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Numerical validation of a concurrent atomistic-continuum multiscale method and its application to the buckling analysis of carbon nanotubes

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ABSTRACT

This work applies the framework of a concurrent multiscale approach to the buckling analysis of carbon nanotubes. In particular, the bridging domain method is used to couple a molecular statics model and a continuum mechanics model. The total potential energy of the entire structure is specified by weighted individual energy contributions of overlapping subdomains. In this handshake region, additional kinematics constraints enforce the compatibility between designated atoms and the continuum body. Three different methods are taken into consideration for the kinematics coupling and the corresponding governing equations are presented. The continuum subdomain is handled by means of a finite element approach and the molecular statics is formulated suitable for a common computational implementation. A series of numerical examples investigates the capability of the bridging domain method for its application in the analysis of carbon nanotubes. Initially, the individual approaches for integrating the kinematics constraints into the global equilibrium equations are compared. Then, in the major contribution of the work, the influences of several modelling parameters of the multiscale model on the buckling analysis of a bent single-walled carbon nanotube are numerically studied. In particular, the size of the atomistic section, the extent of the handshake region and the finite element discretisation are varied. Furthermore, the results obtained by the standard and the relaxed variant of the bridging domain method are compared against each other. In addition, the buckling behaviour of a defective carbon nanotube with varying defect locations is presented. The obtained results of the bridging domain multiscale method are persistently validated against full atomistic molecular statics simulations.

1. Introduction

The undaunted ingenuity of engineers results in an ever increasing demand of structures and, thus, materials that own outstanding properties. For instance, a well-matched combination of specific mechanical, thermal, electrical, electronical and chemical characteristics are requested for a desired application. As a result of the ongoing research to meet these demands, scientists all over the world developed and studied nanoscale structures. For instance, after Iijima [1] brought out details about the microscopic structure of carbon nanotubes, a lot of experimental and computational care (see e.g. [2,3] and references therein) was spent to get a better understanding. Thereby, carbon nanotubes turned out to have a great potential because of their remarkable properties in several areas of interest. The most accurate, but at the same time the most

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expensive methods in regard of computational costs are quantum mechanics approaches. However, these simulations are currently limited to system sizes of essentially only theoretical interest. On the other hand, the concept of continuum mechanics is applied and adapted for the study of nanomaterials. This concept allows the numerical calculations of large volumes of material, however, without being able to cover local events at the length scale of atoms and, thus, with limited accuracy. The principally used computational simulations are based on molecular dynamics or molecular statics offering a good ratio between precision and effort. Nevertheless, molecular mechanics approaches may reach their limits in the numerical study of practical applications in view of computational power as well. With these different methods, carbon nanotubes were studied successfully with a focus on mechanical properties as for instance buckling. By collecting the works of several researchers, Wang et al. [4], Wang et al. [5] and Shima [6] provide a literature survey that gives a review of the progress in the buckling analysis of carbon nanotubes. Moreover, defective carbon nanotubes and graphene were objects of desire (see e.g. [7–13]). The majority of publications with context to computational nanotechnology are based on one of the aforementioned approaches. Thus, they provide inside at different length and time scales and suffer specific limitations. An obvious idea to overcome the drawbacks of the individual formulations and to get an effective simulation method is the combination of several approaches. These multiscale methods are separated in the literature into hierarchical and concurrent multiscale approaches providing emerging and powerful tools. In hierarchical approaches, information is passed between two models valid at different length and time scales as for instance between a molecular dynamics and a continuum mechanics model. Such kind of multiscale approaches may use the atomistic model to obtain material properties essential for the constitutive law of the continuum mechanics from the underlying lattice. In this regard, the Cauchy–Born rule [14] and extensions and modifications therefrom have proven to be useful in the study of carbon nanotubes. The hierarchical methods are advantageous in a manner that no direct coupling of basically distinct physical formulations is necessary. However, they can be strongly limited if defects on the level of atoms such as vacancies and crack tips or, for instance, phase transformations appear. As these are mainly localised phenomena, a full atomistic simulation would overstate the case as essentially only a small subset of the problem needs to be modelled by the sensitive method. This is where the so-called concurrent multiscale approaches come into action that simultaneously consider methods which operate at distinct length and time scales. In the buckling analysis of carbon nanotubes for example molecular dynamics is used to model small subdomains of locally severe deformations whereas the larger portion of the problem with moderate deformations is described by a continuum mechanics approach. Although the idea of concurrent multiscale models is obvious, the main challenge within these models is the proper treatment of the interface between the different simulation approaches for instance the atomistic-continuum transition. In particular, relevant informations between the approaches are exchanged using some kind of handshake region. In this regard, various concurrent multiscale formulations were developed that differ from each other either more or less. A widespread review of these methods can be found in [15,16] with a focus on atomistic-continuum coupling and in a more general form in [3,17]. In the papers mentioned therein, multiscale methods are applied to the computational study of different problems of nanotechnology. Moreover, it turns out that the various methods can be assigned to the classes of energy-based and force-based approaches with their distinct advantages and disadvantages as discussed in [16]. With regard to the buckling analysis of carbon nanotubes two interesting approaches, namely the bridging domain method and the bridging scale method, were applied. In the bridging scale method formulated by Wagner and Liu [18], the solution of the multiscale problem is decomposed into a fine scale and a coarse scale. In particular, the continuum model exists across the entire domain whereas the atomistic model is only present at smaller subdomains where some sort of localised fine scale is important. In order to decouple the two scales, a projection operator between the atomistic and continuum solution is introduced. Initially proposed for one-dimensional problems, the bridging scale method was extended by Qian et al. [19] and applied as a multiscale method for the analysis of carbon nanotubes. The bridging domain method was in a first variant proposed by Belytschko and Xiao [20] for coupling molecular statics with continuum mechanics using an energy-based blending domain partitioning and a finite overlap region. Additional kinematics constraints enforce the compatibility of both models in the handshake region. An advantage of the approach is the fact that the finite element nodes of the continuum model do not need to coincide with the positions of the atoms in the overlap region. Thus, the discretisation of the continuum subdomain does not require finite elements that are as small as the interatomic distances of the atomistic region. Later this idea was extended to dynamics by Xiao and Belytschko [21] and they addressed the positive behaviour of the approach with regard to the problem of spurious wave reflections at the interface of concurrent atomistic-continuum multiscale methods. Moreover, Xu et al. [22], proposed and discussed a modification of the approach, denoted as relaxed bridging domain method, that is about the enforcement of the compatibility condition in multi-lattices. In the works of Belytschko and Xiao [20], Sun and Liew [23] and Zhang et al. [7] the bridging domain method was used to numerically analyse the buckling behaviour of carbon nanotubes.

In this paper, the bridging domain method is applied to carbon nanotubes in order to analyse their buckling behaviour. As the aim is the calculation of equilibrium configurations of the nanostructure at 0 K, the concurrent multiscale model couples a molecular statics approach with a continuum mechanics approach. For the molecular statics portion of the model a formulation following the paper of Wackerfuß [24] is used that allows to efficiently include the atomistic calculation in the computational framework of a finite element implementation. This purely molecular statics approach was previously investigated by the author in a distinct publication [25]. In doing so, the molecular statics model was applied to analyse the buckling behaviour of carbon nanotubes. In this regard, the obtained results were checked against available data from the literature and, thus, the proper implementation of the model was validated. The applied continuum model is based on the local form of the quasi-continuum method. This strategy was proposed by Tadmor et al. [26–28] and allows to define