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Ribbons and groups: a thin rod theory for catheters and filaments

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Abstract. We use the rotation group and its algebra to provide a novel description of deformations of *special Cosserat rods* or thin rods that have negligible shear. Our treatment was motivated by the problem of the simulation of catheter navigation in a network of blood vessels, where this description is directly useful. In this context, we derive the Euler differential equations that characterize equilibrium configurations of stretch-free thin rods. We apply perturbation methods, used in time-dependent quantum theory, to the thin rod equations to describe incremental deformations of partially constrained rods. Further, our formalism leads naturally to a new and efficient finite element method valid for arbitrary deformations of thin rods with negligible stretch. Associated computational algorithms are developed and applied to the simulation of catheter motion inside an artery network.

1. Introduction

Simulation technology is leading to increasingly very fruitful applications in biomedicine. An important example is the simulation of catheter navigation in a network of blood vessels, where a physician/user may practice navigation skills, plan a procedure, or design a new device in a virtual but realistic environment.

A simulation system for this purpose, called *da Vinci* (for visual navigation of catheter insertion) has been constructed at our centre. While the system itself has been discussed elsewhere [1, 2], this paper describes the underlying physics and formalism which was developed in this context. Besides providing efficient computational algorithms, the formalism is interesting in its own right and has useful applications in several other contexts, described elsewhere.

Special Cosserat rods, described in [3], are rods whose deformations are described by the following *strain variables*: flexure (bending), torsion (twist), shear, and dilation (stretch). This paper considers certain types of special Cosserat rods, called *thin rods*, that have negligible shear and possibly negligible stretch. We present a useful description of deformations in terms of Lie groups and Lie algebras, and discuss minimal energy or equilibrium configurations within this framework in the context of constitutively linear elasticity. Related methods for the determination of equilibrium configurations under constrained conditions are applied to the simulation of catheter navigation in an arterial network by using a suitable discretization of the continuum thin rod model.

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2. Comparison with earlier work

The subject of thin rods is an old one, and a classical treatment in terms of curvature and torsion may be found, for instance, in [5], while a more modern analysis is presented in [3]. A nice elaboration of the classical discussion may be found in [6]. The classical treatment has been further applied to rod models of filaments such as DNA molecules, where it leads to a nonlinear Schrödinger equation for equilibrium configurations [7]. These discussions do not make use of the rotation group and its algebra.

Although a formulation similar to the Lie theoretic description proposed here was described in [8, 9], where a quaternionic representation of rotations was used to parametrize the deformations, and, in particular, to develop a computational scheme, we claim several useful and new developments in this paper.

In particular, we wish to emphasize, besides the application to catheter simulation itself, the following novelties and useful consequences of our approach (these are primarily a result of the more complete exploitation of the Lie theoretic features of the formulation):

(1) Our use of the rotation group and its algebra leads to an elegant formulation which lends itself to a direct analysis. Our description has clear advantages for the particular catheter problem that we consider, as well as for several other special—but ubiquitous—cases that we discuss elsewhere.

(2) Our methodology provides a basis for simple and efficient computational algorithms. The Lie algebraic treatment leads to the development of a consistent hierarchical perturbation method (section 5) for solving the equilibrium equations derived in section 4 and allows for fast methods of finding equilibria. These are valid for arbitrary deformations. Since we can work with higher orders in perturbation theory if necessary, large forces can be dealt with easily.

(3) This perturbation method leads directly to a new and easily used finite element description or FEM for the case of rods whose stretch is negligible, where variables can be consistently updated (section 6). We believe our formulation of finite elements is significantly cleaner and clearer than the treatments we have encountered. This method can be directly used for arbitrary deformations, in contrast to conventional FEMs (see [12], for example) which need special schemes for large deformations.

(4) We present in the appendix an analysis of the decoupling in the elastic energy among stretch rate, shear and rotation rate for homogeneous rods (often used without proof in the literature).

In addition to the catheter navigation simulation discussed in this paper, we have applied this formalism to robotics [18] and to networks or *complexes* of thin rods, such as the modelling of protein deformations [19] and cytoskeletal cell mechanics.

3. Kinematics: configurations and deformations

Intuitively, a thin rod is an object that admits a class of physical embeddings into space characterized by two properties: to each embedding there exists a parametrized *central curve* that describes the location of its centre; for each pair of embeddings, the correspondence between material points is *approximated* by a *deformation* that maps normal planes isometrically onto normal planes. The set of deformations is shown below to form an infinite-dimensional Lie group that acts transitively on equivalence classes of embeddings called *configurations*. Bending and twisting of deformed thin rods are described using the associated Lie algebra.

We now define the concept of a framed path or *ribbon* as the analogue of an orthonormal coordinate system to parametrize material points along the the thin rod. For definiteness, we will consider here a rod with endpoints. The centreline may be parametrized by its arclength s as measured from one of the ends of the rod. Everywhere below, we will use a prime to indicate a derivative with respect to arclength.

We define a *director* for a curve $\boldsymbol{r}$ to be a unit vector $\boldsymbol{n}(s)$ (for $s \in [0, L]$) such that

- the derivative $\boldsymbol{n}'$ is square integrable on $[0, L]$,
- $\boldsymbol{n} \cdot \boldsymbol{r}' = 0$ in this interval.

It is clear that for any curve there exists at least one director. Further, the notion of a director may be easily extended to the case of a rod with corners.

The following concept is basic in differential geometry [14]: a *ribbon* is defined to be a pair $(\boldsymbol{r}, \boldsymbol{n})$ where $\boldsymbol{r}$ is a curve and $\boldsymbol{n}$ is a director for $\boldsymbol{r}$.

A ribbon $(\boldsymbol{r}, \boldsymbol{n})$ provides an orthonormal frame $(\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3)$, where

$$\boldsymbol{d}_1 := \boldsymbol{n} \qquad \boldsymbol{d}_3 := \frac{\boldsymbol{r}'}{|\boldsymbol{r}'|} \qquad \boldsymbol{d}_2 := \boldsymbol{d}_3 \times \boldsymbol{d}_1 \tag{1}$$

over the closed interval $[0, L]$. These orthonormal frames, and therefore the ribbons that define them, can be used to parametrize material points sufficiently close to the curve $\boldsymbol{r}$. Our description of thin rod configurations is equivalent to that of the Cosserat theory of rods [4] with one director, or equivalently, the special Cosserat theory with one of the directors chosen to be the unit tangent to the centreline. However, we have not seen elsewhere in this context the full exploitation of the Lie algebraic concepts developed below.

Based on physical considerations, we shall restrict our family of thin tube deformations to require that the deformation derivatives map normal planes into normal planes. This model is a particular case of the special Cosserat theory with one of the directors chosen to lie along the unit tangent to the centreline. That our restriction is a reasonable one may be seen by examining the reduction from three-dimensional linear elasticity to one-dimensional rod theories, which is discussed in the appendix. It is shown there that one can think of rod theories as arising from an expansion in d/L, where d is the cross sectional size and L is the length of the rod. In the limit of small d/L, a description in terms of normal planes alone is seen to be an accurate one. Accordingly, we proceed with our treatment.

Let $SO(3)$ denote the rotation group on three-dimensional space $\mathbb{R}^3$. With respect to a basis for $\mathbb{R}^3$, elements of $SO(3)$ are as usual represented by orthogonal 3×3 matrices with unit determinant.

We define a deformation $d = (\boldsymbol{a}, \alpha, M)$ to consist of

- a translation vector $\boldsymbol{a} \in \mathbb{R}^3$,
- a bounded real function α, and
- a function $M(s) : [0, L] \to SO(3)$ whose derivative is square-integrable.

Let $\mathcal{D}$ denote the set of deformations.

It is straightforward to show that the set $\mathcal{D}$ forms an infinite-dimensional Lie group under the product $(\boldsymbol{a}_1, \alpha_1, M_1)(\boldsymbol{a}_2, \alpha_2, M_2) \equiv (\boldsymbol{a}_1 + \boldsymbol{a}_2, \alpha_1 + \alpha_2, M_1 M_2)$ where addition and multiplication are performed pointwise. Furthermore, $\mathcal{D}$ acts as a group of transformations on the set of ribbons as follows: for a ribbon $(\boldsymbol{r}, \boldsymbol{n})$, and deformation $d = (\boldsymbol{a}, \alpha, M)$

$$d(\boldsymbol{r})(s) = \boldsymbol{r}(0) + \boldsymbol{a} + \int_0^s \mathrm{e}^{\alpha(\tau)} M(\tau) \boldsymbol{r}'(\tau) \, \mathrm{d}\tau \tag{2}$$

and

$$d(\boldsymbol{n})(s) = M(s) \boldsymbol{n}(s). \tag{3}$$

It is clear that for small $\alpha(s)$, this function can be given the interpretation of a local stretch rate along the rod. The rotation matrix $M(s)$ rotates the local frame defining the tangent and the normal plane to a corresponding new frame in the deformed rod; it is the assumption that normal planes are deformed to normal planes that allows us to parametrize the deformations in this manner. Further, it is easy to see that deformations preserve corner angles, if any.

3.1. Rotation rate, bending and twisting

This section defines the rotation rate of a deformation and shows it is a path in the Lie algebra of the rotation group. Then, we define bending and twisting of a deformation acting on a configuration as the normal and tangential components of the rotation rate with respect to the configuration curve.

We note that if a rotation $M(s)$ is differentiable at s, $M'(s)$ lies in the tangent space to $SO(3)$ at $M(s)$. The Lie algebra $\mathcal{A}$ [10] of $SO(3)$ is the tangent space to $SO(3)$ at the identity I; therefore the quantity $\Omega_M(s) \equiv (M(s))^{-1}M'(s) = M^T(s)M'(s)$ takes the tangent space to $SO(3)$ at $M(s)$ to the tangent space to $SO(3)$ at I. Consequently $\Omega_M(s)$ lies in the Lie algebra of $SO(3)$ and is a skew-symmetric matrix.

We shall call $\Omega_M(s)$ the *rotation rate* associated with the path $M(s)$. Clearly if $M'(s)$ is square-integrable (in the interval $[0, L]$), so is $\Omega_M(s)$. Further, given a square-integrable skew-symmetric matrix $\Omega(s)$, a unique rotation $M(s)$ is determined from $M(0)$ and $\Omega(s)$ by integrating the differential equation $M' = M\Omega$.

Notation. We call attention to the following notation that we shall use throughout this paper: for any vector denoted by a lower case boldface letter ($\boldsymbol{\omega} \equiv [\omega_1, \omega_2, \omega_3]^T \in \mathbb{R}^3$), let the corresponding upper case letter denote the skew-symmetric matrix

$$\Omega = \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix} \tag{4}$$

and conversely.

Note that for any $\boldsymbol{v} \in \mathbb{R}^3$ and $\Omega \in \mathcal{A}$, $\Omega\boldsymbol{v} = \boldsymbol{\omega} \times \boldsymbol{v}$. It is also useful to note that for any $N \in SO(3)$ and $\Omega \in \mathcal{A}$, $P \equiv N\Omega N^T \in \mathcal{A}$ and $\boldsymbol{p} = N\boldsymbol{\omega}$. These relations are often invoked later without comment to pass between cross products and matrix similarity transformations.

We also note that given a rotation M through an angle θ about the unit vector $\boldsymbol{n}$, the matrix M may be obtained by exponentiating the matrix (θN); this operation has the expansion

$$M = \exp(\theta N) = I + \sin\theta + (1 - \cos\theta)N^2. \tag{5}$$

We shall now define twisting and bending associated with a thin rod deformation. Let $d = (\boldsymbol{a}, \alpha, M) \in \mathcal{D}$ and $\boldsymbol{r} \in \mathcal{C}$. The twisting (bending) of d relative to $\boldsymbol{r}$ is defined to be the tangential (normal) component of $\boldsymbol{\omega}$ with respect to the curve $\boldsymbol{r}$, where $\Omega(s)$ is the rotation rate associated with $M(s)$. Two examples follow.

Example 1 (helix). *Let $\boldsymbol{p} \in \mathcal{C}$ be defined by $\boldsymbol{p}(s) = s\boldsymbol{u}$ where $\boldsymbol{u}$ is a unit vector and let $d = (0, 1, M) \in \mathcal{D}$ be a deformation such that $M(0) = I$ and $M^T M'$ is a constant $\Omega \in \mathcal{A}$. Then $M(s) = \mathrm{e}^{\Omega s}$ is a rotation by γs about the vector $\boldsymbol{\omega}$ where $\gamma = |\boldsymbol{\omega}|$. Write $\boldsymbol{u} = \beta_1\boldsymbol{u}_1 + \beta_2\boldsymbol{u}_2$ (where $\beta_1^2 + \beta_2^2 = 1$) such that $\boldsymbol{u}_1$ is the unit vector parallel to $\boldsymbol{\omega}$ and $\boldsymbol{u}_2$ is normal to $\boldsymbol{\omega}$ and $\beta_2 > 0$. Then $d(\boldsymbol{p}) = \boldsymbol{q}$ where*

$$\boldsymbol{q}(s) = s\beta_1\boldsymbol{u}_1 + \frac{\beta_2}{\gamma} M\left(s - \frac{\pi}{2\gamma}\right)\boldsymbol{u}_2$$

so that $\boldsymbol{q}$ *forms a helix having axis* $\boldsymbol{u}_1$ *and lying on a cylinder having radius* $\frac{\beta_2}{\gamma}$ *and slope* $\frac{\beta_1}{\beta_2}$. *The curvature* $\kappa = \beta_2\gamma$ *and the torsion* $\tau = \beta_1\gamma$. *The twisting of* M *with respect to* $\boldsymbol{p}$ *equals* τ *(can be positive or negative) and the bending magnitude equals* κ.

Example 2 (horseshoe). *Define the curve* $\boldsymbol{p}(s) = [\cos s, \sin s, 0]^T$, *with unit tangent vector* $\boldsymbol{u}(s) = [-\sin s, \cos s, 0]^T$ *over the interval* $[0, \pi]$ *and define* $M(s) = \mathrm{e}^{U(s)}$. *Then* $M(s)$ *rotates the curve* $\boldsymbol{p}$ *in place and has the effect of bending it at a rate equal to two around the unit vector* $[0, 0, 1] = \boldsymbol{u}' \times \boldsymbol{u}$ *followed by a rigid rotation by* π *about the axis* $[1, 0, 0]$.

4. Equilibrium configurations

This section introduces energy functions and discusses equilibrium configurations, within the context of the kinematical description of deformations discussed so far. The problem of determining physical equilibria under the action of external forces is formulated as a boundary value problem. Although equations equivalent to our final equations (31) and (32) have been known, they have not been presented in the form we have introduced using rotation operators.

4.1. Energy function

Let $(\boldsymbol{r}, \boldsymbol{n})$ be a reference configuration. Given a deformation $d(\boldsymbol{r}, \boldsymbol{n})$, we are interested in energy functions that can be expressed as

$$E(d) = E_{ex}(d(\boldsymbol{r})) + E_{el}(d)$$

where E_{ex} is an *external energy function* that depends only on the configuration curve and $E_{el}(d)$ is an *elastic energy function* that depends only on the shape (i.e. equivalence up to rigid motion) of the configuration (i.e. uniquely specified by the stretching factor α and the rotation rate $\boldsymbol{\omega}$ of the deformation).

The rotation rate $\boldsymbol{\omega}$ and the stretch rate α are the *strain* variables associated with the deformation of the rod.

We express the energy functions as integrals of non-negative energy density functions,

$$E_{ex}(d(\boldsymbol{r})) = \int_0^L J_{ex}(d(\boldsymbol{r}(s)), s)\,\mathrm{d}s \tag{6}$$

and

$$E_{el}(\alpha, \boldsymbol{\omega}) = \int_0^L J_{el}(\alpha(s), \boldsymbol{\omega}(s), s)\,\mathrm{d}s. \tag{7}$$

As stated earlier, this form of the elastic energy corresponds to a particular kind of special Cosserat rod [4]; it is assumed here that cross sections of the rod do not change their shape, so that the single director vector $\boldsymbol{n}$ suffices to characterize the twisting of cross sections as one proceeds along the rod. Rotational and translational invariance dictates that the elastic energy density must depend only on the vector function $\boldsymbol{\omega}$ and on the function α which measures longitudinal stretching.

Choose a basis at position s on the reference curve whose first element is the unit tangent vector, whose second component equals the director, and whose third component equals their cross product and let $z(s)$ represent the size-four column vector $[\alpha(s), \boldsymbol{\omega}(s)]^T$ with respect to this basis. Then the quadratic Taylor approximation for the elastic energy density yields (up to addition of a constant function of s)

$$J_{el}(\alpha(s), \boldsymbol{\omega}(s), s) \approx \tfrac{1}{2}(z(s) - z_0(s))^T Q_4(s)(z(s) - z_0(s))$$

$Q_4(s)$ is a positive definite 4×4 matrix, and $z_0(s) \equiv [\alpha_0(s), \boldsymbol{\omega}_0(s)]^T$ is determined by $Q_4(s)$ and the linear term in the Taylor expansion.

Retaining only the above form of the Taylor expansion corresponds to a linearly elastic model. Then the configuration $z = z_0$ provides the unique (shape equivalence class) configuration of zero elastic energy.

Throughout the remainder of this paper we will assume linear elasticity and that the reference configuration has zero elastic energy (i.e. $z_0(s) = 0$: such a configuration can be observed by placing the rod in a slightly viscous liquid having the same density as the rod material and allowing the rod to assume a stationary state).

We further assume that both the cross sectional geometry and the elastic properties of the rod vary slowly with changes in s that are comparable with the diameter of the rod. Now J_{el} is a quadratic function; then for such rods, it is shown in the appendix that there are no bilinear couplings between α and $\boldsymbol{\omega}$. Thus to quadratic order, the elastic energy density takes the form

$$J_{el}(\alpha, \boldsymbol{\omega}, s) = a\alpha^2 + \tfrac{1}{2}\boldsymbol{\omega}^T Q\boldsymbol{\omega} \tag{8}$$

where $a > 0$ and Q is a 3×3 positive definite *stiffness density* matrix. We also show there that the rotation rate has no coupling to shear variables.

We note here that this form of the elastic energy density is quite general. The further inclusion of appropriate constraints to restrict the degrees of freedom permits the use of this model in describing deformations of protein backbones, where there are constraints on $\boldsymbol{\omega}$. This is best done with the use of a compliance-based formalism discussed in [16].

For rods with rotationally invariant cross sections, the stiffness density, for all s, must further satisfy

$$O^T Q(s) O = Q(s)$$

for every 3×3 matrix O made up of 1 in the upper left entry and a 2×2 rotation matrix in the lower 2×2 block, in a frame with one axis along the unit tangent to the reference curve. This implies Q is a diagonal matrix whose last two entries are equal. In this case, the coefficients in the elastic energy density for arbitrary thin rod deformations and for arbitrary reference curves (in the case of linear elasticity) follow directly from considering the simple case of small deformations of a straight rod [11]; the energy density is

$$J_{el}(\alpha, \omega, s) = \frac{E_Y A}{2}\alpha^2 + \frac{G_S I}{2}|\boldsymbol{\omega}_t|^2 + \frac{E_Y I}{2}|\boldsymbol{\omega}_b|^2. \tag{9}$$

Here $|\boldsymbol{\omega}_t|$ and $|\boldsymbol{\omega}_b|$ denote the magnitude of the twisting and bending components of $\boldsymbol{\omega}$ with respect to the reference configuration (assumed to be an elastic energy minimum); the corresponding twist and bend vectors respectively are $\boldsymbol{\omega}_t \equiv (\boldsymbol{\omega} \cdot \boldsymbol{u})\boldsymbol{u}$ and $\boldsymbol{\omega}_b \equiv \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \boldsymbol{u})\boldsymbol{u}$. Here E_Y is Young's modulus, G_S is twice the shear modulus, A is the cross sectional area, and I is the second moment of area. Note that $\alpha, \boldsymbol{\omega}, A, I$ and the elasticity coefficients E_Y, G_S are in general functions of $s \in [0, L]$. For a thin rod with annular cross section with inner and outer radii R_1 and R_2 respectively (circular for $R_1 = 0$), $A = \pi(R_2^2 - R_1^2)$ and $I \equiv \pi(R_2^4 - R_1^4)/4$.

The quadratic form of the elastic energy of straight *beam elements* which are standard in finite element treatments of thin rod deformations (see, for instance, p 298 in [12]) follows directly from the above elastic energy density for rods with rotationally invariant cross sections. The elements in this description have six degrees of freedom (three positional and three orientational) at each beam endpoint (or node); the 12×12 *stiffness matrix* which describes the energy of a deformed beam element in terms of nodal degrees of freedom is obtained directly by integrating the energy density (9) of a straight rod with a cubic displacement function. We note also that the stiffness of arbitrary *curved* beam elements may be obtained by integrating the perturbation equations (41) developed later in section 5.

In the case when stretch is negligible, one can derive a simplified finite element description with only three degrees of freedom per element (see section 6 below), corresponding to bending and twisting of the element. This may be obtained from the elastic energy density (9) above, or alternatively from the perturbation equations to be derived below.

The following section formulates the determination of equilibrium configurations under specified constraints as a variational problem.

4.2. Thin rod differential equations

Modelling the passage of a thin flexible catheter through a network of tubes with curved walls in a computationally efficient manner is a non-trivial problem. With the important simplifying assumption that the motion is damped sufficiently fast that the catheter may be taken to be instantaneously in equilibrium with the artery walls, the problem may be cast in the form of a quasistatic incremental energy minimization problem.

We shall consider here the problem of determining minimal total energy configurations, which describe deformations of elastic thin rods under external forces and constraints. These are characterized using variational principles to derive differential equations that describe the equilibrium configuration. Further, based on our formalism, efficient techniques to solve for equilibria are presented in subsequent sections.

In order to find minimum energy configurations, we need to minimize the total energy functional, subject to the constraint that the thin rod configuration is a valid deformation of the reference (undeformed) configuration. We shall define an augmented energy functional in order to do this.

We will assume that stretching of the thin rod is negligible, as is indeed the case for real catheters, for instance, during normal use; this means that $\alpha(s) = 0$, to a good approximation.

We will denote by $J_{ex}(\boldsymbol{r}(s), s)$ the corresponding potential energy density due to the interaction of the thin rod with external agents; in the case of a catheter moving inside an arterial wall, the wall may be modelled by means of a steeply rising potential function. Here $\boldsymbol{r}(s)$ is the (deformed) spatial location of a point labelled by length s along the rod; we shall use $\boldsymbol{r}_0(s)$ to denote the undeformed or reference configuration of the catheter.

The total energy of the rod–external agent system is then given by

$$E_{tot}(\boldsymbol{r}, \boldsymbol{\omega}) = \int_0^L \mathrm{d}s\, [J_{el}(\boldsymbol{\omega}(s), s) + J_{ex}(\boldsymbol{r}(s), s)]. \tag{10}$$

Let us denote by $\boldsymbol{u}_0(s)$ the unit tangent vector along the thin rod in its reference or undeformed state.

Since we have assumed that stretching is negligible, deformations of this reference state that we shall consider are then elements of $\mathcal{D}$ of the form $(\boldsymbol{a}, 0, M(s))$, so that the position vector of a point at length s along the thin rod is given from (2) as

$$\boldsymbol{r}(s) = \boldsymbol{r}_0(0) + \boldsymbol{a} + \int_0^s M(t)\boldsymbol{u}_0(t)\, \mathrm{d}t. \tag{11}$$

Notice that $\boldsymbol{r}(0) - \boldsymbol{r}_0(0) = \boldsymbol{a}$. This relationship may be rewritten in differential form as

$$\boldsymbol{r}'(s) = M(s)\boldsymbol{u}_0(s) \tag{12}$$

where the prime indicates differentiation with respect to s.

Recall also that the change of the rotation matrix M along the rod is

$$M'(s) = M(s)\Omega_M(s) \tag{13}$$

where $\Omega_M(s)$ is the instantaneous rotation rate of $M(s)$. Associated with the skew-symmetric matrix Ω_M is the vector $\boldsymbol{\omega}_M$, as discussed earlier.

When a thin rod interacts with external forces, the configuration it assumes is one which minimizes E_{tot}, subject to the above relations, which may be viewed as constraints, for $\boldsymbol{r}'$ and M'. The resulting equilibrium configuration of the thin rod is therefore one which is a stationary state for the following *augmented* energy functional:

$$H = \int_0^L \mathrm{d}s \,(J_{el}(\boldsymbol{\omega}, s) + J_{ex}(\boldsymbol{r}, s) + \boldsymbol{\lambda} \cdot (\boldsymbol{r}' - M\boldsymbol{u}_0) - \boldsymbol{\mu} \cdot (\boldsymbol{\omega} - \boldsymbol{\omega}_M)). \tag{14}$$

We have introduced here the vectors $\boldsymbol{\lambda}(s)$ and $\boldsymbol{\mu}(s)$ which are Lagrange multiplier auxiliary variables which serve to enforce the relations (12) and (13). The dots between vectors indicate scalar products.

The problem of finding the equilibrium configuration of the thin rod is now recast as a constrained optimization problem.

One may choose to simply build the constraints (12) and (13) into the geometry and find equilibrium configurations numerically by a descent on E_{tot}. This was the strategy used in an application described in [17]. Alternatively, we may also derive the Euler–Lagrange equations to find a stationary point of the augmented energy H, as we now do; these equations will make the connection between applied forces and deformations.

The variation in H due to a variation in $\boldsymbol{\omega}$ yields

$$\boldsymbol{\mu} - \frac{\partial J_{el}}{\partial \boldsymbol{\omega}} = 0 \tag{15}$$

as the strong equation for stationarity. The variational equations due to variations in $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ yield the relations

$$\boldsymbol{r}' = M\boldsymbol{u}_0 \tag{16}$$

and

$$M' = M\Omega \tag{17}$$

as required. The associated boundary conditions $\boldsymbol{r}(0)$ and $M(0)$ are assumed known.

A variation in $\boldsymbol{r}$ holding $\boldsymbol{r}(0)$ fixed yields the variational equation

$$\boldsymbol{\lambda}' = \frac{\partial J_{ex}}{\partial \boldsymbol{r}} \tag{18}$$

and the boundary condition $\boldsymbol{\lambda}(L) = 0$.

Next, consider a variation in M. Since we want to preserve the nature of M as a rotation matrix, variations in M are restricted to be of the form $\delta M = M\delta A$, where δA is an antisymmetric matrix (this restriction follows from the fact that $M^T M = I$).

The variation in H due to a variation in M is then

$$\delta H = -\int_0^L \mathrm{d}s \,[\boldsymbol{\lambda} \cdot (M\delta A\boldsymbol{u}_0) - \boldsymbol{\mu} \cdot (\boldsymbol{g} + \delta \boldsymbol{a}')] \tag{19}$$

with

$$\begin{aligned} G &\equiv M^T M'\delta A - \delta A M^T M' \\ &= \Omega\delta A - \delta A\Omega. \end{aligned} \tag{20}$$

This may be rewritten in the form

$$\delta H = \int_0^L \mathrm{d}s[\delta \boldsymbol{a} \cdot ((M^T \boldsymbol{\lambda} \times \boldsymbol{u}_0) + \boldsymbol{\mu} \times \boldsymbol{\omega}) + \boldsymbol{\mu} \cdot \delta \boldsymbol{a}']. \tag{21}$$

Integrating the last term in δH above by parts then yields the variational equation

$$\boldsymbol{\mu}' = \boldsymbol{\mu} \times \boldsymbol{\omega} + (M^T \boldsymbol{\lambda} \times \boldsymbol{u}_0) \tag{22}$$

together with the boundary condition $\boldsymbol{\mu}(L) = 0$.

It is possible to rewrite this equation in a more elegant form by defining a new variable $\boldsymbol{\xi}(s) = M(s)\boldsymbol{\mu}(s)$. Using the above equation for the rate of change of $\boldsymbol{\mu}$, it is easy to see that the rate of change of $\boldsymbol{\xi}$ along the thin rod is given by

$$\boldsymbol{\xi}' = \boldsymbol{\lambda} \times (M\boldsymbol{u}_0) = \boldsymbol{\lambda} \times \boldsymbol{r}'. \tag{23}$$

The auxiliary variables $\boldsymbol{\lambda}$ and $\boldsymbol{\xi}$ have a direct physical interpretation. Consider first the relation

$$\boldsymbol{\lambda}' = \frac{\partial J_{ex}}{\partial \boldsymbol{r}}. \tag{24}$$

The right side here is the gradient of the external potential energy density along the rod; this is therefore the negative of the external force per unit length, $\boldsymbol{f}(s)$, along the rod. Integrating this expression along the entire length of the rod gives

$$\boldsymbol{\lambda}(L) - \boldsymbol{\lambda}(0) = -\int_0^L \mathrm{d}s\, \boldsymbol{f}(s) \tag{25}$$

or, using the boundary condition $\boldsymbol{\lambda}(L) = 0$,

$$\boldsymbol{\lambda}(0) = \boldsymbol{F}_{tot} \tag{26}$$

which is the total external force acting along the length of the thin rod. It is apparent that $\boldsymbol{\lambda}(s)$ may also be interpreted as the *internal* force on the cross section at point s due to internal stress. If the external forces are *concentrated* forces acting only at discrete points, then $\boldsymbol{\lambda}(s)$ must be constant along sections of the rod between such points.

Integrating the equation for $\boldsymbol{\xi}'$, (27), along the length of the rod and using the boundary conditions $\boldsymbol{\lambda}(L) = 0$ and $\boldsymbol{\xi}(L) = 0$ gives

$$\begin{aligned}\boldsymbol{\xi}(0) &= \boldsymbol{\lambda}(0) \times \boldsymbol{r}(0) - \int_0^L \mathrm{d}s\, [\boldsymbol{f}(s) \times \boldsymbol{r}(s)] \\ &= \int_0^L \mathrm{d}s\, (\boldsymbol{r}(s) - \boldsymbol{r}(0)) \times \boldsymbol{f}(s)\end{aligned} \tag{27}$$

which is the total torque $\boldsymbol{\tau}_{tot}$ due to external forces about the initial point $\boldsymbol{r}(0)$ of the rod; therefore $\boldsymbol{\xi}(0) = \boldsymbol{\tau}_{tot}$. It is clear that $\boldsymbol{\xi}(s)$ has the interpretation of being the *internal* moment acting on the cross section at point s. If external moments are applied only at discrete points and there are no applied external forces, then $\boldsymbol{\xi}$ must be constant along sections of the rod between such points.

We shall collect below the system of equations we have derived so far, whose solution yields the equilibrium configuration of the thin rod as a function of the initial point position and orientation $\boldsymbol{r}(0)$ and $M(0)$ respectively:

$$\begin{aligned}\boldsymbol{r}' &= M\boldsymbol{u}_0 \\ M' &= M\Omega \\ \boldsymbol{\lambda}' &= \frac{\partial J_{ex}}{\partial \boldsymbol{r}} \\ \boldsymbol{\xi}' &= \boldsymbol{\lambda} \times \boldsymbol{r}' \\ \boldsymbol{\xi} &= M\boldsymbol{\mu} \\ \boldsymbol{\mu} &= \frac{\partial J_{el}}{\partial \boldsymbol{\omega}}.\end{aligned} \tag{28}$$

If, in addition to forces, there are torques acting along the length of the rod, the fourth equation above has the corresponding torque density appearing on the right side as an additional term:

$$\boldsymbol{\xi}' = \boldsymbol{\lambda} \times \boldsymbol{r}' + \boldsymbol{\tau}' \tag{29}$$

Since J_{el} is quadratic in $\boldsymbol{\omega}$, we can write the equation for $\boldsymbol{\xi}$ in the form

$$\boldsymbol{\xi} = MQ\boldsymbol{\omega} \tag{30}$$

where Q is the symmetric matrix of coefficients in the $\boldsymbol{\omega}$-dependent part of the quadratic form J_{el}; it is the stiffness density of the rod.

To recapitulate, $\boldsymbol{r}$ is the position vector along the thin rod; $\boldsymbol{u}_0$ is the unit tangent vector along the *undeformed* rod; M is the rotation matrix which specifies the deformation from the reference configuration; $\boldsymbol{\omega}$ is the rotation rate vector; $\boldsymbol{\lambda}$ is the internal force on the cross section along the rod, and $\boldsymbol{\xi}$ is the internal moment along its length.

Let us rewrite the above equations in a form which makes the coupled nature of the equations more transparent. Using the relation $\boldsymbol{\xi} = MQ\boldsymbol{\omega}$, we have

$$\begin{aligned}
\boldsymbol{r}' &= M\boldsymbol{u}_0 \\
M' &= M\Omega \\
\boldsymbol{\lambda}' &= \frac{\partial J_{ex}}{\partial \boldsymbol{r}} \\
(Q\boldsymbol{\omega})' &= [(M^T\boldsymbol{\lambda}) \times \boldsymbol{u}_0 - \boldsymbol{\omega} \times Q\boldsymbol{\omega}].
\end{aligned} \tag{31}$$

These four differential equations above along with boundary conditions serve to determine the four unknowns $\boldsymbol{r}$, M, $\boldsymbol{\lambda}$ and $\boldsymbol{\omega}$ upon integration. Notice that knowledge of $M(s)$ along the path s suffices to determine the other variables by integration; however, if $M(s)$ is unknown, these coupled nonlinear equations must be integrated simultaneously.

We note that these equilibrium equations reduce, in the case of rods whose reference configuration is straight, to those given, for instance, in [11].

The last equation in (31) is formally the same as the Euler equation of motion which describes a rotating body; this is the celebrated Kirchoff spinning top analogy (see, for instance, [5]). In this analogy, Q plays the role of the moment of inertia tensor, $\boldsymbol{\omega}$ plays the role of the angular velocity, and the arclength parameter s plays the role of time; the first term on the right side of the last equation in (31) plays the role of a time-dependent torque. This analogy can also be seen to arise from the form of the elastic energy functional (8) with zero stretching, which corresponds to the kinetic energy of a body with moment of inertia Q rotating with instantaneous angular velocity $\boldsymbol{\omega}$. The difference is that while the Euler equation describes the evolution of the configuration in time as an initial value problem, the equilibrium equations for thin rods describe a two-point boundary value problem. The use of a Lie-theoretic description makes the analogy very explicit.

A comparison with a modern treatment such as that in [3] shows that the general and special theories of Cosserat rods discussed there, when specialized to the case of very thin rods, reduce naturally to the rotation group-based theory we have described, as discussed in the appendix.

When there is a free end at $s = L$, the variables $\boldsymbol{\lambda}$ and $\boldsymbol{\xi}$ satisfy the endpoint conditions $\boldsymbol{\lambda}(L) = 0$ and $\boldsymbol{\xi}(L) = 0$; we therefore have a two-point boundary value problem to solve, with initial conditions for $\boldsymbol{r}$ and M, and final conditions for $\boldsymbol{\lambda}$ and $\boldsymbol{\xi}$. In general, shooting methods [13] are needed to solve this boundary value problem.

We note here that when the deformed shape is specified, and the problem is one of computing the corresponding forces, the endpoint conditions $\boldsymbol{\lambda}(L) = 0 = \boldsymbol{\xi}(L)$ must be relaxed, since the shape of the deformed curve is known. Then the total external force along the length is given by

$$\boldsymbol{F}_{tot} = \boldsymbol{\lambda}(0) - \boldsymbol{\lambda}(L)$$

and the force acting on the point of support is $\boldsymbol{\lambda}(0)$. Similarly, as we saw earlier, the moment acting on the support is $\boldsymbol{\xi}(0)$.

For the case of a thin rod acted on by forces as well as torques, the last equation in (31) above is modified to read

$$\omega' = Q^{-1}[(M^T\lambda) \times u_0 - \omega \times Q\omega - Q'\omega + M^T\tau']. \tag{32}$$

5. Perturbation theory

Here we develop a perturbative method for finding equilibrium configurations of a thin rod by an incremental process corresponding to incremental loading. The method has a close analogy with perturbation methods used in time-dependent quantum mechanics. It effectively replaces a nonlinear differential equation by a hierarchy of linear differential equations; the corresponding two-point boundary value problem at each order of perturbation theory is easily solved by a linear shooting method. A similar perturbation theory is also developed for the compliance form of the thin rod equations.

As stated earlier, the arclength parameter s plays the role of time. Taking this analogy a step further, the rotation matrix $M(s)$ may be thought of as playing the role of the time evolution operator in quantum mechanics; developing perturbative versions of the thin rod equations is then analogous to doing time-dependent perturbation theory in quantum mechanics, with the incremental forces playing the role of the perturbing Hamiltonian in quantum mechanics.

We shall consider the general case where the rod is acted on by both forces and torques. Suppose we have found a solution for given force and torque densities λ_0' and τ_0' respectively; denote the corresponding rotation matrix and rotation rate by M_0 and Ω_0 respectively. Let us now apply additional incremental force and torque densities $\epsilon\lambda_1'$ and $\epsilon\tau_1'$ respectively. Here ϵ is a small parameter which reflects the incremental nature of the applied forces and torques. Alternatively, we may regard it as purely a book-keeping device and set it equal to unity later, with the understanding that the applied forces and torques λ_1' and τ_1' are indeed incremental. Let the new configuration have rotation matrix M, with

$$M = NM_0. \tag{33}$$

Therefore N corresponds to a further deformation about the current configuration.

Since there has been only an incremental change in configuration, N can be represented in exponential form as

$$N(s) = \exp(\epsilon T_1(s) + \epsilon^2 T_2(s) + \cdots). \tag{34}$$

This may be expanded order by order in ϵ:

$$N = I + \epsilon T_1 + \epsilon^2\left(T_2 + \frac{T_1^2}{2}\right) + \cdots. \tag{35}$$

The rotation rate of the new matrix M is

$$M^T M' = M_0^T N^T(N'M_0 + NM_0) = \Omega_0 + M_0^T \Omega_N M_0 \tag{36}$$

where $\Omega_N = N^T N'$ is the rotation rate corresponding to the rotation matrix N. Expanding Ω_N as a series in ϵ

$$\Omega_N = \epsilon\Omega_1 + \epsilon^2\Omega_2 + \cdots \tag{37}$$

and substituting in $\Omega_N = N^T N'$ gives the sequence of relations

$$\begin{aligned} \Omega_1 &= T_1' \\ \Omega_2 &= T_2' + \tfrac{1}{2}(T_1'T_1 - T_1T_1') \end{aligned} \tag{38}$$

and so on, order by order in ϵ.

Equation (36) above gives the new rotation rate vector as

$$\boldsymbol{\omega} = \boldsymbol{\omega}_0 + M_0^T(\epsilon\boldsymbol{\omega}_1 + \epsilon^2\boldsymbol{\omega}_2 + \cdots) \tag{39}$$

with $\boldsymbol{\omega}_1$ and $\boldsymbol{\omega}_2$ given by

$$\begin{aligned}\boldsymbol{\omega}_1 &= \boldsymbol{t}_1' \\ \boldsymbol{\omega}_2 &= \boldsymbol{t}_2' + \tfrac{1}{2}\boldsymbol{t}_1' \times \boldsymbol{t}_1\end{aligned} \tag{40}$$

respectively.

We may use these expansions in the thin rod equations to obtain a sequence of *linear* differential equations for T_1, T_2 and so on, order by order in the perturbation ϵ. The incremental method therefore replaces a set of nonlinear differential equations by a hierarchy of linear differential equations that may be solved to desired accuracy at each incremental step. We shall give here the corresponding equations to first and second order in perturbation theory. Perturbing equation (29) to first order in ϵ yields the system of first-order differential equations

$$\begin{pmatrix} M_0QM_0^T\boldsymbol{\omega}_1 \\ \boldsymbol{t}_1 \end{pmatrix}' = \begin{pmatrix} \Xi_0 & \Xi_0' - \Lambda_0M_0U_0M_0^T \\ I & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{\omega}_1 \\ \boldsymbol{t}_1 \end{pmatrix} + \begin{pmatrix} -M_0U_0M_0^T & I \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{\lambda}_1 \\ \boldsymbol{\tau}_1' \end{pmatrix} \tag{41}$$

where I is the 3×3 identity matrix and Ξ_0 is the skew-symmetric matrix corresponding to $\boldsymbol{\xi}_0$, etc. This system may be written in several equivalent forms. It must of course be supplemented by appropriate boundary conditions. If the orientation at one end (say at $s = 0$) is fixed and the (change in) torque at the other end is specified, then the boundary conditions are

$$\begin{aligned}&\boldsymbol{t}_1(0) = 0 \\ &\boldsymbol{f}(L) \equiv [\boldsymbol{t}_1 \times \boldsymbol{\xi}_0 + M_0QM_0^T\boldsymbol{\omega}_1]_{s=L} = \boldsymbol{\tau}_1(L)\end{aligned} \tag{42}$$

where $\boldsymbol{\tau}_1(L)$ is the specified change in applied torque at $s = L$.

It is apparent here that only the *rotated* stiffness density $M_0QM_0^T$ (i.e. of the deformed configuration as seen in a fixed external reference frame) and the *rotated* unit tangent $M_0\boldsymbol{u}_0$ (whose matrix representation is $M_0U_0M_0^T$) enter these equations; this is as it should be since the variable $\boldsymbol{t}_1$ defines an incremental rotation measured in the fixed frame.

Since equation (41) is linear in the variables $\boldsymbol{\omega}_1$ and $\boldsymbol{t}_1$, it may be solved by a linear shooting method for the specified final point condition. This involves making a guess for $\boldsymbol{\omega}_1(0)$, solving the differential equation, measuring the deviation from the desired final point condition, and correcting the guess accordingly. This correction requires knowledge of the 3×3 matrix expressing the linear relationship between the final point value $\boldsymbol{f}(L)$ and the initial value $\boldsymbol{\omega}_1(0)$, whose three columns may be found numerically by integrating the equation for three orthogonal unit vector choices of $\boldsymbol{\omega}_1(0)$.

For completeness, we give the form of the equation one gets at the next order in perturbation theory. This is clearly a relation for $\boldsymbol{t}_2$; we get the first-order differential equation system

$$\begin{pmatrix} M_0QM_0^T\boldsymbol{\omega}_2 \\ \boldsymbol{t}_2 \end{pmatrix}' = \begin{pmatrix} \Xi_0 & \Xi_0' - \Lambda_0M_0U_0M_0^T \\ I & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{\omega}_2 \\ \boldsymbol{t}_2 \end{pmatrix} + \begin{pmatrix} \boldsymbol{b} \\ -\frac{1}{2}T_1'\boldsymbol{t}_1 \end{pmatrix} \tag{43}$$

where we have defined the quantity $\boldsymbol{b}$ as

$$\boldsymbol{b} \equiv (\Lambda_1T_1 + \tfrac{1}{2}\Lambda_0T_1^2) + \tfrac{1}{2}(T_1\Xi_0'\boldsymbol{t}_1 + (\Xi_0T_1' - T_1'\Xi_0)\boldsymbol{t}_1 + T_1\Xi_0\boldsymbol{t}_1'). \tag{44}$$

Given that we have already solved for $\boldsymbol{t}_1$ at the previous order of perturbation theory, this is again a linear system of equations. The boundary conditions at this order are

$$\boldsymbol{t}_2(0) = 0 \tag{45}$$

and

$$[\boldsymbol{t}_2 \times \boldsymbol{\xi}_0 + \tfrac{1}{2}\boldsymbol{t}_1 \times (\boldsymbol{t}_1 \times \boldsymbol{\xi}_0) + \boldsymbol{t}_1 \times M_0QM_0^T\boldsymbol{t}_1' + M_0QM_0^T\boldsymbol{\omega}_2] = 0. \tag{46}$$

To summarize, the perturbation method replaces a set of highly nonlinear differential equations corresponding to a two-point boundary value problem with a hierarchy of linear differential equations, each of which is easily solved, at every incremental step in the deformation. At each deformation step, it is clear that more accurate solutions may be obtained by working at higher orders in the perturbing forces, and the process has a close analogy with the time-dependent perturbation theory often employed in quantum mechanical problems.

6. Stretch-free finite elements

In this section we describe a new finite element discretization for stretch-free rods that provides an effective method of computing equilibrium configurations.

Consider a rod with arbitrary reference curve, with homogeneous material properties and circularly symmetric cross section, discretized into a sequence of elements straight in their reference states. The element *stiffness* matrix which describes the linear response of each element to applied incremental forces and torques, $K_{el,i}$ in equation (60) below, as well as the equation for equilibrium (66) (for a single element) may be obtained directly by integration of the differential equation (41) assuming a constant rotation rate along the element. In the following, we will make the derivation of an incremental equilibrium equation of the discretized rod more explicit by directly expanding the elastic energy of the rod.

Let its Young's modulus and rigidity modulus be E and G respectively; let I be the second moment of area of the cross section and let $J = 2I$. For the case of zero stretch, the elastic energy density of the rod (9) may be written in terms of the rotation rate $\boldsymbol{\omega}$ as

$$J_{el} = \frac{EI}{2}|\boldsymbol{\omega}_b|^2 + \frac{GJ}{2}|\boldsymbol{\omega}_t|^2 \tag{47}$$

where $\boldsymbol{\omega}_t \equiv (\boldsymbol{\omega} \cdot \boldsymbol{u})\boldsymbol{u}$ and $\boldsymbol{\omega}_b \equiv \boldsymbol{\omega} - \boldsymbol{\omega}_t$ are the twisting and bending components respectively of the rotation rate.

The deformation of the rod may be expressed in terms of only the new orientations at the nodal points; the degrees of freedom for incremental deformations are nodal orientational changes in this case.

Thus, let element $(i, i+1)$ be aligned with the x-axis in the reference state and let s be the arclength parameter along this element. The pulled-back deformed element has an orientation $N(s)$ (for $0 \leqslant s \leqslant L_i$ where L_i is the length of the element) relative to that at node i; for small strain ($\boldsymbol{\omega}$) we can write $N(s) \approx I + \tilde{\theta}(s)$ where $\tilde{\theta}(s)$ is skew-symmetric. Clearly we can write (see figure 1)

$$\tilde{\theta}(L_i) = M_i^T M_{i+1} - I. \tag{48}$$

For each such element, the vector $\boldsymbol{\theta}(s)$ corresponding to $\tilde{\theta}$ may be expanded as a linear function of the arclength along the element:

$$\boldsymbol{\theta}(s) = \boldsymbol{b}s \tag{49}$$

where there is no constant term since $\boldsymbol{\theta}(0) = 0$. Since the rotation rate along the element is, to leading order, given by $\boldsymbol{\omega} = \mathrm{d}\boldsymbol{\theta}/\mathrm{d}s = \boldsymbol{b}$, this approximation of linear $\boldsymbol{\theta}(s)$ corresponds to constant rotation rate deformations for the elements.

If we write $\boldsymbol{\theta}(L_i) \equiv \boldsymbol{\theta}_i = (\theta_1, \theta_2, \theta_3)$, then we have $\boldsymbol{b} = \boldsymbol{\theta}_i / L_i$. We shall refer to $\boldsymbol{\theta}_i$ as the strain associated with the element $(i, i+1)$.

Since the strain is small, derivatives of displacements of the element in the y and z

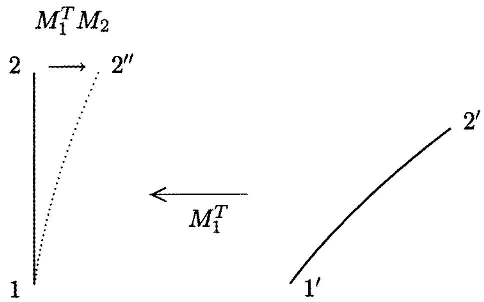

Figure 1. A pulled-back deformation showing the relative orientation between endpoints of the pulled-back deformed element.

directions are well approximated by

$$\frac{\mathrm{d}y}{\mathrm{d}s} = \theta_z(s) \qquad \frac{\mathrm{d}z}{\mathrm{d}s} = -\theta_y(s) \tag{50}$$

where the minus sign in the second equation accounts for the sense of rotation. These equations may be integrated to give

$$\begin{pmatrix} y(L) \\ z(L) \end{pmatrix} = \frac{L}{2}\begin{pmatrix} \theta_3 \\ -\theta_2 \end{pmatrix}. \tag{51}$$

Analogously, for an element aligned with a unit vector $\boldsymbol{u}_i$ in its reference state, the pulled-back transverse displacement is

$$\begin{aligned} \boldsymbol{y}_\perp &= \frac{L_i}{2}\boldsymbol{\theta}_i \times \boldsymbol{u}_i \\ &= \frac{L_i}{2}(M_i^T M_{i+1} - I)\boldsymbol{u}_i. \end{aligned} \tag{52}$$

There is no longitudinal displacement to leading order since there is no stretching. The pulled-forward transverse displacement is

$$\begin{aligned} \boldsymbol{y}_{\perp,f} &= \frac{L_i}{2}M_i(M_i^T M_{i+1} - I)\boldsymbol{u}_i \\ &= \frac{L_i}{2}(M_{i+1} - M_i)\boldsymbol{u}_i. \end{aligned} \tag{53}$$

In the deformed state, each element $(i, i+1)$ is rigidly rotated by M_i and bent and twisted; thus the position of node $(i+1)$ is related to that of node i by

$$\begin{aligned} \boldsymbol{x}_{i+1} &= \boldsymbol{x}_i + L_i M_i \boldsymbol{u}_i + \boldsymbol{y}_{\perp,f} \\ &= \boldsymbol{x}_i + \frac{L_i}{2}(M_i + M_{i+1})\boldsymbol{u}_i. \end{aligned} \tag{54}$$

Writing $\boldsymbol{b} \equiv (b_1, b_2, b_3)$, it is easy to see that the twisting component of the rotation rate is given by $b_1 = \theta_1/L_i$, while $b_2 = \theta_2/L_i$ and $b_3 = \theta_3/L_i$ make up the bending component. From equation (47), it follows by integration over the element arclength that the elastic energy of the element is

$$E_{el,i} = \tfrac{1}{2}\boldsymbol{\theta}_i^T K_{ele,i}\boldsymbol{\theta}_i \tag{55}$$

with the 3×3 stiffness matrix

$$K_{ele,i} = \begin{pmatrix} GJ/L_i & 0 & 0 \\ 0 & EI/L_i & 0 \\ 0 & 0 & EI/L_i \end{pmatrix}. \tag{56}$$

When the element in its reference state is not aligned with the x-axis, the above stiffness matrix $K_{ele,i}$ must be conjugated by a rotation matrix which rotates the global x-axis to the direction defined by the reference element.

Note that the strains $\boldsymbol{\theta}_i$ are usually small even when the deformation of the rod is large. We may find equilibrium configurations incrementally by relating changes in the strains $\boldsymbol{\theta}_i$ to changes in the nodal degrees of freedom (nodal orientations). A small change in current orientation at node i may be written as $\delta M_i = \delta\Phi_i M_i$ where $\delta\Phi_i$ is a skew-symmetric matrix. From the definition (48), it then follows to leading order in incremental quantities that

$$\delta\boldsymbol{\theta}_i = M_i^T(\delta\boldsymbol{\phi}_{i+1} - \delta\boldsymbol{\phi}_i). \tag{57}$$

The incremental change in the elastic energy of the element is

$$\delta E_{el,i} = \tfrac{1}{2}\delta\boldsymbol{\theta}_i^T K_{ele,i}\delta\boldsymbol{\theta}_i + \boldsymbol{\theta}_i^T K_{ele,i}\delta\boldsymbol{\theta}_i. \tag{58}$$

To quadratic order, using (57) and the assumption of small strain, we may write the incremental elastic energy in terms of the global incremental orientational degrees of freedom $\delta\boldsymbol{\phi}_i$ and $\delta\boldsymbol{\phi}_{i+1}$:

$$\delta E_{el,i} = \frac{1}{2}[\delta\boldsymbol{\phi}_i \delta\boldsymbol{\phi}_{i+1}]K_{el,i}\begin{bmatrix}\delta\boldsymbol{\phi}_i \\ \delta\boldsymbol{\phi}_{i+1}\end{bmatrix} - L_{el,i}^T\begin{bmatrix}\delta\boldsymbol{\phi}_i \\ \delta\boldsymbol{\phi}_{i+1}\end{bmatrix} \tag{59}$$

with

$$K_{el,i} = H_i^T K_{ele,i} H_i \tag{60}$$

and

$$L_{el,i} = -H_i^T K_{ele,i}\boldsymbol{\theta}_i \tag{61}$$

where we have defined the 3×6 matrix $H_i \equiv [-M_i^T \; M_i^T]$.

The 6×6 matrix $K_{el,i}$ and the 6×1 vector $L_{el,i}$ are the stiffness matrix and load vector respectively associated with the element $(i, i+1)$. The total elastic stiffness matrix and load vector for the rod's entire set of degrees of freedom (orientation changes at each node) may be assembled from these elemental quantities by adding for each node the corresponding stiffness and load contributions respectively from all the edges (elements) connected to that node.

It is worth noting that the element stiffness matrix $K_{el,i}$ and the equation for equilibrium (66) may also be obtained directly by integration of the differential equation (41).

External torques applied at the nodes contribute a term $\tau^T[\delta\phi]$ to the incremental total energy where $[\delta\phi]$ is the concatenated vector of incremental orientational degrees of freedom for all the nodes and τ is the vector of applied external torques at all the nodes.

In the incremental total energy, external *forces* at the nodes couple to the incremental nodal positions; nodal positions depend on all the orientations up to that node, as in equation (54). The incremental version of this equation may be written in the form

$$\begin{pmatrix}\delta\boldsymbol{x}_1 \\ \delta\boldsymbol{x}_2 \\ \cdot \\ \cdot \\ \delta\boldsymbol{x}_N\end{pmatrix} = \begin{pmatrix}\delta\boldsymbol{x}_1 \\ \delta\boldsymbol{x}_1 \\ \cdot \\ \cdot \\ \delta\boldsymbol{x}_1\end{pmatrix} + T\begin{pmatrix}\delta\boldsymbol{\phi}_1 \\ \delta\boldsymbol{\phi}_2 \\ \cdot \\ \cdot \\ \delta\boldsymbol{\phi}_N\end{pmatrix} \tag{62}$$

where T is the lower triangular matrix given by

$$T = \begin{pmatrix} 0 & 0 & \cdot & \cdot & \cdot & 0 \\ P_1 & R_1 & 0 & \cdot & \cdot & 0 \\ P_1 & P_2 & R_2 & 0 & \cdot & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ P_1 & P_2 & \cdot & \cdot & P_{N-1} & R_{N-1} \end{pmatrix}. \tag{63}$$

Here we have defined

$$\begin{aligned} P_i &\equiv -\tfrac{1}{2}(L_{i-1}V_{i-1} + L_i V_i) \\ R_i &\equiv -\frac{L_i V_i}{2} \end{aligned} \tag{64}$$

where V_i is the skew-symmetric matrix corresponding to the unit vector $\boldsymbol{v}_i = M_i \boldsymbol{u}_i$.

Then if F_{ex} is the vector of applied external forces at all the nodes, the incremental energy due to external forces and torques at the nodes, F_{ex} and τ respectively, is

$$\delta E_{ex} = -F_{ex}^T[\delta x_1] - (F_{ex}^T T + \tau^T)[\delta\phi] \tag{65}$$

where $[\delta x_1]$ is the first term in (62).

When loads at the nodes are specified directly (usually with the first node held fixed, $\delta \boldsymbol{x}_1 = 0$), incremental equilibria may be obtained from minimizing the quadratic expansion of the total incremental energy $(\delta E_{el} + \delta E_{ex})$; this yields the system

$$K_{el}[\delta\phi] = (L_{ex} + L_{el}) \tag{66}$$

where $L_{ex} = (T^T F_{ex} + \tau)$; note that the total load on the right side is an incremental quantity since F_{ex} and τ are applied incrementally.

Catheters are generally made of polyurethane with a typical Young's modulus value of about 6×10^6 N m^{-2} and a Poisson's ratio of about 0.45. Typical inner and outer diameters are 1 mm and 2.5 mm, respectively. Figure 2 compares results for a loading experiment (a downward force applied at one end with the other end fixed) using the three degree of freedom (d.o.f.) finite element method (FEM) described here with a more precise six d.o.f. FEM which allows for stretch (discussed in [16]). In both cases, 20 elements were used. It can be seen that the agreement between the two methods is excellent, although the three d.o.f. method uses only half the number of degrees of freedom.

Figure 3 shows the large deformation result of applying a force and torque in steps at one end, with position and orientation fixed at the other end (clamped boundary conditions).

When there is a position-dependent external potential field interacting with the rod, associated with it is an external stiffness matrix and an external load vector (arising from the quadratic and linear parts respectively of the Taylor expansion of the incremental external energy); then the total stiffness matrix $(K_{el} + T^T K_{ex} T)$ must be used on the left side of (66).

7. Simulating catheter navigation

An important biomedical application is the realistic simulation of catheter motion within a network of blood vessels. Assuming that the vessel wall is quite rigid, the constraint that the catheter is contained within the vessel walls may be represented by a steeply rising potential function. Given the severe damping present in the system, the process of insertion may be treated to good approximation as an adiabatic or quasistatic one, so that at every instant the catheter assumes a shape which minimizes the sum of the elastic deformation energy and the wall potential energy. Using the finite element discretization described in the previous section,

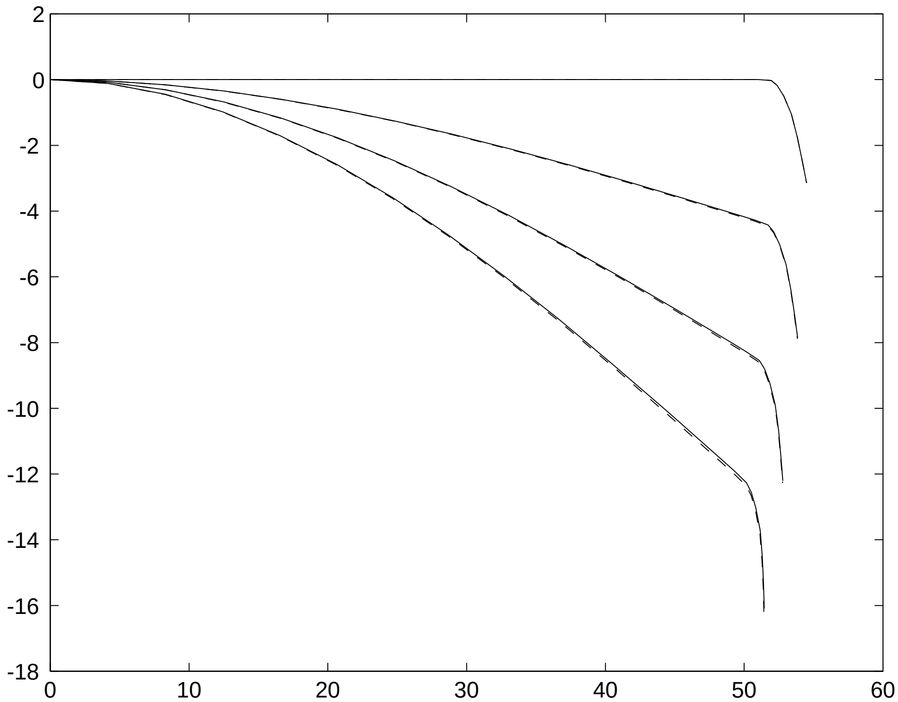

Figure 2. A loading experiment with a catheter which compares results from the three d.o.f. FEM used here (full curves) with a six d.o.f. FEM which allows for stretch (broken curves). A downward force was applied; length units are in cm.

equilibrium catheter configurations may be computed incrementally as the catheter is pushed in, withdrawn, or twisted at the entry point; these are the degrees of freedom actually accessible to the physician performing the procedure.

The total elastic energy E_{el} is obtained by integrating the elastic energy density, which as discussed earlier is a quadratic function of the rotation rate (strain) $\boldsymbol{\omega}$. The external energy E_{ex}, that enforces the arterial wall constraint, is obtained by integrating the wall potential P_{ex}; this potential is zero inside the inner artery wall and increases quadratically with distance from this wall outside. At every (small) insertion step, the total energy may be expanded to quadratic order in the configuration variables, so that we have a quadratic minimization to perform at every step, as discussed in section 6.

7.1. Wall potential

We characterize the artery by a central curve (parametrized by t), assume that the artery has a circular cross section with slowly varying cross sectional radius r, and that the catheter has a circular cross section of radius R. The catheter is outside the vessel wall when the signed distance $d(\boldsymbol{p})$ from a point $\boldsymbol{p}$ on the catheter to the artery wall,

$$d(\boldsymbol{p}) = |\boldsymbol{p} - \boldsymbol{q}| + R - r \tag{67}$$

is positive, where $\boldsymbol{q}$ is the closest point to $\boldsymbol{p}$ on the central curve of the artery, and r is the arterial radius at $\boldsymbol{q}$. It is clear that d is positive if and only if the catheter penetrates the arterial wall.

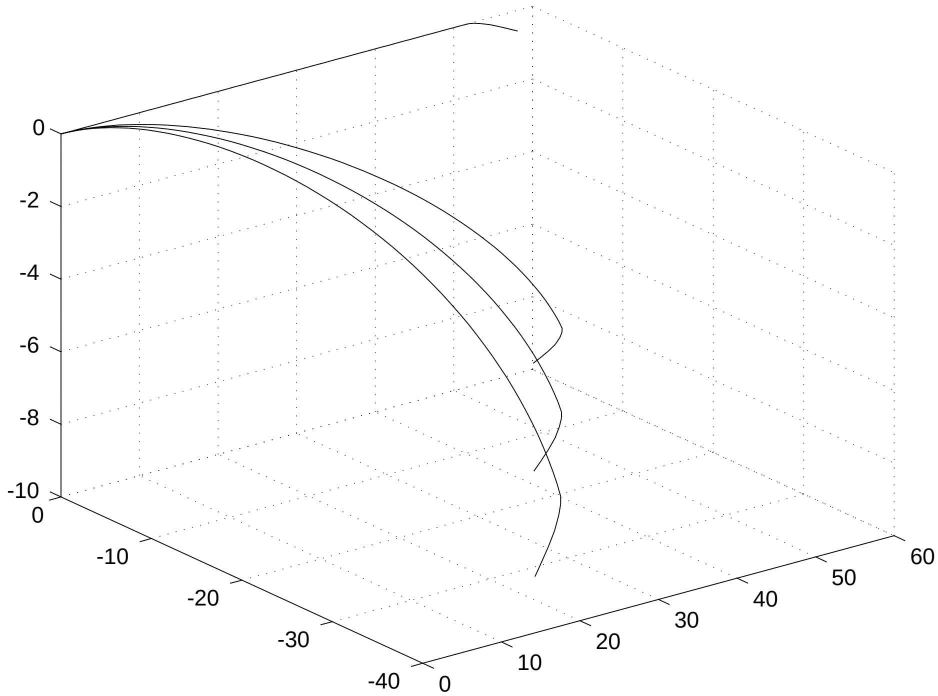

Figure 3. A loading experiment with a catheter which results in a large deformation; a force and torque were applied at the free end and the three d.o.f. FEM was used. Length units are in cm.

The wall potential function P_{ex} increases quadratically with the catheter's distance from the surface of the arterial tube. The potential function is thus defined by

$$P_{ex}(\boldsymbol{p}) := \frac{a}{2} d^2 \tag{68}$$

for $d > 0$, and $P = 0$ for $d \leqslant 0$. The gradient and Hessian (matrix of second derivatives) of the wall potential function with respect to the catheter's position variables $\boldsymbol{p}$ are respectively

$$\bigtriangledown P_{ex}(\boldsymbol{p}) \equiv a d(\boldsymbol{p}) \frac{\boldsymbol{p} - \boldsymbol{q}}{|\boldsymbol{p} - \boldsymbol{q}|} \qquad \text{if} \quad d \geqslant 0, \quad \text{else} \ \equiv 0 \tag{69}$$

and

$$\text{Hessian } P_{ex}(\boldsymbol{p}) \equiv a \frac{d(\boldsymbol{p})}{|\boldsymbol{p} - \boldsymbol{q}|} I - a \frac{(R - r)(\boldsymbol{p} - \boldsymbol{q})(\boldsymbol{p} - \boldsymbol{q})^T}{|\boldsymbol{p} - \boldsymbol{q}|^3} \tag{70}$$

where I is the 3×3 identity matrix and $(\boldsymbol{p} - \boldsymbol{q})^T$ denotes the row vector obtained by transposing the column vector $(\boldsymbol{p} - \boldsymbol{q})$.

We have included here the explicit expressions for the gradient (negative force density) and Hessian of the wall potential since these quantities are needed in the determination of equilibria by minimizing the quadratic expansion of the incremental energy. These are the coefficients of the linear and quadratic terms in the Taylor expansion of the incremental external energy density.

The gradient and Hessian of the wall potential in (69) and (70) above may be integrated to get the total external *load* and *stiffness* associated with an element in terms of its endpoint positional degrees of freedom. As for the elastic load and stiffness in the previous section, these may be assembled into a total external stiffness matrix K_{ex} and load vector L_{ex}.

We have in effect reduced the computation of the *force* density at each point $\boldsymbol{p}$ on the central curve of the catheter to the problem of computing the nearest point $\boldsymbol{q}$ on the central curve of the artery. For this, we need a geometric model for the central curve of the artery and its wall. The inner arterial wall is accordingly represented by a tubular surface, a *cylindrical swept surface* having the parametrized form

$$W_{cyl}(\boldsymbol{c}, r) := \{\boldsymbol{c}(t) + r(t)\cos(\theta)\boldsymbol{v}(t) + r(t)\sin(\theta)\boldsymbol{w}(t) : t \in [0, 1], \theta \in [0, 2\pi]\} \tag{71}$$

where $\boldsymbol{c}(t)$ is a continuously differentiable function on the arterial central curve. We assume that the artery radius $r(t)$ is less than the radius of curvature of the central curve at each point; $\boldsymbol{v}$ and $\boldsymbol{w}$ are unit vectors that are normal to the curve and to each other (they span the cross section).

Let $\boldsymbol{h}(t)$ denote the unit tangent to the curve at $\boldsymbol{c}(t)$ and define the *orthogonal plane* $P(t)$ to the curve $\boldsymbol{c}$ at $\boldsymbol{c}(t)$ by

$$P(t) \equiv \{\boldsymbol{q} : (\boldsymbol{q} - \boldsymbol{c}(t)) \cdot \boldsymbol{h}(t) = 0\}.$$

If $\boldsymbol{p}$ is close to the arterial wall, we may compute the nearest point on the arterial central curve to $\boldsymbol{p}$, $\boldsymbol{q} = \boldsymbol{c}(t(\boldsymbol{p}))$, where $t(\boldsymbol{p}) \in [0, 1]$ is the smallest value of t such that

$$|\boldsymbol{p} - \boldsymbol{c}(t(\boldsymbol{p}))| \leqslant r(t(\boldsymbol{p})) \tag{72}$$

and

$$(\boldsymbol{p} - \boldsymbol{c}(t(\boldsymbol{p}))) \cdot \boldsymbol{h}(t) = 0. \tag{73}$$

Since we represent the arterial central curve $\boldsymbol{c}(t)$ by piecewise cubic functions in t and $\boldsymbol{h}(t)$ is the tangent to this curve, this last equation yields a fifth-degree polynomial equation in t. It can be solved using a standard optimization method such as the Newton–Raphson method.

A network of arteries is represented by a union of such tubular surfaces.

7.2. Energy minimization

The quadratic minimization process is essentially a Newton method for finding a minimum. The control variables in the problem whose changes lead to new configurations are the position and orientation changes at the point of insertion, determined by the user. The Newton method for incremental energy minimization is very sensitive to moderately large increments in the control variables. Initial placement methods, that estimate plausible (i.e. low energy) deformed equilibria consistent with control variable increments, are required to ensure stability and speed.

For initial placement, we use the *tangential placement method* which minimizes incremental elastic energy subject to the constraint that points on the catheter which contact the artery wall move tangentially (to the wall). This assumption is exact for a catheter pushed against a flat frictionless wall; it is natural to use it in the context of a catheter in a blood vessel as well.

Consider a node i on the catheter which is in contact with the wall. Tangential placement for this node means that

$$\delta\boldsymbol{x}_i \cdot \boldsymbol{n} = 0 \tag{74}$$

where $\boldsymbol{n}$ is the outward normal to the artery wall at the point of contact. We need to rewrite this constraint in terms of the incremental orientational degrees of freedom. Using (62), it may be written in the form

$$\boldsymbol{n} \cdot \delta\boldsymbol{x}_1 + \sum_{j=1}^{i-1}(P_j\delta\boldsymbol{\phi}_j) \cdot \boldsymbol{n} + (R_{i-1}\delta\boldsymbol{\phi}_i) \cdot \boldsymbol{n} = 0. \tag{75}$$

Using the skew-symmetric nature of P and R, this equation may be rewritten as

$$\sum_{j=1}^{i-1}(\boldsymbol{p}_j \times \boldsymbol{n}) \cdot \delta\boldsymbol{\phi}_j + (\boldsymbol{r}_{i-1} \times \boldsymbol{n}) \cdot \delta\boldsymbol{\phi}_i = \boldsymbol{n} \cdot \delta\boldsymbol{x}_1 \tag{76}$$

with (see equation (64))

$$\begin{aligned} \boldsymbol{p}_j &= -\tfrac{1}{2}(L_{j-1}\boldsymbol{v}_{j-1} + L_j\boldsymbol{v}_j) \\ \boldsymbol{r}_j &= -\frac{L_j}{2}\boldsymbol{v}_j. \end{aligned} \tag{77}$$

If there are m nodes on the catheter which contact the wall, then we have m constraints of the form (76). This system of constraints may be written in matrix form as

$$B[\delta\phi] = b \tag{78}$$

where the matrix B and the vector b are built from the left and right sides respectively of (76).

Given position and orientation changes $\delta\boldsymbol{x}_1$ and $\delta\boldsymbol{\phi}_1$ at the insertion point, tangential placement minimizes the incremental *elastic* energy subject to the constraint (78). The constraint may be implemented by adding a Lagrange multiplier to the energy, so that the

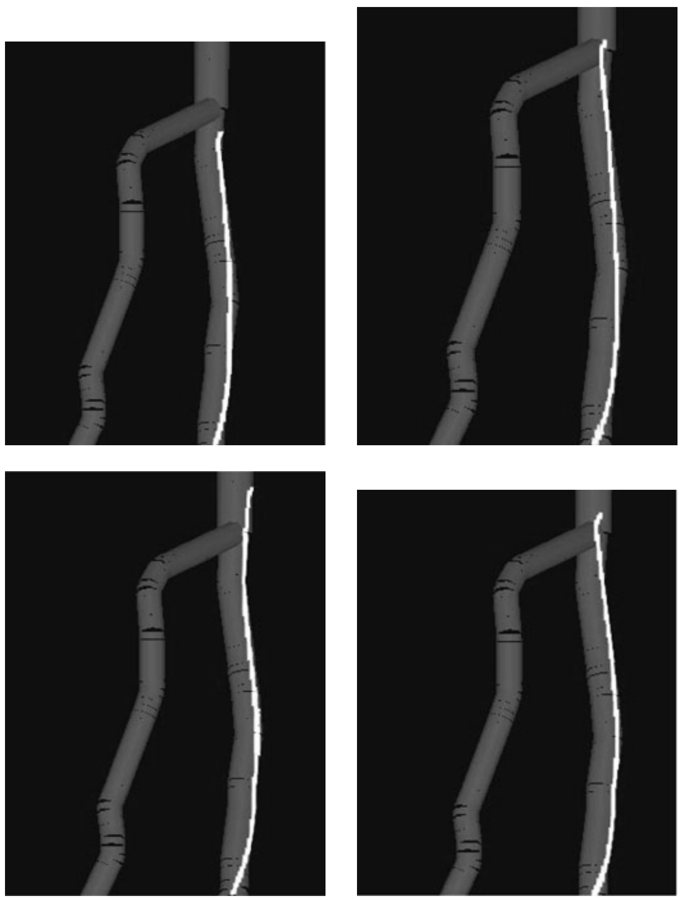

Figure 4. A sequence of simulated catheter moves in an artery, shown clockwise from top left.

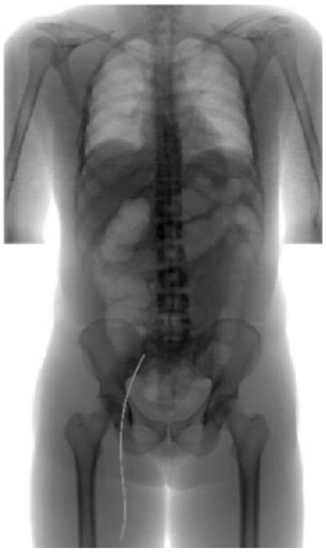

Figure 5. A simulated fluoroscopic image of a simulated catheter in an anatomical context. The catheter is inserted from the thigh and is visible as a curve.

function to be optimized is (since increments are applied from an equilibrium, elastic and external loads balance)

$$\delta H = \tfrac{1}{2}[\delta\phi]^T K_{el}[\delta\phi] + \lambda^T (B[\delta\phi] - b) \qquad (79)$$

where λ is a vector of constraint forces. This function is optimized when the linear system [15]

$$\begin{pmatrix} K_{el} & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} [\delta\phi] \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ b \end{pmatrix} \qquad (80)$$

is solved. The tangential placement procedure thus gives us an initial estimate $[\delta\phi]_0$ from the solution of this linear system.

The Taylor expansion of the total incremental energy (elastic plus external) must be minimized to find an equilibrium configuration; to quadratic order in the energy, minimization is achieved when the linear system

$$(K_{el} + \tilde{K}_{ex})[\delta\phi] = (L_{el} + L_{ex}) \qquad (81)$$

is satisfied, as discussed at the end of section 6, where $\tilde{K}_{ex} = T^T K_{ex} T$. Since the incremental energy generally contains terms higher order than quadratic, this system must be iterated to find a true equilibrium. In practice, for small increments of the control variables, this only requires a few iterations.

The process may be summarized as follows:

(1) Given user-specified changes of control variables at the insertion point, if there are nodes contacting the artery wall, use tangential placement to find an initial estimate of orientational changes $[\delta\phi]_0$. If there are no contacting nodes, displace the catheter rigidly.
(2) Construct correspondingly updated stiffness matrices (elastic and external) and load vectors and solve the linear system (81). Update variables and iterate (81) until convergence is achieved, i.e., the total load becomes very small.

A catheter (the same as that used in the loading experiments in section 6) inserted into an artery by using the above process is shown in figure 4, where the deformation of the shape to fit inside the artery is clearly visible. Figure 5 shows a simulated fluoroscopic view, with a catheter inserted by the simulation procedure described here, of the kind that a physician usually works with in an actual catheterization procedure. For details about the simulation system, the reader is referred to [1]. The system uses anatomical data reconstructed from the Visible Human^{TM} database. Catheters are usually hollow and are used in conjunction with guidewires which pass through them. The determination of equilibrium shapes of such a composite object, particularly in the catheter's head region, is also required. A discretization with circular arcs may be used for this purpose and is described in [17]. This method directly builds the constraints (12) and (13) into the description of the geometry and finds equilibria by minimizing the total energy. We are developing the incorporation of the guidewire into the FEM formalism discussed in this paper as well and will discuss this elsewhere.

To conclude, we have described a formalism for the description of thin rod deformations and applied it to the problem of simulating catheter navigation. The description applies across the wide range of scales at which chain-like objects are found, from proteins and the cell cytoskeleton to catheters and bridges made of beams. By the addition of an inertial term (d'Alembert's principle) we can extend the formalism detailed here to the dynamics of flexible rods [18]. A discretized treatment is directly applicable to the control of 'tentacles' or flexible robot arms with joints.

Acknowledgments

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Appendix. Reduction from three-dimensional elasticity

Here we show that equation (8), and related results marked (a) and (b) at the end of this appendix, arise from the reduction of three-dimensional continuum mechanics to a thin rod model. Although these consequences may be part of 'folk' knowledge in the elasticity community, we have not seen these results derived before (see, for example, chapters 8 and 9 in [3], where Cosserat rods are discussed).

The elastic energy in three dimensions, to quadratic order in the strains u_{ij}, takes the form

$$E_{el} = \int_V C_{ijkl} u_{ij} u_{kl}\, \mathrm{d}v \tag{82}$$

where the integral is over the volume of the rod and the C are elasticity coefficients; C is symmetric under exchange of $\{ij\}$ and $\{kl\}$. We shall consider, for convenience, the case of *isotropic* materials, in which case the C satisfy $C_{ijkl} = 0$ for $i = j$ and $k \neq l$. Specifically, the energy density J_3 in this case takes the form

$$J_3 = \mu_s \,\mathrm{Tr}(u_s u_s^T) + \frac{K}{2} (\mathrm{Tr}\, u)^2 \tag{83}$$

where u_s is the traceless part of the strain tensor which describes volume-preserving or shear deformations,

$$u_{s,ij} = u_{ij} - \tfrac{1}{3}\delta_{ij}\,\mathrm{Tr}\, u. \tag{84}$$

The elastic constants μ_s and K are the shear modulus and the bulk modulus, respectively.

Consider a normal cross section of the rod which forms one side of an infinitesimal slab of rod. Choose orthonormal coordinates (x_1, x_2, x_3) such that the x_1 axis is tangent to the centreline and choose the origin so that

$$\int_A x_i \,\mathrm{d}x_2\, \mathrm{d}x_3 = 0 \qquad i = 2, 3 \tag{85}$$

where A denotes the cross section. We shall assume that the geometry of the rod varies slowly enough that the centreline forms a continuous piecewise smooth curve.

We shall write down now a general expression for the deformation of material in the neighbourhood of the section A, up to quadratic order in the coordinates. Denoting displacements in the x_1, x_2 and x_3 directions by u_1, u_2 and u_3 respectively, we write

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} k_1 & h_1 & g_1 & a_1 & b_1 & c_1 & d_1 & e_1 & f_1 \\ k_2 & h_2 & g_2 & a_2 & b_2 & c_2 & d_2 & e_2 & f_2 \\ k_3 & h_3 & g_3 & a_3 & b_3 & c_3 & d_3 & e_3 & f_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_1^2 \\ x_1 x_2 \\ x_1 x_3 \\ x_2 x_3 \\ x_2^2 \\ x_3^2 \end{pmatrix}. \tag{86}$$

We shall assume that the strain tensor (with components $u_{ij} = (\partial_i u_j + \partial_j u_i)/2$) obtained from this deformation varies only slowly along the rod; this assumption (a natural one for a rod whose cross sectional extent is much smaller than its length) implies that the strain tensor, up to quadratic order in the local coordinates, is reflection invariant under $x_1 \to -x_1$. This requirement gives $a_1 = 0$, as well as the three relations

$$\begin{aligned} a_2 &= -b_1/2 \\ a_3 &= -c_1/2\,. \\ b_3 &= -c_2 \end{aligned} \tag{87}$$

Further, we can make overall rotations of the axes to set the coefficients h_1, g_1 and g_2 to zero. Then the independent components of the strain tensor are:

$$\begin{pmatrix} u_{11} \\ u_{22} \\ u_{33} \\ u_{12} \\ u_{13} \\ u_{23} \end{pmatrix} = \begin{pmatrix} k_1 \\ h_2 \\ g_3 \\ k_2/2 \\ k_3/2 \\ h_3/2 \end{pmatrix} + \begin{pmatrix} b_1 & 0 & c_1 \\ 0 & 2e_2 & d_2 \\ 0 & d_3 & 2f_3 \\ 0 & 2e_1 & (d_1 + c_2) \\ 0 & (d_1 - c_2) & 2f_1 \\ 0 & (2e_3 + d_2) & (2f_2 + d_3) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{88}$$

The stress tensor $\boldsymbol{\sigma}$ obtained from this strain tensor must satisfy the equilibrium equations

$$\operatorname{div} \boldsymbol{\sigma} = 0 \tag{89}$$

which hold in the absence of body forces (which we neglect). In addition, we shall assume that since the rod is thin, the force densities (derived from surface stresses) on the sides of the rod are zero almost everywhere on the surface (under normal loading conditions), and that where they are non-zero, they scale like (d/L), where d is a measure of cross sectional extent and L is the length of the rod. We shall see presently that this is a consistent assumption.

For isotropic materials, the independent components of the stress tensor may be written in terms of those of the strain tensor [11] in the form

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix} = \frac{Y}{(1+\nu)(1-2\nu)}$$

$$\times \begin{pmatrix} (1-\nu) & \nu & \nu & 0 & 0 & 0 \\ \nu & (1-\nu) & \nu & 0 & 0 & 0 \\ \nu & \nu & (1-\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & (1-2\nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & (1-2\nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & (1-2\nu) \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{22} \\ u_{33} \\ u_{12} \\ u_{13} \\ u_{23} \end{pmatrix} \tag{90}$$

where $Y = 9K\mu_s/(3K+\mu_s)$ is Young's modulus and $\nu = \frac{1}{2}(3K-2\mu_s)/(3K+\mu_s)$ is Poisson's ratio.

With the use of these expressions, the above requirements place further constraints on the coefficients. They tell us that we must have the relations

$$\begin{aligned} e_2 &= -\nu b_1/2 \\ d_2 &= -\nu c_1 \\ d_3 &= -\nu b_1 \\ f_3 &= -\nu c_1/2. \end{aligned} \tag{91}$$

They also yield, to this order, the equations

$$h_2 = g_3 = -\nu k_1. \tag{92}$$

All of the above follow from setting $\sigma_{22} = 0$ and $\sigma_{33} = 0$ on the boundary of the cross section. Where these stresses on the surface are non-zero, the strain tensor must be expanded to higher order, in general, to satisfy the boundary conditions. It is easy to see that these corrections to the strain tensor from higher-order terms are significant only near the boundary. In addition, in these stressed regions, the constant terms in the strain tensor may be independently non-zero, so that for instance (92) need not hold; equation (91) may be modified as well. These corrections are generally of order d/L.

In regions with zero boundary stresses, corrections to equation (92) are of quadratic order in d/L. This may be seen by an expansion away from a stressed region into an unstressed region that includes broken reflection symmetry.

We also find the general relations

$$\begin{aligned} e_1 &= f_1 = 0 \\ e_3 &= -d_2/2 = \nu c_1/2\ . \\ f_2 &= -d_3/2 = \nu b_1/2 \end{aligned} \tag{93}$$

These follow from the equilibrium equations (89) upon assuming that the elastic moduli vary only slowly along the rod. At higher order in d/L, these equalities are modified and in any case tell us that e_3 and f_2 are not independent quantities. The quantities e_1 and f_1 remain zero at higher order as well; this follows from the equilibrium equations and from the zero surface force density requirement on the x_1 component of the surface force, which reads

$$\sigma_{12}m_2 + \sigma_{13}m_3 = 0. \tag{94}$$

Here $\boldsymbol{m}$ is the outward normal at the rod surface or the boundary of the section (this has zero x_1 component due to our choice of coordinates). These relations are also consistent, as they should be, with the boundary condition $\sigma_{23} = 0$ on the surface. Equation (94) also yields the boundary condition

$$(d_1 + c_2)x_3m_2 + (d_1 - c_2)x_2m_3 = 0 \tag{95}$$

on the boundary contour. For a circular cross section, this yields $d_1 = 0$; there is no warping of the cross section in this particular case. For an arbitrary cross sectional shape, equation (95) cannot be satisfied as it stands and in general must be augmented by additional terms (arising from extra terms in u_1 that are higher order in the transverse coordinates) due to warping of the cross section. It is to be noted that these warping terms are only present when $c_2 \neq 0$; in general, to leading order we therefore have $d_1 \propto c_2$.

In order to make the connection with standard treatments of Cosserat theories, we shall now relabel some of the coefficients and interpret them. So we shall write $\alpha \equiv k_1$, $\beta_1 \equiv h_2$, $\beta_2 \equiv g_3$, $\omega_1 \equiv c_2$, $\omega_2 \equiv c_1$, $\omega_3 \equiv -b_1$ and $d_1 \equiv \omega_1 \bar{d}_1$; then the constraints we have derived tell us that $d_2 = -\nu\omega_2$, $2e_2 = \nu\omega_3$, $d_3 = \nu\omega_3$, $2f_3 = -\nu\omega_2$, $2e_3 = \nu\omega_2$ and $2f_2 = -\nu\omega_3$.

With these definitions, the independent components of the strain tensor in three dimensions finally take the form (to leading order in d/L)

$$\begin{pmatrix} u_{11} \\ u_{22} \\ u_{33} \\ u_{12} \\ u_{13} \\ u_{23} \end{pmatrix} = \begin{pmatrix} k_1 \\ h_2 \\ g_3 \\ k_2/2 \\ k_3/2 \\ h_3/2 \end{pmatrix} + \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ 0 & \nu\omega_3 & -\nu\omega_2 \\ 0 & \nu\omega_3 & -\nu\omega_2 \\ 0 & 0 & \omega_1(\bar{d}_1 + 1)/2 \\ 0 & \omega_1(\bar{d}_1 - 1)/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{96}$$

It is apparent from here that the variable k_1 measures stretch in the longitudinal direction and that h_2 and g_3 measure stretch in the transverse directions. It is also clear that k_2, k_3 and h_3 measure shear in the $x_1 - x_2$, $x_1 - x_3$ and $x_2 - x_3$ planes, respectively. The vector $\boldsymbol{\omega} \equiv (\omega_1, \omega_2, \omega_3)$ measures strain due to twisting and bending deformations along the rod; it is clear from the form of the strain tensor that it expresses a *rate* of twisting and bending. The variable $\bar{d}_1$ measures warping of the cross section; it effectively contributes a factor to the twist modulus. More correctly, this variable receives higher-order corrections which it needs to satisfy the boundary condition (95).

We mention again that corrections to these equations come from higher-order terms (of order higher than quadratic in the transverse coordinates) in the expansion of the deformation (86); these are expected to be small under normal loading conditions. In particular, it is clear that changes in the cross sectional *geometry* are of quadratic or higher order in the transverse coordinates.

This form of the strain tensor corresponds exactly to the *general* theory of Cosserat rods described in terms of two transverse directors, for example, in [3]. This model allows for stretching in the transverse and longitudinal directions, changes in angles between the two directors and the tangent to the centreline, and rotation along the curve of the plane defined by the transverse directors. The nine parameters which quantify the strains in equation (96) correspond to a $GL(3)$ general affine transformation of the three directors in this model.

A specialization of this $GL(3)$ model is the theory of *special Cosserat* rods. In addition to bending, twisting and stretch of the centreline, this model allows for the plane defined by the two transverse directors to change its angle with respect to the unit tangent to the centreline. This model is therefore described by the strain variables of rotation rate $\boldsymbol{\omega}$, longitudinal stretch k_1, and shear strains k_2 and k_3 which quantify shear in two non-transverse planes.

Using the strain tensor (96) in the elastic energy density (83) and using the centreline definition (85), the following facts emerge upon integration over the cross sectional variables:

(a) In the resulting quadratic one-dimensional energy density, there is no coupling of the rotation rate $\boldsymbol{\omega}$ with either stretch or shear.

(b) The terms in the one-dimensional energy density involving stretch and shear have a coefficient proportional to $(\mu_s A)$, while the terms depending on the rotation rate have a coefficient proportional to $(\mu_s I)$; here $A \sim d^2$ is the area of cross section, $I \sim d^4$ is a second moment of area. The rotation rate has an average value determined roughly by the total angular change of the unit tangent along the rod (say ϕ) divided by its length L. Since ϕ is typically a number of order one, assuming a roughly equal distribution of energies says that average stretch and shear rates therefore have magnitudes of order d/L; thus for instance $k_1 \sim (d/L)$. As d becomes very small relative to L, stretch contributes very little to change in geometry.

Further, one expects from this analysis that in general various stretch and shear rates are all of comparable magnitude. Since it is the bending modes of deformation which cost least energy for small d/L, our earlier assumption that force densities on the sides of the rod are generically small is justified.

A further specialization of the special Cosserat theory is one which considers the rotation rate alone as the strain variables. Given the small value of d/L, the effect on the cross sectional *geometry* remains very small, as we have noted earlier; to a good approximation one can indeed assume that normal sections are deformed to normal sections. This description in terms of the centreline and an associated rotation rate alone, which intuition suggests is reasonable, is therefore easily justified.

While our analysis used isotropic elasticity for convenience, it is easy to see that the conclusions above remain valid even upon removing this restriction. All changes are only in the coefficients of the resulting one-dimensional energy density. We used homogeneity as well in the above. When there are departures from homogeneity, there are in general couplings between rotation rate and the stretch and shear variables in the one-dimensional energy density. However, as long as variations in properties are slow, our results continue to hold to a good approximation.

The foregoing analysis serves to make precise the notion of 'thinness'. With the model used in this paper as an initial approximation, an expansion in powers of d/L could be developed to provide successively more refined models of 'thicker' rods.

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