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Nanoscale vibration and buckling of single-walled carbon nanotubes using the meshless local Petrov–Galerkin method

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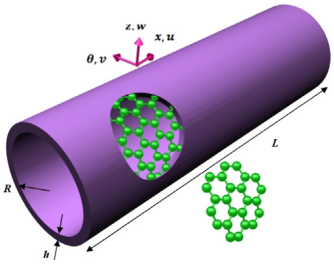
HIGHLIGHTS

- Developing a meshless nonlocal shell model for vibration and buckling analysis of SWCNTs.
- Applying the MLPG method to numerically solve the problem.
- Exploring the effects of nonlocal parameter and geometry and boundary conditions.
- Calibrating the nonlocal parameter with MD simulations.

GRAPHICAL ABSTRACT

A size-dependent meshfree shell model is developed to describe vibration and buckling characteristics of SWCNTs. The model is validated by MD simulations.



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ABSTRACT

The meshless local Petrov–Galerkin (MLPG) method is implemented to analyze the free vibration and axial buckling characteristics of single-walled carbon nanotubes (SWCNTs) with different boundary conditions. To this end, a nonlocal shell model accounting for the small scale effect is used. In the theoretical formulations, a variational form of the Donnell shell equations is constructed over a local subdomain which leads to derivation of the mass, stiffness and geometrical stiffness matrices. Comprehensive results for the resonant frequencies and critical axial buckling loads of SWCNTs are presented. The influences of boundary conditions, nonlocal parameter and geometrical parameters on the mechanical behavior of SWCNTs are fully investigated. The results obtained from the present numerical scheme are shown to be in good agreement with those from exact solution for simply-supported SWCNTs and those of molecular dynamics simulations. It is shown that the natural frequencies and critical axial buckling loads of SWCNTs are strongly dependent on the small scale effect and geometrical parameters.

1. Introduction

In the past two decades, nano-sized structures have gained considerable interest in the research community as reflected by the surge of the nano-related publications. Since the publication of Iijima's paper in 1991 on carbon nanotube (CNT) [1], this nanostructure has become one of the hottest frontiers in different fields of science due to its superior mechanical and electrical properties. The fundamental building block of CNTs is single-walled carbon nanotubes (SWCNTs) which are the cylinders with the thickness of one atom and can be described as a rolled-up graphene sheet. One of the efficient techniques that usually used to understand the behavior of nanostructures is continuum-based modeling [2]. To incorporate the small size effects into the continuum models, some researchers have suggested the application of nonlocal version of continuum mechanics proposed by Eringen [3,4]. The nonlocal continuum theory was initially introduced to nanotechnology by Peddieson et al. [5] which motivated many other researchers to use nonlocal models in the analysis of nanostructures [6–24]. Considerable studies on vibrational and buckling

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responses of CNTs using nonlocal continuum mechanics have been carried out, in which some have been organized on the basis of beam models [6–17] and some others based on the shell models [18–24]. By adjusting the nonlocal parameter, the nonlocal shell models have the capability to predict accurate results, which are comparable to those of atomistic approaches such as molecular dynamics (MD) simulations. As seen from the previous studies on the behaviors of CNTs, most of them have been limited to simply-supported nanotubes for which exact solution exists. In the computational nanomechanics, developing influential techniques capable of treating various boundary conditions are clearly indispensable. Recently, meshless methods have become attractive alternatives for solving problems, as they do not rely on a grid or a mesh and employ a set of scattered nodes to discritize the problem domain. They are proposed to overcome some shortcomings of classical mesh-based methods such as finite element method (FEM), including the need for re-mesh to be more accurate, inaccuracy near the boundaries of problem, mesh distortion in large deformation problems, etc. [25]. The meshless methods were originated in 1977 by Lucy who used the smooth particle hydrodynamics (SPH) method for modeling astrophysical phenomena [26]. At present, there are many meshfree methods including the diffuse element method (DEM) [27], the element-free Galerkin (EFG) [28], the point interpolation method (PIM) [29], the reproducing kernel particle (RKP) [30], the partition of unity method (PUM)[31], hp-clouds [32], the natural element method (NEM) [33], the meshless local Petrov–Galerkin (MLPG) [34,35], the local point interpolation method (LPIM) which is based on the idea of the MLPG approach [36] and so on, in which different interpolation techniques are used. Unlike the MLPG, most of the meshless methods are not truly meshless techniques due to using background cells for integration of a weak form over the problem domain. In the MLPG method, no element is used for interpolation and integration. Also, the nodal trial and test functions can be chosen from different spaces which classified the MLPG method as MLPG1 to MLPG6 [37,38]. The MLPG method has been applied for the static analysis of two-dimensional solids and one-dimensional beams in [39]. Gu and Liu [40] proposed the MLPG formulation for the free vibration and forced vibrations of two-dimensional structures by using the moving least squares approximation as the shape function. Their results demonstrated the convergence, efficiency and flexibility of the MLPG approach. In the present work, as an applicable computational method in the area of nanotechnology, the moving least squares (MLS) interpolation is employed to construct both trial and test functions which labeled as MLPG6. The main purpose of this study is to analyze the free vibration and axial buckling characteristics of SWCNTs with arbitrary boundary conditions via a nonlocal shell model in which the small length-scale effect is taken into account. The obtained results from the present model are assessed by those of MD simulations and the appropriate nonlocal parameters are proposed for each chirality and boundary condition. Moreover, the evaluated results of the simply-supported SWCNT are compared with those of obtained by exact analytical solution.

2. Meshless local Petrve–Galerkin method

In the meshless local Petrove–Galerkin method, the global domain of problem Ω constructed from a set of scattered nodes, as shown in Fig. 1. This method is conventionally based on a local approximation or interpolation to introduce the trial function and a local weak form through the use of weighted-residual procedure. In the present study, the local variational form is constructed over a local sub-domain Ω_s bounded by Γ_s (see Fig. 1). The sub-domains which have very simple shapes such as a linear support domain for one-dimensional problems and a circle or a rectangular in two-dimensional problems, entirely situated on the global domain and could overlap each other. The variational form over a local quadrature domain is integrated in which the domains of other nodes are not taken into account. Since there is no need for any meshes or background cells for interpolation or integration purpose, the method is known as a "truly" meshless one. Thus, there are two local domains centered by node i: local integration domain Ω_Q and local interpolation domain Ω_i for Guass integration point x_Q, as shown in Fig. 1. It should be noted that for performed local variational forms, the test function and local integration domains are the same. The implementation of this method for vibration and buckling analysis of a SWCNT will be discussed later on.

2.1. Moving least squares approximation

In the present MLPG method, the nodal trial function and test function are chosen from the same function space and correspond to the Moving Least Squares (MLS) approximation. A function $v(x)$ can be approximated by $v^h(x)$ in the sub-domain Ω_s as

$$v^h(x) = \sum_{I=1}^{n} q_I(x) b_I(x) = q^{\mathbf{T}}(x) b(x) \tag{1}$$

where $q_I(x)$ are the monomial basis functions, $b_I(x)$ are the corresponding coefficients and n is the number of nodes located in the local interpolation domain. The commonly used monomial basis functions and the first derivation of them are given as

$$q^{\mathbf{T}} = [1, x, x^2, \ldots, x^M] \tag{2}$$

$$q_x^{\mathbf{T}} = [0, 1, 2x, \ldots, Mx^{M-1}] \tag{3}$$

in which M is the number of basis functions.

The unknown coefficients $b_I(x)$ are obtained by the minimization of a weighted discrete L_2 norm

$$\Gamma = \sum_{I=1}^{n} \omega(x - x_I) \, [q^{\mathbf{T}}(x_I) b(x) - v_I]^2 \tag{4}$$

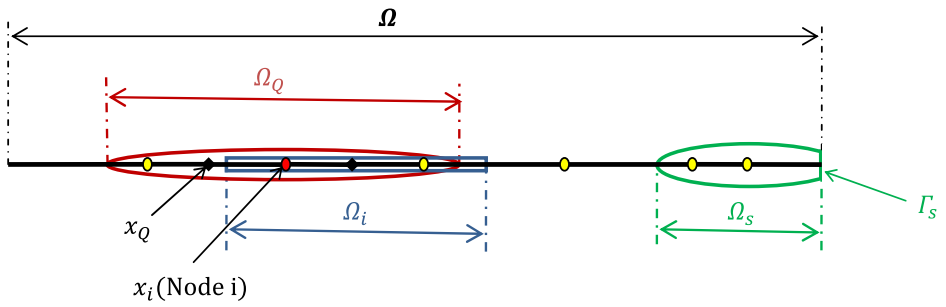

Fig. 1. Different sub-domains Ω_s for each node consist of the local integration domain Ω_Q for node x_i and local interpolation domain Ω_i for Guass integration point x_Q