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Analysis of single-walled carbon nanotubes using the moving Kriging interpolation

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ABSTRACT

The higher-order Cauchy–Born rule is applied to predict the mechanical response of single-walled carbon nanotubes (SWCNTs). As second-order deformation gradients can describe the bending effect of C–C bond vectors involved in the theoretical scheme of the higher-order gradient continuum, the established constitutive model accords extremely well with physical behavior. From the constitutive relationship constructed, a novel computational method is proposed for numerical simulation of buckling behaviors of SWCNTs. In this study, a new mesh-free method developed from the moving Kriging (MK) interpolation is employed to implement numerical simulation of mechanical properties of SWCNTs under axis-symmetrical loadings. As the mesh-free shape function constructed using the MK interpolation has the delta function property, the shape functions satisfy the essential boundary conditions automatically. Therefore, the essential boundary conditions can be easily implemented. Several numerical examples of buckling behaviors of SWCNTs are presented to test the effectiveness and efficiency of this method. The numerical results are also compared with those obtained from the full atomistic simulation method, and are found to be in agreement. Moreover, this computational method can largely reduce the degrees of freedom of the system, and thus save a large amount of computational resources. As a result, this is a very attractive approach, which has great potential in the engineering field. This mesh-free method is further applied to the study of post-buckling of SWCNTs. The results are compared with those obtained from full atomistic simulation, and demonstrate that this method is truly effective and efficient.

1. Introduction

Due to the exceptional mechanical, chemical and electrical properties of carbon nanotubes (CNTs), various researchers in different research fields have sought to understand the diverse aspects of CNT properties. The landmark paper on CNTs was reported in the last century by Iijima of the NEC Corporation [1]. Generally speaking, CNTs are studied and simulated using atomistic modeling approaches [2–9] since these modeling approaches can capture the microscale physical mechanisms of nanostructures. However, they require tremendous computational resources and time and, therefore, their applications have been quite limited. Liew et al. [5,6] spent 36 h studying the buckling behavior of a (10,10) single-walled CNT (SWCNT) containing 2000 atoms with molecular dynamics simulation in a single SGI origin 2000 CPU; investigation of a four-walled CNT containing 15097 atoms required 4 months. In view of these problems, there is an urgent need to establish an effective and efficient computational method. Researchers have sought to adopt alternative approaches, e.g. continuum simulation methods [10–17], instead of working from an atomic perspective. Continuum simulation has been found to be computationally very efficient. These continuum simulation methods, which can largely reduce the degrees of freedom, are much faster than molecular simulations for analyzing nanostructures. Thus, they are much more attractive in studying large systems. Govindjee and Sackman [10] applied the Euler beam theory to simulate mechanical properties of CNTs. Ru [11,12] treated a SWCNT as a single-layer shell with an effective bending stiffness and modeled mechanical responses of CNTs under axial compression. Li and Chou [13] employed a molecular structural mechanics method to predict elastic properties of SWCNTs. He et al. [14] and Liew et al. [15] employed a continuum cylindrical shell model to account for the van der Waals interaction between different walls of CNTs. Wang and Hu [16] and Wang et al. [17] investigated the longitudinal and flexural wave propagation in CNTs by modeling a CNT as a non-local elastic cylindrical shell and employing continuum mechanics. One continuum modeling approach, traced back to the quasi-continuum method [19–21] for two-dimensional problems, was constructed from the Cauchy–Born rule [18,19], where the constitutive relationship is derived by linking atomic structure of material to a continuum level. Due to the lack of centrosymmetry of the hexagonal lattice structures in CNTs,

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internal relaxation needs to be adopted to ensure the minimum energy of the atomic system. Zhang et al. [22,23] proposed this internal relaxation method when studying CNTs. They recommended a combination of interatomic potentials with a continuum model and studied linear elastic modulus fracture nucleation. However, as Arroyo and Belytschko [24,25] suggested, this application of the standard Cauchy–Born rule may be inadequate. Essentially, SWCNTs are curved crystalline sheets with a one-atom thickness. Therefore, the curved effect should not be neglected. Arroyo and Belytschko's numerical simulation demonstrated that the constitutive relationship constructed based on an exponential Cauchy–Born rule can truly describe buckling behaviors of CNTs, while modeling based on the standard Cauchy–Born rule cannot, since the standard Cauchy–Born rule cannot describe the bending effect. Sunyk and Steinmann [26] noted that deformations of the underlying crystal must be sufficiently homogeneous when the Cauchy–Born rule is to be applied. Thus, they introduced the second-order deformation gradient to capture inhomogeneous deformations. Later, Guo et al. [27] and Wang et al. [28] proposed a higher-order Cauchy–Born rule for analysis of elastic properties of SWCNTs by considering the effect of the second order gradient. The mesh-free method using the moving least square (MLS), recently proposed by Liew et al. [29] and Peng et al. [30], has been shown to have great potential in solving large deformation and buckling of SWCNTs.

This paper focuses principally on numerical computational validity and efficiency of the constitutive relationship constructed using the higher order Cauchy–Born rule through the moving Kriging (MK) interpolation approach [31–34]. We model the nanostructure in the theoretical framework of the higher order gradient continuum, in which the strain energy density depends not only on the first order but also the second order deformation gradient. After considering the second order deformation gradient in simulation of mechanical properties of CNTs, the effect of bending stiffness is captured and buckling behaviors are described. With the higher-order Cauchy–Born rule mapping the reference configuration to the current configuration, deformation energy of a representative cell can be obtained and the average strain energy density is equal to the energy of an equivalent volume of the continuum. We select an equilibrium graphite sheet and an undeformed SWCNT as the reference and the current configuration. Then the rolling process mapping from the planar sheet to the cylindrical structure is described by the three optimization parameters λ_1, λ_2 and θ, corresponding to the uniform longitudinal and circumferential stretches and the twist angle, respectively. Moreover, as described before, due to the crystalline lattice structures in CNTs without centrosymmetry, an inner shift η should be introduced to ensure the minimum energy of the system.

Subsequently, based on the higher-order gradient theory, an approximate numerical technique should be used to implement the numerical simulation. However, as the second order gradient involved in the theory requires C^1-continuity [35,36] of interpolation of displacements, it is difficult to establish the elements and construct the interpolation function using the finite element method (FEM). Recently, scholars have employed the mesh-free method to study nanostructures. The mesh-free method is a newly-developed technique with higher-order continuous interpolation of displacement that is superior to traditional computational techniques. Sun and Liew [37,38] and Liew and Sun [39] applied the higher-order Cauchy–Born rule to simulate mechanical responses of SWCNTs under axial-symmetrical loadings. Their simulations demonstrated that a small number of meshless nodes could achieve a good effect when deformation of the crystalline structures was homogeneous, and with an increase in number of nodes, the buckling pattern can be accurately displayed. However, using this method, it was difficult to implement the boundary conditions, due to lack of the delta function. The Kriging interpolation has advantages of both higher order continuity and delta function property and thus is used to construct the mesh-free shape function. Moreover, by employing the semivariogram model for numerical calculations, the constructed shape function is easy to express and convenient for first- and second-order differentiation. In the present work, we have constructed a meshless computational framework using moving Kriging interpolation to conduct numerical calculation of SWCNTs, in order to overcome the delta issue.

The remainder of the paper is organized as follows. In Section 2, the moving Kriging interpolation is reviewed. Section 3 presents the higher-order gradient continuum theory and the constitutive relationship of the present model. By employing the Brenner potential, the constitutive relationship is also derived by the higher-order Cauchy–Born rule. This rule links the atomistic level to continuum deformation of a SWCNT. This section describes how to establish the reference configuration and provide an original image of the cell structure. In Section 4, the meshless computational framework developed is illustrated in detail. First, several numerical results of axial buckling behaviors of SWCNTs are provided to demonstrate the efficiency and effectiveness of this method. Then post-buckling behaviors under axial compression and other types of buckling behaviors under bending, torsion and hydrostatic pressure are also simulated, using the mesh-free method. Section 5 presents conclusions of the present research.

2. The moving Kriging interpolation

Kriging was first applied in geostatistics for spatial interpolation and was used for construction of the shape function and its derivatives. Like the moving least square approximation (MLS), Kriging interpolation can also be extended to any sub-domain $\Omega(x_i)$-termed moving Kriging. We consider a distribution function $u(x_i)$ in a sub-domain $\Omega(x_i)$. The sub-domain is represented by a series of dispersive nodes $x_i (i = 1,2,\ldots,n)$, where n is the total number of nodes of the sub-domain. With n given field values $u(x_1)$, $u(x_2),\ldots,u(x_n)$, the approximate field function $\hat{u}(x)$ can be interpolated by a weighted linear combination:

$$\hat{u}(x) = \sum_{i=1}^{n} \lambda_i(x) u(x_i), \tag{1}$$

where $\lambda_i(x)$ is the weight function of the ith node. There are two conditions which should be satisfied when selecting coefficients $\lambda_i(x)$, i.e. unbiasedness and minimum variance.

The first term is unbiasedness, which implies that the expected value of approximate function $\hat{u}(x)$ must be equivalent to that of $u(x)$:

$$E[u(x)] = E[\hat{u}(x)], \tag{2}$$

Substitution of Eq. (1) into Eq. (2) yields:

$$E[u(x)] = E\left[\sum_{i=1}^{n} \lambda_i(x) u(x_i)\right]. \tag{3}$$

A polynomial drift model $p_l(x)$ is summarized by

$$\sum_{i=1}^{n} \lambda_i(x) p_l(x_i) = p_l(x), \quad 1 \leqslant l \leqslant m, \quad p_1(x) = 1, \tag{4}$$

A commonly used linear basis in one-, two- and three-dimensional space is given as:

$$\boldsymbol{p}^T(\boldsymbol{x}) = (1, x_1), \quad m = 2, \tag{5}$$

$$\boldsymbol{p}^T(\boldsymbol{x}) = (1, x_1, x_2), \quad m = 3, \tag{6}$$

$$\boldsymbol{p}^T(\boldsymbol{x}) = (1, x_1, x_2, x_3), \quad m = 4, \tag{7}$$

and a quadratic basis is: