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# A nonlinear theory of prestressed elastic stick-and-spring structures

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ABSTRACT

The discrete modeling of a large class of mechanical structures can be based on a stick-and-spring concept. We here present a stick-and-spring theory with potential application to the statics and the dynamics of such nanostructures as graphene, carbon nanotubes, viral capsids, and others. A key feature of our theory is its geometrical nonlinearity: we combine exactly defined strain measures with a general linear stress response; another, rarely found feature is a careful account of prestress states. A linear version is firstly proposed, where attention is restricted to study small displacements from an unstressed reference placement. Next, a theory linearized about a prestressed (preloaded or not) placement is displayed, which is based on a careful analysis of the tangent stiffness operator and its two parts, the elastic and prestress stiffness operators. Finally, two examples are proposed and solved; when an analytical solution is of prohibitive complication, numerical solutions are given, by the use of a specifically implemented 'stick-and-spring' code.



## 1. Introduction

In this paper we propose a theory of elastic molecular structures that may be in a stressed state before their static response to applied loads and imposed nodal displacements is determined, or their free vibrations are studied. In addition to hoping it to be of interest *per se*, we believe that this theory is applicable in many contexts, both statical and dynamical, where the objects whose mechanical behavior is under scrutiny are carbon allotropes (nanotubes, graphene sheets, nanoribbons), molecules, protein complexes, *et cetera*.

We regard a molecular structure as a collection of *nodes*, *edges*, and *wedges*: edges are imagined as node-to-node inflexible but extensible straight *sticks*, acting as *axial springs* when extended; wedges are imagined as complexes of two sticks sharing one end node, equipped by a *torsion spring* reacting to relative rotations of the wedge sticks in their common plane. Accordingly, we call the structures we model *Stick-and-Spring structures* (S&S). Similar but simpler molecular structures are the so-called *elastic networks*, that is, roughly speaking, sets of nodes pair-wise connected by edges, a concept used to model generally small displacements from an equilibrium configuration of protein complexes (see e.g. Radez, Chennubothla, Yang, & Bahar, 2006). Another class of molecular structures comprises the *molecular dynamics models*, where a two- or three-body

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potential accounts for the interactions among particles whose relative distance is less than a prescribed cut-off length (Abell, 1985; Brenner, 1990; Brenner et al., 2002; Finnis & Sinclair, 1984; Tersoff, 1988).

Stick-and-spring models have been widely used to predict the mechanical behavior of Carbon NanoTubes (CNTs) and graphene. The linear model exploited in Chang and Gao (2003) to obtain closed-form expressions for the elastic properties of armchair and zigzag CNTs has been extended in Xiao, Gama, and Gillespie (2005) to study torsion loading and handle non-linearities, by means of a modified Morse potential. A similar approach is used in Shen and Li (2004) to investigate various loading conditions, and in Wang (2004) to evaluate effective in-plane stiffness and bending rigidity of armchair and zigzag CNTs. Molecular mechanics has also been employed as a scale-bridging method to build shell theories (Bajaj, Favata, & Podio-Guidugli, 2013; Chang, 2010; Favata & Podio-Guidugli, 2014). In Chang, Geng, and Guo (2005), the model of Chang and Gao (2003) is extended to chiral CNTs, an issue addressed also in Chang, Geng, and Guo (2006). Recently, a new formulation of the stick-and-spring model has been proposed (Merli, Lázaro, Monléon, & Domingo, 2013), allowing for general load conditions, arbitrary chirality, and an initial stressed state. It is worth mentioning the computational methods presented in Meo and Rossi (2006), where non-linear torsional spring elements are adopted and implemented in a Finite Element (FE) code. The mechanical properties of graphene sheets and nanoribbons have been analyzed with a similar approach; in particular, FE formulations have been given, employing both linear (Georgantzinos, Giannopoulos, & Anifantis, 2010) and non-linear springs (Geng & Chang, 2006; Georgantzinos, Giannopoulos, Katsareas, Kakavas, & Anifantis, 2011; Giannopoulos, Liosatos, & Moukanidis, 2011, 2012).

The method of structural analysis we propose is fairly general and versatile. Although it can be profitably adopted for all of the above mentioned applications (and many others), here we only give a description of its general features, illustrated by an analysis of simple concept structures of no special applicative significance, except for the cyclohexane isomers considered in Remark 4, Section 4.2; real applications will be dealt with elsewhere. The main novelty of our approach consists in handling prestress without neglecting geometrical nonlinearities; a careful account of prestress is important in various contexts where our theory is potentially applicable: see e.g. (Edwards, Wagner, & Gräter, 2012) for globular proteins, and Shi, Peng, Pugno, and Gao (2012), where certain aspects of the mechanical phenomenolgy of graphene and CNTs are investigated.

Here is a summary of the contents of our paper. In Section 2, we describe the topology and the kinematics of stick-and-spring structures; in particular, we define *exact* strain measures and derive their *linearized* version. Then, in Section 3, we use a virtual power argument to derive the nodal equations that must be satisfied by all stress states compatible with the data, that is, balancing the applied load in the given reference placement. These equations implicitly define the *equilibrium operator* and its transpose, the *kinematic compatibility operator*. Just as for any other discrete structural system, the dimensions of the null spaces of these operators provide a useful classification criterion for the structural systems under study: e.g., the set of admissible self-stress states can be identified with the nullspace of the equilibrium operator. A linear theory of elastic S&S structures consists in coupling the nodal equilibrium equations with a linear constitutive equation delivering edge and wedge stresses in terms of linearized edge and wedge strain measures; such an equation is tantamount of specifying the *linear stiffness operator*.

However, the effects of prestress on a system's response cannot be predicted within a fully linear setup. To account for these effects, in Section 4 we derive an expression for the *tangent stiffness operator*, that is, the Hessian of the stored energy. This operator admits an additive decomposition into an *elastic stiffness operator* (the analog of the stiffness operator encountered in the linear theory) plus a *prestress stiffness operator*. While the former operator accounts for first-order changes in the strain measures, the latter accounts for orientational changes of edges and wedges and for the stresses they carry; thus, its contribution to balancing the service loads can be nonnull even when the accompanying displacements entail null linearized strains. Such contribution is especially important when it comes to assessing the stability of an equilibrium placement, which is connected with the sign-definiteness of the tangent stiffness operator, when seen as a quadratic form. In this connection, we borrow from rigidity theory (Connelly, 1999) (see also Micheletti, 2013) the notions of *prestress stability* and *super-stability*, and we restate them for S&S structures.

Knowledge of the equilibrium and tangent stiffness operators allows for application of standard numerical machineries to solve a number of structural problems, such as computing load–displacement paths, performing buckling analyses, determining natural frequencies and vibration modes, and integrating the nonlinear motion equations. In Section 5, two simple concept structures are analyzed, in the linear, linearized, and nonlinear setups of our theory; in particular, the numerical results obtained by the use of a specifically implemented 'stick-and-spring' code are presented. Some directions of future research are mentioned in our final Section 6.

## 2. Topology and kinematics

### 2.1. Topology

A S&S structure is a triplet $\mathcal{S} = (\mathcal{N}, \mathcal{E}, \mathcal{W})$, consisting of: (i) a collection $\mathcal{N}$ of $N$ points, called *nodes*, of the three-dimensional Euclidean space; (ii) a collection $\mathcal{E}$ of $E$ *edges*, that is, two-elements subsets of $\mathcal{N}$; (iii) a collection $\mathcal{W}$ of $W$ *wedges*, that is, three-elements subsets of $\mathcal{N}$. We say that $ij \in \mathcal{E}$ is the edge connecting nodes $i, j \in \mathcal{N}$, and that $ijk \in \mathcal{W}$, with $i, j, k \in \mathcal{N}$, is the wedge with *head node* $i$ and *tail nodes* $j$ and $k$.