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A MULTISCALE COMPUTATIONAL FRAMEWORK FOR THE MODELING OF CARBON NANOTUBES

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Summary. *A multiscale computational framework is presented for developing a coupled self-consistent system of equations involving molecular mechanics at the small scale and quasi-continuum mechanics at the very large scale. The finite element method developed on the multiscale variational framework furnishes a two level statement of the problem. It provides the multiple-scale analysis capability by concurrently feeding the information at the molecular scale, formulated in terms of the nano-scale material moduli, into the quasi-continuum equations. Interatomic interactions are incorporated into the model through a set of analytical equations with internal variables that are a function of the local state of deformation [1]. Multi-body potentials of the Tersoff-Brenner type are employed to model point defects that affect atomic structure locally, and therefore generate localized displacements with localized force fields. The nano-scale material moduli are integrated into a modified form of the Geometrically Exact Shell Model [2] to model nanotubes. Representative numerical examples are shown to validate the model and demonstrate its range of applicability.*

1 INTRODUCTION

A mathematically consistent multiscale computational framework is presented for bridging the scales between molecular mechanics and nanoscale based quasi-continuum mechanics. Instead of employing the commonly practiced "computational" nesting of information from smaller scales into the larger ones, we propose a novel mathematical nesting of scales that yield the proposed multi-scale method. We employ two concurrent domains: a nanoscale continuum domain for the defect free nanotube, and an atomic scale domain that models the localized defects in graphene sheets and nanotubes. The stick-slip model of Gao and co-workers [1] is employed to yield nanoscale material moduli that are a function of internal variables which are in turn based on the changes in the bond lengths and bond angles that occur because of the local state of deformation. Multi-body interatomic potentials of the Tersoff-Brenner type are employed to generate localized force fields around point defects in the graphene sheets and nanotubes.

2 A MULTISCALE COMPUTATIONAL FRAMEWORK

This section illustrates the multiscale method and presents the key ideas underlying the proposed method. Let $\mathcal{L}$ be the differential operator of the partial differential equation that governs the deformation of the nano-structure.

$$\mathcal{L}\boldsymbol{u}=\boldsymbol{f} \quad \text{in} \quad \Omega \tag{1}$$

The corresponding variational form obtained via standard procedure can be expressed as:

$$(\boldsymbol{w}, \mathcal{L}\,\boldsymbol{u}) = (\boldsymbol{w}, \boldsymbol{f}) \tag{2}$$

We assume an additive decomposition of the total solution into coarse scales $\widetilde{\boldsymbol{u}}$ (i.e., meso-to-micro scales) and fine scales $\boldsymbol{u}'$ (i.e., micro-to nano scales).

$$\boldsymbol{u}=\widetilde{\boldsymbol{u}}+\boldsymbol{u}' \tag{3}$$

We assume a similar decomposition of the weighting function

$$\boldsymbol{w}=\widetilde{\boldsymbol{w}}+\boldsymbol{w}' \tag{4}$$

where $\widetilde{\boldsymbol{w}}$ are the weighting functions for the coarse scales and $\boldsymbol{w}'$ are the weighting functions for the fine scales. In addition, we assume an additive decomposition of the forcing function into coarse scales $\widetilde{\boldsymbol{f}}$ (meso-to-micro) and fine scales $\boldsymbol{f}'$ (micro-to-nano) components.

$$\boldsymbol{f}=\widetilde{\boldsymbol{f}}+\boldsymbol{f}' \tag{5}$$

Substituting $\boldsymbol{u}, \boldsymbol{w}$ and $\boldsymbol{f}$ in (2) we get

$$(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \mathcal{L}(\widetilde{\boldsymbol{u}}+\boldsymbol{u}'))=(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \widetilde{\boldsymbol{f}}+\boldsymbol{f}') \tag{6}$$

The proposed additive decomposition of the forcing function gives rise to a further decomposition of the coarse and fine scale solutions such that

$$\widetilde{\boldsymbol{u}}=\widetilde{\boldsymbol{u}}_{\widetilde{f}}+\widetilde{\boldsymbol{u}}_{f'} \tag{7}$$

$$\boldsymbol{u}'=\boldsymbol{u}'_{\widetilde{f}}+\boldsymbol{u}'_{f'} \tag{8}$$

Wherein $\widetilde{\boldsymbol{u}}_{\widetilde{f}}$ and $\boldsymbol{u}'_{\widetilde{f}}$ are the coarse and fine scale components of the solution that arise because of microscale force terms $\widetilde{\boldsymbol{f}}$. Similarly, $\widetilde{\boldsymbol{u}}_{f'}$ and $\boldsymbol{u}'_{f'}$ are the coarse and fine scale components of the solution that arise because of $\boldsymbol{f}'$. Substituting (7) and (8) in (6) we get

$$\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \mathcal{L}\left((\widetilde{\boldsymbol{u}}_{\widetilde{f}}+\widetilde{\boldsymbol{u}}_{f'})+(\boldsymbol{u}'_{\widetilde{f}}+\boldsymbol{u}'_{f'})\right)\right)=\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \widetilde{\boldsymbol{f}}+\boldsymbol{f}'\right) \tag{9}$$

Employing bi-linearity in (9), and assuming $\widetilde{\boldsymbol{f}}$ and $\boldsymbol{f}'$ to be linearly independent we obtain a split of the problem that leads to the following two sub-problems.

Meso-Micro Scale Problem: $$\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \mathcal{L}(\widetilde{\boldsymbol{u}}_{\widetilde{f}}+\boldsymbol{u}'_{\widetilde{f}})\right)=\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \widetilde{\boldsymbol{f}}\right) \tag{10}$$

Micro-Nano Scale Problem: $$\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \mathcal{L}(\widetilde{\boldsymbol{u}}_{f'}+\boldsymbol{u}'_{f'})\right)=\left(\widetilde{\boldsymbol{w}}+\boldsymbol{w}', \boldsymbol{f}'\right) \tag{11}$$

It is important to note that if we sum (10) and (11), we recover equation (9). In (11) the components $\widetilde{\boldsymbol{u}}_{f'}$ and $\boldsymbol{u}'_{f'}$ are associated with the meso-to-micro and the micro-to-nano displacement fields, respectively, that arise because of $\boldsymbol{f}'$. In this framework $\widetilde{\boldsymbol{u}}_{f'}$ and $\boldsymbol{u}'_{\widetilde{f}}$ are the displacement components that transfer information between scales, and thus act as the bridging scales. Consequently, this framework provides a neat merger of the two

displacement fields arising because of the nano forcing function $\boldsymbol{f}'$ that is obtained from the MD model and the micro forcing function $\widetilde{\boldsymbol{f}}$ that arises because of the loading environment.

3 NUMERICAL RESULTS

The multiscale method is employed for studying the mechanical properties of defect-free and defective carbon nanotubes. Various types of nanotube, e.g., zigzag tubes, armchair tubes, and nanotubes with arbitrary chirality are investigated. Figures 1 presents the Poisson's ratio and Young's modulus for the nanotubes, wherein the multi-body interatomic potentials are incorporated into the nano-structural model via a set of analytical equations [1]. These equations yield nanoscale material moduli (for the defect-free carbon nanotube) that are a function of internal variables and are based on the changes in the bond lengths and bond angles occurring because of the local state of deformation. The nano-scale based material moduli are embebed in a modified form of the geometrically exact shell model by Simo and co-workers [2]. Figure 2 presents the bending collapse of a carbon nanotube, modeled via the multiscale method, while Figure 3 presents stretch loading, elastic stretching, and elastic "localization" in the carbon nanotube.

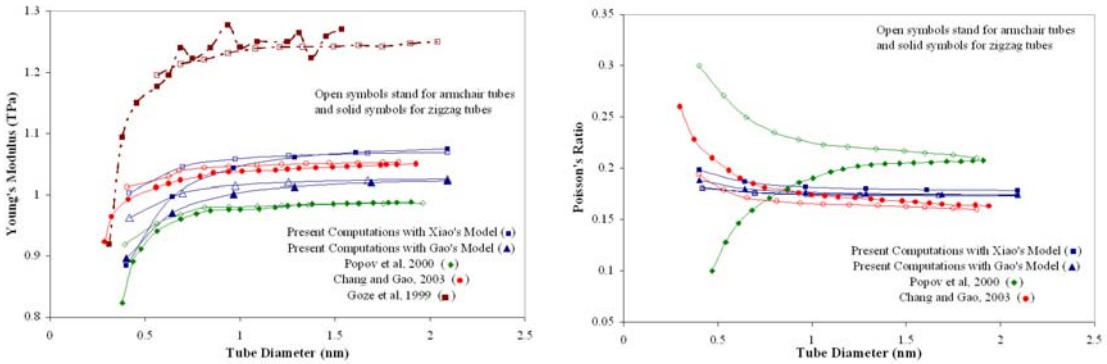

Figure 1. Nano-tube: Young's modulus and Poisson ratio

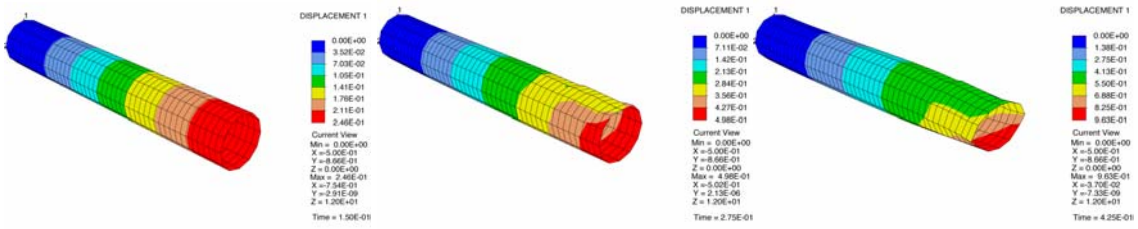

Fig. 2. The bending collapse of a carbon nanotube, modeled via the multiscale method.

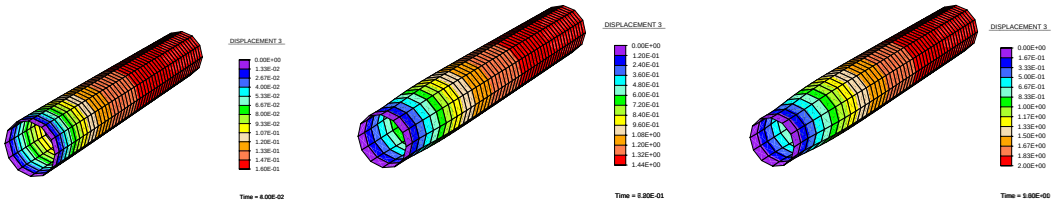

Fig. 3. Stretch loading and elastic stretching of the nanotube.

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