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A neural network-based surrogate model for carbon nanotubes with geometric nonlinearities

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Abstract

This paper presents a neural network (NN)-based surrogate modeling approach suitable for the geometrically nonlinear analysis of carbon nanotubes (CNTs). In this work we propose an NN-based equivalent beam element (NN-EBE) which is capable of accurately predicting the high-order phenomena caused by size-effects that characterize the behavior of CNTs at the nano-scale and can only be predicted by micro-mechanical models. The basic idea is to approximate the residual forces of the Newton–Raphson incremental-iterative formulation of the classical Euler or Timoshenko beams of the EBE model by an NN prediction, which is based on the response of the detailed MSM model of a CNT portion. Several numerical examples are presented for straight and wavy CNTs under bending and compression, which demonstrate that the proposed methodology is possible to efficiently predict the nonlinear response of large-scale CNT structures in a fraction computing time compared to the full-scale problem.

Keywords: Surrogate model; Carbon nanotubes; Molecular structural mechanics; Nonlinear geometry; Artificial neural networks

1. Introduction

Since their discovery by Iijima [1] in 1991, carbon nanotubes (CNTs) have attracted much attention because of their great mechanical, electrical and thermal properties. Composite nano-materials that consisted of some polymer matrix reinforced with CNTs can potentially achieve significantly improved properties [2–7] and for this reason their use in telecommunications, aerospace, biomedical and construction applications has been increasing rapidly.

The prediction of the mechanical properties as well as the development of modeling techniques capable of capturing the behavior of the isolated CNTs is of high interest among researchers. There are three major categories of modeling techniques as defined in [8]: (a) the atomistic modeling, which consists of the molecular dynamics (MD) simulations [9–12] and the ab initio approaches [13–16]; (b) the equivalent continuum modeling (ECM), that assumes the CNT lattice as an equivalent continuum medium [17–26]; (c) the nano-scale continuum modeling

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(NCM), in which the Carbon–Carbon bonds are replaced by mechanically equivalent structural elements, constructing a CNT three-dimensional lattice structure. Many NCM methods have been proposed [27–32] but among them the so called molecular structural mechanics (MSM) approach is the most efficient and widely used method due to its simplicity [33–35].

The nonlinear structural response of isolated CNTs has been the subject of extensive research. Their buckling behavior under axial compression, torsion and/or bending has been mainly explored in the framework of MD simulations [17,36–40]. ECM with FEM or nonlocal elasticity [41–51] and NCM [44,52,53] approaches have also been utilized in this context. However, the NCM models exhibit computational intractability, especially when modeling a large number of CNTs, i.e. embedded CNTs in representative volume elements (RVEs) with realistic mesoscale dimensions, as well as in the context of stochastic multiscale optimization problems, where such structural analyses have to be repeated for a large number of times.

In order to address the aforementioned computational demands, a neural network (NN)-based surrogate modeling approach is proposed that is suitable for the geometrically nonlinear analysis of carbon nanotubes (CNTs). The proposed methodology can also be applied to a series of problems in nonlinear structural mechanics, achieving a substantial reduction in the required computational effort. CNTs with a relative small length to diameter aspect ratio exhibit cross-sectional distortions, which lead to local phenomena that cannot be captured even by advanced beam theory approaches. On the other hand, the detailed simulation of CNTs with micro-mechanical models leads to an exponentially large-scale problem, which is computationally very expensive. In this work we propose an NN-based equivalent beam element (NN-EBE) modeling technique that is capable of accurately predicting the high-order phenomena that detailed micro-mechanical models are able to capture, with orders of magnitude less computational effort. The basic idea is to approximate the residual forces of the Newton–Raphson incremental-iterative formulation by an NN prediction of the response of the detailed micro-mechanical CNT model. The NN surrogate model is properly trained to return accurate enough estimates of the elements nodal internal forces, in the range of the applied CNT deformations. Several numerical examples are presented for straight and wavy CNTs under bending and compression. It is demonstrated that using the proposed methodology it is possible to efficiently predict the nonlinear response of complex systems in a fraction computing time compared to the full-scale problem.

The paper is organized as follows: In Section 2 we briefly present the molecular structural mechanics approach as proposed in [33–35] where the covalent bonds are replaced by three-dimensional circular Euler–Bernoulli or Timoshenko beams. In Section 3 the procedure of simulating the nonlinear behavior of CNTs using a series of equivalent beam elements (EBE), as presented in [54], is enhanced with the use of NN predictions of the internal nodal forces. In this section, the basic theoretical aspects of the artificial neural networks and their implementation for the formulation of the NN-based nonlinear EBE are also examined. In Section 4, three test examples are examined in detail and the computational performance of the proposed methodology is presented in Section 5. Finally, in Section 6 the conclusions and some future research directions are discussed.

2. Molecular structural mechanics approach

This section addresses the correlation between molecular and structural mechanics taking into account the nonlinearities caused by the deformation of the lattice of carbon nanotubes when subjected to any type of loading or deformation. This correlation can be achieved by the equivalence of the total potential energy that is known from molecular mechanics with the strain energy caused by deformation that is known from structural mechanics, as described in [28] and in [33], see Fig. 2.

Assuming small deformations and by adopting the harmonic representation, the axial, bending and torsional potential energies of a covalent C–C bond, as shown in Fig. 2(a), can be expressed as:

$$U_r = \frac{1}{2}k_r(r - r_0)^2 = \frac{1}{2}k_r(\Delta r)^2 \tag{1}$$

$$U_\theta = \frac{1}{2}k_\theta(\theta - \theta_0)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2 \tag{2}$$

$$U_\tau = \frac{1}{2}k_\tau(\phi - \phi_0)^2 = \frac{1}{2}k_\tau(\Delta\phi)^2 \tag{3}$$