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Modeling and numerical treatment of elastic rods with frictionless self-contact

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1. Introduction

In the last three decades, the theory of elastic rods has witnessed great development because of its various industrial and biomechanical applications. Among the types of elastic rods used in practical applications we mention beams in civil constructions, cables in marine industries [1–3], pipelines in the oil industries, and fragments of the DNA molecule in the modeling of live sciences, see e.g. [4–8]. Several models of elastic rods were employed for the study of the deformations and supercoiling of fragments of the DNA molecules. The elastic rod models in the context of DNA modeling has experienced an increasing sophistication and successfully produced detailed information on the deformations of the DNA molecules. Nevertheless, there are several problems that remain to be studied for a good understanding of the supercoiling process of DNA fragments. The field of open problems in this context is still very vast.

The problem of self-contact in elastic rod has attracted, in at least the last two decades, a continuous attention. Several

ABSTRACT

In this paper we present a hyperelastic rod model that takes into account self-contact forces. The model is based on Cosserat rod theory that incorporates shear, elongation, flexure and twist deformations. The problem of avoiding self-penetration of parts of the rod is handled by the introduction of a contact distance function and the incorporation of associated contact forces. We present a penalty method for the treatment of the multi-valued and non-differentiable contact law. We also describe an augmented Lagrangian formulation of this problem. We then give the details of the finite-element discretization of the elastic rod self-contact problem as well as some numerical examples.

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researchers addressed this challenging problem using different approaches. Coleman and Swigon [4] have used an analytical approach to obtain equilibrium configurations of uniform elastic rods with self-contact points under terminal loads. Thompson et al. [9] studied the mechanics of uniform ply in which two strands coil around one another in the form of a helix. van der Heijden et al. [7] studied the self-contact problem in clamped rods using numerical continuation. Goyal et al. [10] used a computational approach to study looping and supercoiling of DNA fragments. Coyne [11] addressed the problem of loop formation and elimination in twisted cables.

In the present work, we propose to study the modeling and numerical aspects of the equilibrium configurations of an elastic rod, subject to terminal loads and which might contains points or regions of self-contact not known *a priori*. The dominant classical theories of elastic rods are local ones and do not account for the global behavior of the configuration of the rod. In particular, the equations resulting from these theories cannot foresee nor avoid the self-penetration of different parts of the rod. We describe a uni-dimensional model for the treatment of self-contact in elastic rod that is based on the Cosserat theory. The particularity of the model we propose is the introduction of a simplified contact distance that takes into account the geometric description of the rod. We make the mathematical analysis of this contact problem





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by giving an existence theorem. We first note that the computation of the contact distance is equivalent to an orthogonal projection computation of a point on a curve. By minimizing the elastic energy under the constraint that the contact distance is non-positive we avoid self-penetration of different parts of the rod. We present numerical results using a four-node curved finite element and a multiplicative method for updating rotations as described by Simo and Vu-Quoc [12] and Ibrahimbegović [13]. This updating procedure has the advantage of automatically taking care of the constraints of orthonormality of the directors.

The paper is organized as follows. In Section 2, we review the kinematics, equilibrium equations and constitutive law of the theory of elastic rods based on the Cosserat model. Section 3 is devoted to the mathematical formulation of an elastic rod theory that accounts for large deformations as well as self-contact forces. We define a contact distance and use it to give a variational formulation of the problem of self-contact in elastic rods. In Section 4, we present the finite-element formulation of the problem of elastic rods with self-contact. Some numerical examples of planar and 3D configurations of elastic rods with self-contact are presented in Section 5.

2. Cosserat theory of rods

2.1. Preliminaries

Let $\{O; e_1, e_2, e_3\}$ be a fixed frame, with origin O and righthanded orthonormal basis $\{e_1, e_2, e_3\}$, of the Euclidean space \mathbb{R}^3 . For any two vectors $a, b \in \mathbb{R}^3$, the scalar and vector products are denoted $a \cdot b$ and $a \times b$, respectively. We denote by ||a|| the Euclidean norm of the vector a, i.e., $||a|| = (a \cdot a)^{1/2}$. The tensor product $a \otimes b$ of the vectors a and b is the second-order tensor defined by $(a \otimes b)c = (c \cdot b)a$ for all vectors $c \in \mathbb{R}^3$. For a vector a, we denote by a^{\times} the skew-symmetric tensor such that $(a^{\times})b = a \times b$ for all vectors $b \in \mathbb{R}^3$. We denote by axial(A) the axial vector associated with a skew-symmetric tensor A, i.e., such that $(axial(A))^{\times} = A$. Throughout the article, the summation convention for repeated Latin indices is employed with range 1–3.

2.2. Geometric description

We employ the director theory of rod based on the model introduced almost hundred years ago by the Cosserat brothers [14], used in the abstract framework proposed by Antman [15], and exploited by Simo and Vu-Quoc [16]. We consider an elastic rod \mathcal{R} of length L and circular cross-sections of a uniform diameter 2ε . The configuration of the rod is described by specifying, for each $s \in [0, L]$, a position vector $\mathbf{r}(s)$ and a right-handed triad of orthonormal directors $\{d_1(s), d_2(s), d_3(s)\}$, see Fig. 1. The curve $\mathscr{C} \equiv \{\mathbf{r}(s), s \in [0, L]\}$ represents the line of centroids of the crosssections, in the deformed configuration of *R*. The triad $\{d_1(s), d_2(s), d_3(s)\}$ gives the orientation of the material cross-section at *s* of \mathcal{R} . We take **R**(*s*) to denote the proper orthogonal tensor $\mathbf{R}(s) = \mathbf{d}_i(s) \otimes \mathbf{e}_i$. Throughout, quantities that are associated with the reference configuration are denoted with the same symbol as those associated with the deformed configuration but with a superposed hat, e.g., \hat{r} instead of r. We shall assume that s is an arclength parameter for the curve $\widehat{\mathscr{C}}$, i.e., the center line of the rod in its reference configuration.

The space of all possible configurations of the rod is

$$\mathscr{C} = \{ (\boldsymbol{r}, \boldsymbol{R}) \in H^1([0, L]; \mathbb{R}^3 \times SO(3)) \},$$
(1)

where SO(3) is the Lie group of special orthogonal tensors in \mathbb{R}^3 . This configuration space is not linear but rather a differentiable manifold. The tangent space $T_{(\mathbf{r},\mathbf{R})} \mathcal{C}$ to \mathcal{C} at (\mathbf{r},\mathbf{R}) is



Fig. 1. Geometric descriptions of the reference (left) and current (right) configurations of a Cosserat elastic rod.

$$T_{(\mathbf{r},\mathbf{R})}\mathscr{C} = \{ (\mathbf{p}, \mathbf{q}^{\times}\mathbf{R}) \text{ where } (\mathbf{p}, \mathbf{q}) \in H^1([\mathbf{0}, L]; \mathbb{R}^3 \times \mathbb{R}^3) \}.$$
(2)

The space of kinematically and physically (impenetration) admissible configurations of the rods is a subset of \mathscr{C} whose elements satisfy prescribed boundary conditions and impenetration constraints to be discussed later.

2.3. Kinematics and strains measures

The kinematics of the rod are encapsulated in the following two equations:

$$\boldsymbol{r}'(\boldsymbol{s}) = \boldsymbol{v}(\boldsymbol{s}),\tag{3a}$$

$$\boldsymbol{R}'(\boldsymbol{s}) = \boldsymbol{u}^{\times}(\boldsymbol{s})\boldsymbol{R}(\boldsymbol{s}),\tag{3b}$$

where here and throughout ' denotes differentiation with respect to *s*. The vector $\boldsymbol{u}(s)$ is the axial (also called Darboux) vector associated with the skew-symmetric tensor $\boldsymbol{R}'(s)\boldsymbol{R}^T(s)$.

Following Antman [15], we introduce the following strain measures

$$\mathbf{V}(s) = \mathbf{R}^{T}(s)\mathbf{r}'(s) = \mathbf{R}^{T}(s)\mathbf{v}(s), \tag{4a}$$

$$\mathbf{U}^{\times}(s) = \mathbf{R}^{T}(s)\mathbf{R}'(s) = \mathbf{R}^{T}(s)\mathbf{u}^{\times}(s)\mathbf{R}(s).$$
(4b)

We note here that the components v_i and u_i of the vectors \mathbf{v} and \mathbf{u} in the basis { \mathbf{d}_i , i = 1, 2, 3} have the following mechanical interpretation: u_1 and u_2 measure the flexure in the planes ($\mathbf{d}_2, \mathbf{d}_3$) and ($\mathbf{d}_3, \mathbf{d}_1$), respectively, and u_3 is a measure of the twist of the rod; v_1 and v_2 measure the shear deformations in the \mathbf{d}_1 and \mathbf{d}_2 directions, respectively, while v_3 represents the elongation of the rod. We say that the rod is unshearable if $v_i = \mathbf{v} \cdot \mathbf{d}_i = 0$, i = 1, 2; inextensible if $v_3 = \mathbf{v} \cdot \mathbf{d}_3 = 1$; and inextensible and unshearable if $\mathbf{v} = \mathbf{d}_3$.

Under a superposed rigid-body motion, defined by a proper orthogonal tensor Q and a translation vector c, the position vector r(s) transforms according to

$$\boldsymbol{r}^*(\boldsymbol{s}) = \boldsymbol{Q}\boldsymbol{r}(\boldsymbol{s}) + \boldsymbol{c},$$

and the directors $d_i(s)$ transform as

$$\boldsymbol{d}_i^*(s) = \boldsymbol{Q} d_i(s)$$

It follows that the rotation tensor $\mathbf{R}(s)$ transforms to $\mathbf{R}^*(s) = \mathbf{Q}R(s)$, and hence it is straightforward to check that the strain measures (4) are unaffected by the superposed rigid-body motion.

Because $\mathbf{V} \cdot \mathbf{e}_i = \mathbf{R}^T \mathbf{v} \cdot \mathbf{e}_i = \mathbf{v} \cdot \mathbf{R}\mathbf{e}_i = \mathbf{v} \cdot \mathbf{d}_i$, the components of the vector \mathbf{V} with respect to the fixed frame $\{\mathbf{e}_i\}$ coincide with the components of the vector \mathbf{v} with respect to the moving frame $\{\mathbf{d}_i\}$. Similarly, the components in the fixed frame $\{\mathbf{e}_i\}$ of the vector

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