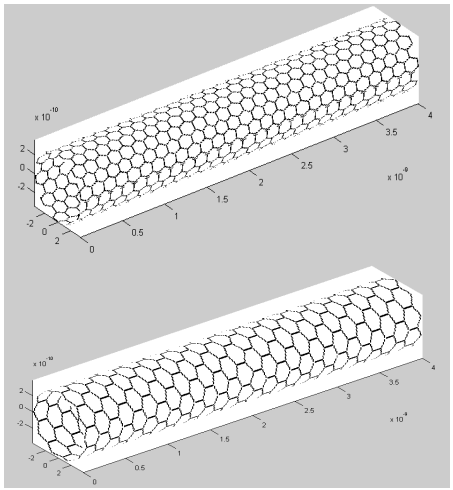

Figure 4: Reduced-order lumped CNT model can be used to quickly simulate larger or systems of CNTs without a reduction in accuracy. Shown here are (a) graphical display for Armchair (10,10) CNT and (b) Zigzag (10,0) CNT of length 4nm each.

3.2 SugarCube Models

The models for the two kinds of symmetrical CNTs are also available for use in SugarCube [7], which is a novice-friendly online tool for manipulating parameter values of ready-made N/MEMS that were initially configured using Sugar. The user can change various parameters like chirality, length and magnitude and direction of applied nodal forces. The model outputs the displaced structure and the displacements of the desired node. See Figure 5.

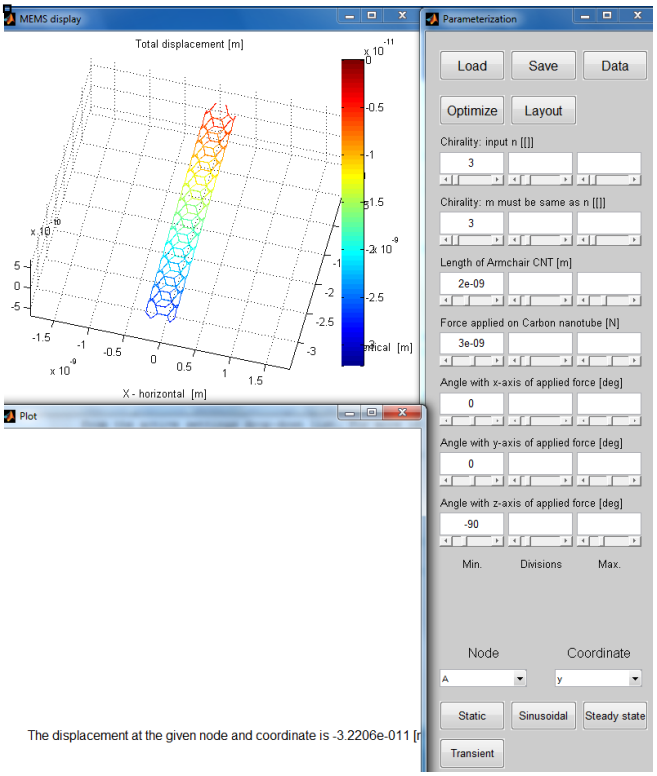

Figure 5: SugarCube. The Armchair CNT **is simulated. A**n axial force of 3nN applied on a (3,3) CNT of length 2nm. A displacement of 3.2e-11 nm is obtained.

4. APPLICATIONS

In this section, we discuss a few examples to demonstrate the application of our CNT model in N/MEMS. We exemplify a nanomaterial testing device based on [8], nanomotor based on [9], and a proposed NEMS comb drive resonator.

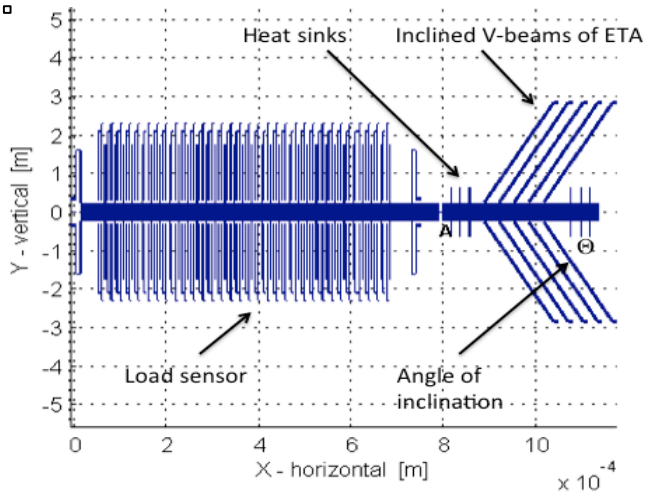

Figure 6: MEMS nanomaterial testing device modeled in Sugar [10]. The CNT test specimen is placed at node A. The CNT has a diameter of 0.78nm and length of 5nm. The user is able to optimize the thermal actuator and electrostatic sensor of the MEMS device to suit the expected properties of test specimens.

Nanomaterial tester. As a first example, we demonstrate the use of the CNT model for performance optimization of the MEMS-based Nanomaterial testing device developed by Espinosa et al. [8]. The chosen stiffness of the actuator and the load sensor are a strong function of the properties of the nanoscale specimen to be investigated. Hence, these properties need to be tailored for the prescribed nanostructure specimen in order to obtain sufficient or optimal performance.

We have modeled the material testing device in Sugar (see Figure 6). Here, at node A is a CNT of diameter 0.78nm and length 5nm. A specimen elongation of 172.8nm was obtained from the Sugar CNT model, for an average temperature rise of 150deg of the V-beams. For the same specimen, the elongation was found to be 149.6nm from the analytical model. Refer [8], [10] for details on the complete analysis.

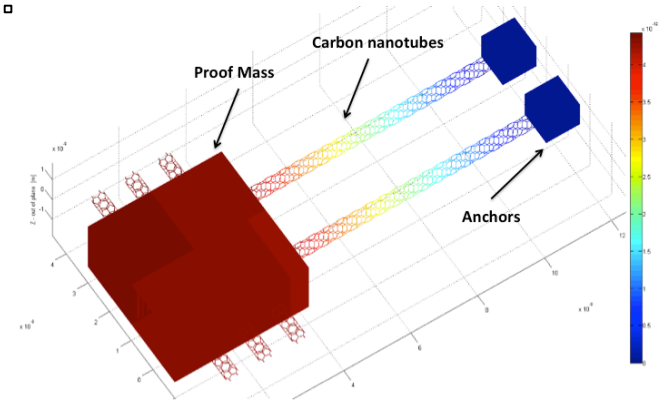

Figure 7: CNT comb drive resonator. The proposed NEMS resonator consists of CNT flexures and comb drive fingers. The anchors and proof mass may be deposited bulk material.

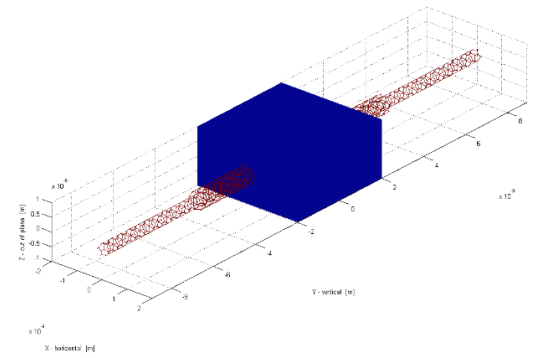

Figure 8: Nanomotor. A design of a nanomotor is shown. Full 3D electric field analysis has yet to be implemented for complete analysis of the nanomotor.

NEMS resonator. The CNT model can be used to explore the design of a NEMS comb drive resonator. In Figure 7 we show a proposed resonator with flexures and comb fingers composed of CNTs. The CNTs flexures have a diameter of 0.39nm and length of 6nm. The proof mass is a poly-silicon deposit of length, width, and height of 3nm each.

As a last example, in Figure 8 we exemplify our CNT model used in the design of a nanomotor. The original nanomotor was demonstrated by [9]. It consists of an outer CNT sleeve surrounding a central CNT support.

5. CONCLUSIONS

In this paper we introduce a new online tool for simulating the geometry and dynamic behavior of carbon nanotubes. The CNT models are implemented in both Sugar and SugarCube. The models do not require any programming or extensive training to use. They allow novice users to analyze the dynamic response of the CNT structure to small applied forces. The user can either use the original CNT models for analyzing small structures, or the more computationally efficient reduced-order model for simulating larger CNTs.

Currently, models for static analysis of symmetrical CNTs (zigzag and armchair) are available. This work will be extended to model CNTs of asymmetrical chirality. The transient model is also currently under construction.

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