

# A Reduced-Order General Continuum Method for Dynamic Simulations of Carbon Nanotube

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## ABSTRACT

*In this paper, a reduced-order general continuum method for simulating the three-dimensional transient mechanical behaviors of carbon nanotube (CNT) is presented. The method builds the potential energy density for carbon nanotubes by applying the macroscopic deformation gradient to the atomistic energy potential based on a modified Cauchy-Born rule. The minimum energy principle in finite element methods can be used to obtain the equilibrium solution of the resulting equations. To compute the dynamic behaviors of carbon nanotubes, an explicit Newmark time integration scheme is applied to augment the static formulation. Details of the proposed formulation to study CNT dynamics are described. The results of simulation cases are then presented. The cases include a two-dimensional carbon atomic ring interacting with carbon substrate, static deformation of carbon nanotube, such as elongation, buckling, and twisting, and dynamic deformation of CNT-AFM probe with point force loading. Where possible, the results are compared with those obtained by molecular dynamics and atomic based finite element methods. The comparison shows that the current method can capture unique nonlinear characteristics of CNTs and provide predictions of the CNT's transient behaviors.*

*Keywords:* Atomistic-Based Finite Element, Carbon Nanotube, Cauchy-Born Rule, Dynamical Behavior, Mechanical Properties

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## INTRODUCTION

Since first found in the form of multi-walled carbon nanotubes (MWNTs) by Iijima (1991) carbon nanotubes (CNT) have gained overwhelming attention in many areas of science and engineering for their outstanding and unique properties. CNTs are small size, low density, high stiffness, and high strength materials. CNTs can be used to produce, for example, enhanced

composite materials for efficient heat removal, and precise drug delivery. These and other potential applications of CNT have provided strong drivers to develop numerical methods to better predict their mechanical behavior.

Two major types of computational approach can be recognized in the literature. They are the classical molecular dynamics (MD) methods (Iijima et al., 1996) and those that link atomistic constitutive laws to the finite element framework (Tadmor et al., 1996; Miller & Tadmor, 2009; Arroyo & Belytschko, 2002;

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Pantano et al., 2004; Garg et al., 2007; Tadmor et al., 1999). It is well known that the MD method excels at modeling structural details of a crystal at the lattice level. Its computational cost, however, can be prohibitive for large systems. For example (Tadmor et al., 1999), a MD simulation of a system with the number of atoms in the order of  $10^9$ , corresponding to less than a few hundred nanometers in dimension, lends itself to a significant challenge to computing capacity. Given the fact that the mean diameter of an MWNT is in the range of 5 to 100 nm and the length is about several micrometers (Tadmor et al., 1999), the MD method is less than an ideal candidate for routine use to simulate the mechanical and dynamic behavior of CNTs. On the other hand, the results obtained by using the MD method have suggested that the majority of the lattice deforms smoothly and closely obeys continuum elasticity. Yakobson et al. (1996) used the MD method to study CNTs under three basic mechanical loads: axial compression, bending, and torsion. They reported a remarkable synergism between the results of MD and those of macroscopic structural mechanics. Arroyo et al. (2005) used a two-dimensional atomic rope deformation case to study the convergence property of an atomistic based finite element method (or continuum method). It was shown that, with increasing number of atoms simulated, the strain energy of the rope obtained from the continuum method converged to that from a parent atomic model. Consequently, continuum methods with constitutive laws constructed upon atomistic energy functions can play an important role in CNT simulations.

In what follows we present a brief review of two types of reduced-order continuum schemes, i.e. the general continuum method and the elastic model-based continuum method used in the prediction of the mechanical behavior of CNTs. For a more general review readers are referred to Miller and Tadmor (2009) where fourteen different reduced-order schemes were compared for a static Lomer dislocation dipole problem in face centered cubic aluminum.

A general continuum method develops the constitutive law from an atomistic energy function using intrinsic geometric quantities to describe deformation. The earliest work in this regard was, to the authors' knowledge, Tadmor et al. (1996), which was designed for defect analysis in solids. The concepts of local and nonlocal formulations were introduced to account for inhomogeneous phenomena of material, such as stacking faults and dislocations. If the size of a finite element is larger than the crystallite radius, then the homogeneity can be assumed for the element, or, in other words, the deformation gradient  $\mathbf{F}$  is uniform over the element. The status of the element is considered local. The total strain energy can be calculated by summing up the contribution from the local elements, which, in turn, defines the first Piola-Kirchhoff stress tensor and the Lagrangian tangent stiffness tensor. The local formulation can thus be built upon these quantities. If the size of a finite element is smaller than the crystallite radius then the motion of atoms in the crystallite can not be described by a uniform local deformation gradient  $\mathbf{F}$  and the element is considered nonlocal. The actual displacement of each atom is needed for the construction of strain energy. Coupling the local and the nonlocal formulations can be effective in computing material defects in that, at the grain boundaries where the inhomogeneous structural events are expected, the nonlocal formulation can be invoked, while the local formulation is applied in regions of lower strain.

Geometrically, a CNT is essentially a curved lattice structure or a two-dimensional manifold embedded in three-dimensional space. A bond of CNT is the chord of the curved surface rather than its tangent. A direct application of the Cauchy-Born rule (Zanzotto, 1996; Ericksen, 2008) in the form of  $\mathbf{w}=\mathbf{F}\mathbf{A}$ , where  $\mathbf{w}$  denotes the tangent vector of the CNT surface and  $\mathbf{A}$  the undeformed carbon-carbon bond on the rectangular graphene sheet, is therefore invalid for CNT modeling. In an application of a general continuum method to CNT simulation the exponential Cauchy-Born rule (Arroyo &

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