

# Mathematical and numerical treatments of elastic rods with frictionless self contact

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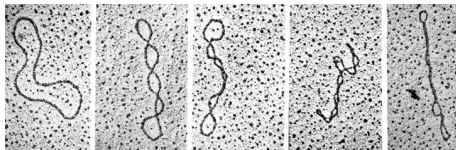
**Ecole Nationale d'Ingénieurs de Tunis**

**Joint work with Mourad Chamekh & Saloua Mani-Aouadi**

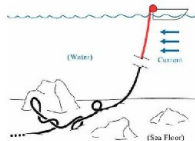
**7th Meeting on Unilateral Problems in Structural Analysis  
Palmanova, June 2010**

# Motivation

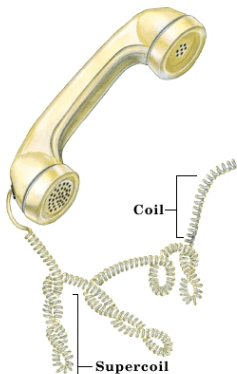
- Supercoiling of the DNA molecule



- Satellite and submarine cables



## Telephone cable

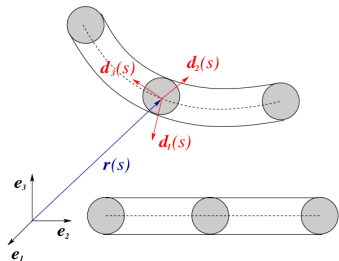


# Cosserat theory of rods

We consider an elastic rod  $\mathcal{R}$  of length  $L$  and circular cross sections of a uniform diameter  $2\varepsilon$ .

The configuration of the rod is described by specifying for each  $s \in [0, L]$ :

- **position vector**  $\mathbf{r}(s)$  with respect to a fixed orthonormal frame  $\{O; \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ .
- right-handed triad of orthonormal **directors**  $\{\mathbf{d}_1(s), \mathbf{d}_2(s), \mathbf{d}_3(s)\}$ , or equivalently, the proper orthogonal tensor  $\mathbf{R}(s) = \mathbf{d}_i(s) \otimes \mathbf{e}_i$ .



# Kinematics

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

$$\begin{aligned}\mathbf{r}'(s) &= \mathbf{v}(s), \\ \mathbf{R}'(s) &= \mathbf{u}^\times(s)\mathbf{R}(s),\end{aligned}$$

where  $'$  denotes differentiation with respect to  $s$ .

$$\mathbf{u}^\times(s) = \begin{bmatrix} 0 & -u_3(s) & u_2(s) \\ u_3(s) & 0 & -u_1(s) \\ -u_2(s) & u_1(s) & 0 \end{bmatrix}.$$

The vector  $\mathbf{u}(s)$  is the axial (also called Darboux) vector associated with the skew-symmetric tensor  $\mathbf{R}'(s)\mathbf{R}^T(s)$ .

## Strains measures

We introduce the following **strain measures**

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

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

- \*  $\mathbf{v} \cdot \mathbf{d}_1$  and  $\mathbf{v} \cdot \mathbf{d}_2$  represent shear strains.
- \*  $\mathbf{v} \cdot \mathbf{d}_3$  represents elongation.
- \*  $\mathbf{u} \cdot \mathbf{d}_1$  and  $\mathbf{u} \cdot \mathbf{d}_2$  represent flexures.
- \*  $\mathbf{u} \cdot \mathbf{d}_3$  represents twist.

These strain measures are invariant under translations and rotations.

## Balance equations

Let  $\mathbf{n}(s)$  be the resultant force (of the material with  $\sigma > s$  on the material with  $\sigma < s$ ) acting across the cross section at  $s$  of  $\mathcal{R}$ .

Let  $\mathbf{m}(s)$  be the resultant couple acting across the cross section at  $s$  of  $\mathcal{R}$  about the point  $\mathbf{r}(s)$ .

The local form of the balance of forces and moments for the rod write

$$\begin{aligned}\mathbf{n}' + \mathbf{f} &= \mathbf{0}, \\ \mathbf{m}' + \mathbf{r}' \times \mathbf{n} + \mathbf{t} &= \mathbf{0},\end{aligned}$$

where  $\mathbf{f}$  and  $\mathbf{t}$  are external distributed force and torque per unit length of the reference configuration.

## Constitutive relations

We assume that the rod is made of a **hyperelastic** material, i.e., there exists an elastic energy density  $\mathcal{W}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}})$  such as

$$\begin{aligned} \mathbf{m}(s) &= \mathbf{R} \frac{\partial \mathcal{W}}{\partial \mathbf{u}}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}), \\ \mathbf{n}(s) &= \mathbf{R} \frac{\partial \mathcal{W}}{\partial \mathbf{v}}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}), \end{aligned}$$

where  $\hat{\mathbf{u}}(s)$  and  $\hat{\mathbf{v}}(s)$  are the strains in the unstressed reference configuration.



## Boundary value problem

$$\mathbf{r}'(s) = \mathbf{R}(s)\mathbf{v}(s),$$

$$\mathbf{R}'(s) = \mathbf{R}(s)\mathbf{u}^\times(s),$$

$$\mathbf{n}'(s) + \mathbf{f}(s) = \mathbf{0},$$

$$\mathbf{m}'(s) + \mathbf{r}'(s) \times \mathbf{n}(s) + \mathbf{t}(s) = \mathbf{0},$$

$$\mathbf{m}(s) = \mathbf{R} \frac{\partial \mathcal{W}}{\partial \mathbf{u}}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}),$$

$$\mathbf{n}(s) = \mathbf{R} \frac{\partial \mathcal{W}}{\partial \mathbf{v}}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}),$$

$\mathbf{R}(0)\mathbf{d}_i(0)$  or  $\mathbf{m}(0) \cdot \mathbf{d}_i(0)$  is prescribed,

$\mathbf{r}(0) \cdot \mathbf{d}_i(0)$  or  $\mathbf{n}(0) \cdot \mathbf{d}_i(0)$  is prescribed,

$\mathbf{R}(L)\mathbf{d}_i(L)$  or  $\mathbf{m}(L) \cdot \mathbf{d}_i(L)$  is prescribed,

$\mathbf{r}(L) \cdot \mathbf{d}_i(L)$  or  $\mathbf{n}(L) \cdot \mathbf{d}_i(L)$  is prescribed.

## Configuration space

The space of all possible configurations of the rod is

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

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

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

## First variation operator

For a scalar-, vector- or tensor-valued function, say  $\xi(s)$ , we consider a smooth one-parameter family of curves  $\xi_\epsilon(s)$  such that

$$\xi_0(s) = \xi(s).$$

We denote by  $\delta\xi$  the derivative of  $\xi_\epsilon$  with respect to the parameter  $\epsilon$  evaluated at  $\epsilon = 0$ , i.e.,

$$\delta\xi = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \xi_\epsilon.$$

## Perturbed configurations

For a given configuration  $(\mathbf{r}, \mathbf{R}) \in \mathcal{C}$ , we construct a perturbed configuration  $(\mathbf{r}_\epsilon, \mathbf{R}_\epsilon) \in \mathcal{C}$  by setting

$$\begin{aligned}\mathbf{r}_\epsilon(s) &= \mathbf{r}(s) + \epsilon \mathbf{p}(s), \\ \mathbf{R}_\epsilon(s) &= \exp(\epsilon \mathbf{q}^\times(s)) \mathbf{R}(s),\end{aligned}$$

where  $\mathbf{p}(\cdot)$  and  $\mathbf{q}(\cdot)$  are vector-valued functions on  $[0, L]$ .

- The vector-valued function  $\mathbf{p}(\cdot)$  is interpreted as a superposed infinitesimal displacement on the center line  $\mathbf{r}(\cdot)$ .
- The skew-symmetric tensor-valued function  $\mathbf{q}^\times(\cdot)$  is interpreted as an infinitesimal rotation superposed on the rotation  $\mathbf{R}(\cdot)$ .

It then follows that

$$\begin{aligned}\delta \mathbf{r} &= \mathbf{p}, \\ \delta \mathbf{R} &= \mathbf{q}^\times \mathbf{R}.\end{aligned}$$

## Principle of virtual work

The principle of virtual work writes

$$\delta \mathcal{J}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) = 0, \quad \forall (\mathbf{p}, \mathbf{q}) \text{ admissible variation,}$$

where

$$\mathcal{J}(\mathbf{r}, \mathbf{R}) = \int_0^L [\mathcal{W}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}) - \mathbf{f} \cdot \mathbf{r}] ds.$$

$\delta \mathcal{J}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q})$  is the sum of:

- The virtual work of the internal forces and moments

$$\delta \mathcal{J}_{\text{int}}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) := \int_0^L \{ \mathbf{n} \cdot (\mathbf{p}' + \mathbf{r}' \times \mathbf{q}) + \mathbf{m} \cdot \mathbf{q}' \} ds$$

- The work of the applied loads

$$\delta \mathcal{J}_{\text{ext}}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) := \int_0^L \mathbf{f} \cdot \mathbf{p} ds$$

## Variational Formulation

The space of **kinematically admissible** configurations is

$$\mathcal{C}_a = \{(\mathbf{r}, \mathbf{R}) \in \mathcal{C} \mid (\mathbf{r}, \mathbf{R}) \text{ satisfies BC}\}.$$

The problem of finding the configurations that satisfy the equilibrium equations together with the constitutive law leads to the following nonlinear minimization problem

$$\begin{cases} \text{Find } (\mathbf{r}, \mathbf{R}) \in \mathcal{C}_a \text{ such that} \\ \mathcal{J}(\mathbf{r}, \mathbf{R}) \leq \mathcal{J}(\tilde{\mathbf{r}}, \tilde{\mathbf{R}}), \quad \forall (\tilde{\mathbf{r}}, \tilde{\mathbf{R}}) \in \mathcal{C}_a. \end{cases}$$

## Gap function for the self-contact problem

**Impenetrability condition:** In a **physically admissible configuration** two points of the rod **cannot** have the same placement.

To take this (nonlocal) condition, we introduce a (signed) distance of contact by the distance between the points on the central curve of the rod.

This distance is called **gap function** or **self-penetration function** and is given by

$$d_r(s) = 2\varepsilon - \min_{\sigma \in I(s)} \|\mathbf{r}(s) - \mathbf{r}(\sigma)\|,$$

where  $I(s)$  is a subset of  $[0, L]$  associated with the portion

$$\{\mathbf{r}(\tau), \tau \in I(s)\}$$

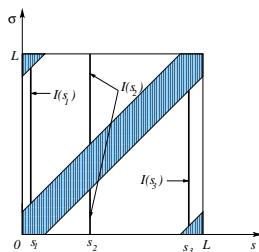
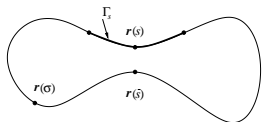
of the curve  $\mathcal{C} = \{\mathbf{r}(s), s \in [0, L]\}$  which can be in contact with  $\mathbf{r}(s)$ .

# Gap function for the self-contact problem

For a closed rod, the set  $I(s)$  is

$$I(s) = \begin{cases} [s^+, L + s^-], & \text{if } s \in [0, \delta], \\ [0, s^-] \cup [s^+, L], & \text{if } s \in [\delta, L - \delta], \\ [s^+ - L, s^-], & \text{if } s \in [L - \delta, L], \end{cases}$$

where  $s^+ = s + \delta$  and  $s^- = s - \delta$ , and  $\delta$  is a fixed constant that depends on  $\varepsilon$ .





## Closest point

The problem of finding the arclength  $\bar{s}$  of the closest point on  $\mathcal{C} \setminus \Gamma_s$  to the point  $\mathbf{r}(s)$  is equivalent to the following minimization problem

$$\min_{\sigma \in I(s)} \|\mathbf{r}(\sigma) - \mathbf{r}(s)\|^2.$$

As the curve  $\mathbf{r}([0, L])$  is continuous and the set  $I(s)$  is compact, this minimization problem admits at least one solution.

When  $\bar{s} \notin \partial I(s)$ , or when the curve  $\mathbf{r}([0, L])$  is closed, then  $\mathbf{r}(\bar{s})$  is an orthogonal projection of  $\mathbf{r}(s)$  on  $\mathcal{C} \setminus \Gamma_s$ . We can therefore write

$$\mathbf{r}'(\bar{s}) \cdot [\mathbf{r}(\bar{s}) - \mathbf{r}(s)] = 0.$$

Thus, the unit vector  $\boldsymbol{\nu}(s) = \frac{\mathbf{r}(s) - \mathbf{r}(\bar{s})}{\|\mathbf{r}(s) - \mathbf{r}(\bar{s})\|}$  is orthogonal to  $\mathbf{r}'(\bar{s})$ .

## Variational formulation of the self-contact problem

The space of **kinematically admissible** configurations is

$$\mathcal{C}_a = \{(\mathbf{r}, \mathbf{R}) \in \mathcal{C} \mid (\mathbf{r}, \mathbf{R}) \text{ satisfies BC}\}.$$

As self-penetration of different parts of the rod is physically impossible, we shall impose the constraint

$$d_{\mathbf{r}}(s) \leq 0, \quad \forall s \in [0, L].$$

We therefore introduce the space of **kinematically and physically admissible** configurations

$$\mathcal{C}_c = \{(\mathbf{r}, \mathbf{R}) \in \mathcal{C}_a, \text{ such that } d_{\mathbf{r}}(s) \leq 0, \forall s \in [0, L]\}.$$

## Nonlinear self-contact problem

The problem of finding the configurations that satisfy the equilibrium equations together with the constitutive laws leads to the following nonlinear minimization problem

$$\begin{cases} \text{Find } (\mathbf{r}, \mathbf{R}) \in \mathcal{C}_c \text{ such that} \\ \mathcal{J}(\mathbf{r}, \mathbf{R}) \leq \mathcal{J}(\tilde{\mathbf{r}}, \tilde{\mathbf{R}}), \quad \forall (\tilde{\mathbf{r}}, \tilde{\mathbf{R}}) \in \mathcal{C}_c, \end{cases}$$

where

$$\mathcal{J}(\mathbf{r}, \mathbf{R}) = \int_0^L [\mathcal{W}(s, \mathbf{u} - \hat{\mathbf{u}}, \mathbf{v} - \hat{\mathbf{v}}) - \mathbf{f} \cdot \mathbf{r}] ds,$$

is the total energy.

## Treatment of the constraints

The self-contact problem is formulated on the space  $\mathcal{C}_c$  of kinematically and physically admissible configurations which contains two types of constraints:

- the rotation  $\mathbf{R}$  must be in  $SO(3)$ .
- the gap function  $d_r$  must be nonpositive.

We handle constraint which is related to  $SO(3)$  using **differential-geometric tools**.

We use a **penalty method** to relax the constraint expressing the impenetration.

## Penalized energy

For this, we introduce the following energy functional defined on the space of kinematically admissible configurations  $\mathcal{C}_a$ :

$$\mathcal{J}_{\text{total}}(\mathbf{r}, \mathbf{R}) = \mathcal{J}(\mathbf{r}, \mathbf{R}) + \mathcal{J}_c(\mathbf{r})$$

where

$$\mathcal{J}_c(\mathbf{r}) := \frac{1}{2}\mu \int_0^L \langle d_{\mathbf{r}}(s) \rangle^2 ds,$$

is a term that penalizes self penetration.

$\mu$  is a (large) penalty parameter

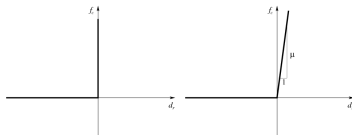
$\langle \cdot \rangle$  is the Macauley bracket representing the positive part of its operand  $\langle x \rangle = \max(0, x) = \frac{1}{2}(x + |x|)$ .

# Mechanical interpretation of the penalized energy

In the penalty method, the compression force  $f_c^\mu$  is taken to be

$$f_c^\mu(s) = \mu \langle d_{\mathbf{r}}(s) \rangle.$$

This constitutive-like equation replaces the (multivalued non differentiable) contact law.



With the introduction of the contact pressure  $f_c^\mu$ , the penalty energy can be written as

$$\mathcal{J}_c(\mathbf{r}) = \frac{1}{2} \int_0^L f_c^\mu(s) d_{\mathbf{r}}(s) ds,$$

which can be seen as expressing the **work of the contact pressure**.

## The Karuch-Kuhn-Tucker conditions

The non-penetration constraint yields a contact force  $f_c$  between the material at  $s$  and that at  $\bar{s}$ . Under the assumption of frictionless contact, this force is a normal pressure, i.e.,

$$f_c(s) = f_c(s)\nu(s),$$

where  $f_c(s)$  is non negative.

The frictionless self-contact law

$$d_r(s) \leq 0,$$

$$f_c(s) \geq 0,$$

$$d_r(s) f_c(s) = 0,$$

describes the Karuch-Kuhn-Tucher conditions.

## Principle of virtual work for the penalized problem

The necessary condition for minimizing the total energy in the space  $\mathcal{C}_a$  is

$$\delta \mathcal{J}_{\text{total}}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) = \delta \mathcal{J}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) + \delta \mathcal{J}_c(\mathbf{r}; \mathbf{p}) = 0.$$

To obtain the expression for  $\delta \mathcal{J}_c(\mathbf{r}; \mathbf{p})$  we note that, although  $\langle \cdot \rangle$  is not differentiable at 0, the function  $\langle \cdot \rangle^2$  is differentiable and

$$\frac{d\langle x \rangle^2}{dx} = 2\langle x \rangle.$$

We obtain

$$\delta \mathcal{J}_c(\mathbf{r}; \mathbf{p}) = \int_0^L f_c^\mu(s) \delta d_r(s) ds.$$

This equation states that  $\delta \mathcal{J}_c(\mathbf{r}; \mathbf{p})$  is given by the virtual work developed by the contact force through a variation of the contact distance.



## The first variation of $\delta \mathcal{J}_c$

The gap function can be written as

$$d_r(s) = 2\varepsilon - (\mathbf{r}(s) - \mathbf{r}(\bar{s})) \cdot \boldsymbol{\nu}(s),$$

from which we obtain

$$\delta d_r(s) = [\delta \bar{s} \mathbf{r}'(\bar{s}) - \mathbf{p}(s) + \mathbf{p}(\bar{s})] \cdot \boldsymbol{\nu}(s) - [\mathbf{r}(s) - \mathbf{r}(\bar{s})] \cdot \delta \boldsymbol{\nu}(s).$$

As  $\boldsymbol{\nu}(s)$  is a unit vector  $\Rightarrow \mathbf{r}(\bar{s}) - \mathbf{r}(s) \perp \delta \boldsymbol{\nu}(s)$ .

Since  $\mathbf{r}'(\bar{s}) \perp \boldsymbol{\nu}(s)$ ,  $\delta \bar{s}$  need not be computed.

Accordingly, the expression of  $\delta d_r(s)$  simplifies to

$$\delta d_r(s) = (\mathbf{p}(\bar{s}) - \mathbf{p}(s)) \cdot \boldsymbol{\nu}(s).$$

In conclusion we have

$$\delta \mathcal{J}_c(\mathbf{r}; \mathbf{p}) = \int_0^L f_c^\mu(s) (\mathbf{p}(\bar{s}) - \mathbf{p}(s)) \cdot \boldsymbol{\nu}(s) ds.$$

## The penalized nonlinear problem

Now let  $\mathcal{G}$  denote the nonlinear functional defined by

$$\mathcal{G}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) := \delta \mathcal{J}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) + \delta \mathcal{J}_c(\mathbf{r}; \mathbf{p}).$$

Then the penalized problem that we propose to solve writes

$$\left\{ \begin{array}{l} \text{Find } (\mathbf{r}, \mathbf{R}) \in \mathcal{C}_a \text{ such that} \\ \mathcal{G}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}) = 0, \quad \forall (\mathbf{p}, \mathbf{q}) \text{ such that } (\mathbf{p}, \mathbf{q}^\times \mathbf{R}) \in T_{(\mathbf{r}, \mathbf{R})} \mathcal{C}_a, \end{array} \right.$$

where  $T_{(\mathbf{r}, \mathbf{R})} \mathcal{C}_a$  is the tangent space to  $\mathcal{C}_a$  at  $(\mathbf{r}, \mathbf{R})$ .

This is a nonlinear problem which we propose to solve it iteratively by Newton method (on manifolds).

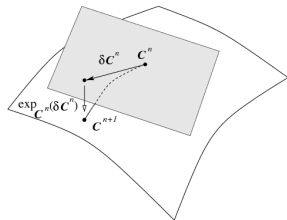
## Newton's method on a nonlinear space

In the classical Newton's method, at each iteration the correction vector is added to the previous estimate of the solution.

In the case where the solution space is nonlinear, such as  $\mathcal{C}_a$ , the update procedure is based on the **exponential map**:

At the iteration  $n$ , the estimate of the solution  $\mathbf{C}^n$  belongs to the **nonlinear space**, whereas the correction vector  $\delta\mathbf{C}^n$  lies in the **tangent space**.

The new estimate  $\mathbf{C}^{n+1}$  of the solution is obtained by the exponential map at  $\mathbf{C}^n$  of  $\delta\mathbf{C}^n$ .



## Newton method on $\mathcal{C}_a$

At the iteration  $n$  we start with an estimate  $(\mathbf{r}^n, \mathbf{R}^n)$  and then we solve for  $(\boldsymbol{\eta}, \boldsymbol{\theta})$  the linearized problem

$$\mathcal{G}(\mathbf{r}^n, \mathbf{R}^n; \mathbf{p}, \mathbf{q}) + \Delta \mathcal{G}(\mathbf{r}^n, \mathbf{R}^n; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) = 0,$$

where the symbol  $\Delta$  denotes the directional derivative defined for any scalar-, vector- or tensor-valued function  $F(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q})$  by

$$\Delta F(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) := \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} F(\mathbf{r} + \epsilon \boldsymbol{\eta}, \exp(\epsilon \boldsymbol{\theta}^\times) \mathbf{R}; \mathbf{p}, \mathbf{q}).$$

The estimate at the next iteration step is then

$$(\mathbf{r}^{n+1}, \mathbf{R}^{n+1}) = (\mathbf{r}^n + \boldsymbol{\eta}, \exp(\boldsymbol{\theta}^\times) \mathbf{R}^n).$$

The iterative process continues until the norm of the correction term  $(\boldsymbol{\eta}, \boldsymbol{\theta})$  of the current iteration falls below a prescribed value.

# Linearization of the virtual work of internal forces and moments

We have

$$\Delta \delta \mathcal{J}_{\text{int}}(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) = \int_0^L (\mathbf{Q}_m(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) + \mathbf{Q}_g(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta})) ds,$$

where

$$\mathbf{Q}_m(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) = \begin{pmatrix} \boldsymbol{\eta}' \\ \boldsymbol{\theta} \\ \boldsymbol{\theta}' \end{pmatrix} \cdot \begin{pmatrix} \mathbf{V} & \mathbf{V}\mathbf{r}'^\times & \mathbf{W} \\ -\mathbf{r}'^\times \mathbf{V} & -\mathbf{r}'^\times \mathbf{V}\mathbf{r}'^\times & -\mathbf{r}'^\times \mathbf{W} \\ \mathbf{W}^T & \mathbf{W}^T \mathbf{r}'^\times & \mathbf{U} \end{pmatrix} \begin{pmatrix} \mathbf{p}' \\ \mathbf{q} \\ \mathbf{q}' \end{pmatrix},$$

$$\mathbf{Q}_g(\mathbf{r}, \mathbf{R}; \mathbf{p}, \mathbf{q}; \boldsymbol{\eta}, \boldsymbol{\theta}) = \begin{pmatrix} \boldsymbol{\eta}' \\ \boldsymbol{\theta} \\ \boldsymbol{\theta}' \end{pmatrix} \cdot \begin{pmatrix} \mathbf{0} & -\mathbf{n}^\times & \mathbf{0} \\ \mathbf{n}^\times & \mathbf{n}^\times \mathbf{r}'^\times & \mathbf{m}^\times \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{p}' \\ \mathbf{q} \\ \mathbf{q}' \end{pmatrix}.$$

# Linearization of the virtual work of self-contact forces

We obtain

$$\Delta \delta \mathcal{J}_c(\mathbf{r}; \mathbf{p}; \boldsymbol{\eta}) = \int_0^L \frac{\mu H(d_r)}{2\varepsilon - d_r(s)} \mathbf{Q}_c(\mathbf{r}; \mathbf{p}; \boldsymbol{\eta}) ds,$$

where

$$\begin{aligned} \mathbf{Q}_c(\mathbf{r}; \mathbf{p}; \boldsymbol{\eta}) &= \check{\boldsymbol{\eta}}(s) \cdot (2\varepsilon \boldsymbol{\nu}(s) \otimes \boldsymbol{\nu}(s) - d_r(s) \mathbf{I}) \check{\mathbf{p}}(s) \\ &+ \frac{d_r(s)}{\|\mathbf{r}'(\bar{s})\|^2 + \mathbf{r}''(\bar{s}) \cdot \check{\mathbf{r}}(s)} \begin{pmatrix} \check{\boldsymbol{\eta}}(s) \\ \boldsymbol{\eta}'(\bar{s}) \end{pmatrix} \cdot \begin{pmatrix} \mathbf{r}'(\bar{s}) \otimes \mathbf{r}'(\bar{s}) & \mathbf{r}'(\bar{s}) \otimes \check{\mathbf{r}}(s) \\ \check{\mathbf{r}}(s) \otimes \mathbf{r}'(\bar{s}) & \check{\mathbf{r}}(s) \otimes \check{\mathbf{r}}(s) \end{pmatrix} \begin{pmatrix} \check{\mathbf{p}}(s) \\ \mathbf{p}'(\bar{s}) \end{pmatrix} \end{aligned}$$

with for any vector-valued function  $\mathbf{h}(\cdot)$ , the function  $\check{\mathbf{h}}(\cdot)$  is defined by  $\check{\mathbf{h}}(s) = \mathbf{h}(s) - \mathbf{h}(\bar{s})$ .

## Finite element discretization

Let  $0 = s_0 < s_1 < \dots < s_N = L$  be a uniform subdivision of the interval  $[0, L]$  with meshsize  $h = L/N$ .

We approximate the field variable  $\mathbf{g}$  (such as  $\mathbf{r}$ ,  $\mathbf{p}$ ,  $\mathbf{q}$ ,  $\boldsymbol{\eta}$  and  $\boldsymbol{\theta}$ ) with  $\mathbf{g}_h$  by using Lagrangian cubic finite elements.

Then the restriction to a typical element  $I_h^e = [s_{e-1}, s_e]$  of the field variable  $\mathbf{g}_h$  is given by

$$\mathbf{g}_h^e(s) = \sum_{n=1}^4 \phi_n^e(s) \mathbf{g}_h^{e,n},$$

- $\phi_n^e(s)$ ,  $n = 1, \dots, 4$  are the cubic interpolation functions.
- $\mathbf{g}_h^{e,n}$  represents the value at node  $n$  of element  $e$  of the field  $\mathbf{g}_h^e(s)$ .

# Discretization of the linearized virtual work of internal forces and moments

The discretization of the linearized internal virtual work writes

$$\Delta \delta \mathcal{J}_{\text{int}} = \sum_{e=1}^N \Delta \delta \mathcal{J}_{\text{int}}^e = \sum_{e=1}^N \sum_{n=1}^4 \sum_{m=1}^4 (\mathbf{P}_{(k)}^{e,n})^T \left[ \mathbb{K}_{\text{mat},(k)}^{e,nm} + \mathbb{K}_{\text{geo},(k)}^{e,nm} \right] \mathbf{H}_{(k)}^{e,m}.$$

The material part is given by

$$\mathbb{K}_{\text{mat},(k)}^{e,nm} = \int_{I_h^e} (\Xi_{(k)}^{e,n})^T(s) \begin{bmatrix} \mathbf{V}_{(k)}^e(s) & \mathbf{W}_{(k)}^e(s) \\ (\mathbf{W}_{(k)}^e)^T(s) & \mathbf{U}_{(k)}^e(s) \end{bmatrix} \Xi_{(k)}^{e,m}(s) ds.$$

The geometric part is given by

$$\mathbb{K}_{\text{geo},(k)}^{e,nm} = \int_{I_h^e} \begin{bmatrix} \mathbf{0} & -\phi_n^{e'}(s) \phi_m^e(s) (\mathbf{n}_{(k)}^e(s))^\times \\ \phi_n^e(s) \phi_m^{e'}(s) (\mathbf{n}_{(k)}^e(s))^\times & \phi_n^e(s) (\phi_m^{e'}(s) (\mathbf{m}_{(k)}^e(s))^\times + \phi_m^e(s) (\mathbf{n}_{(k)}^e(s))^\times (\mathbf{r}_{(k)}^e)'(s))^\times \end{bmatrix} ds.$$



## Discretization of the virtual work of external loads

The discretized form of the virtual work of external loads writes

$$\delta \mathcal{J}_{\text{ext}} = \sum_{e=1}^N \delta \mathcal{J}_{\text{ext}}^e = \sum_{e=1}^N \sum_{n=1}^4 (\mathbf{F}_{\text{ext}}^{e,n})^T \mathbf{P}^{e,n}, \quad (1)$$

where

$$\mathbf{F}_{\text{ext}}^{e,n} = \lambda \int_{I_h^e} \begin{bmatrix} \tilde{\mathbf{f}}(s) \phi_n^e(s) \\ \tilde{\mathbf{c}}(s) \phi_n^e(s) \end{bmatrix} ds. \quad (2)$$

Here  $\lambda$  is a loading parameter, and  $\tilde{\mathbf{f}}$  and  $\tilde{\mathbf{c}}$  are scaled versions of the external loads  $\mathbf{f}$  and  $\mathbf{c}$ , i.e.,

$$\mathbf{f} = \lambda \tilde{\mathbf{f}} \text{ and } \mathbf{c} = \lambda \tilde{\mathbf{c}}.$$

## Discretization of the contact energy

Discretization by the finite-element approximation of the linearized contact energy yields

$$\Delta \delta \mathcal{J}_c = \sum_{v=1}^N \Delta \delta \mathcal{J}_c^v \simeq \sum_{v=1}^N \sum_{i=1}^3 (\Delta \boldsymbol{\rho}^{(v,e_i)})^T \mathbb{K}_{\text{cont}}^{v,i} \delta \boldsymbol{\rho}^{(v,e_i)},$$

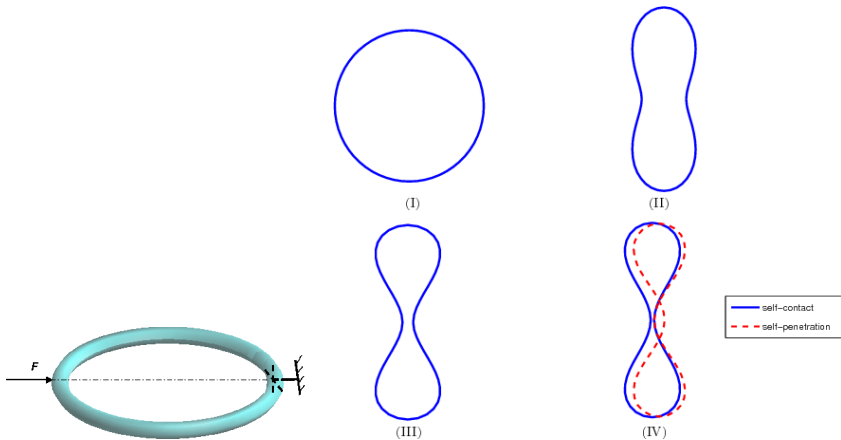
where  $\mathbb{K}_{\text{cont}}^{v,i}$  is the contact element stiffness matrix. It is given by

$$\mathbb{K}_{\text{cont}}^{v,i} = \mu \omega_i \frac{H(d_{\mathbf{r}}^v(\sigma_i))}{2\varepsilon - d_{\mathbf{r}}^v(\sigma_i)} (\boldsymbol{\Sigma}^{(v,e_i)}(\sigma_i))^T \boldsymbol{\Gamma}^{(v,e_i)}(\sigma_i) \boldsymbol{\Sigma}^{(v,e_i)}(\sigma_i),$$

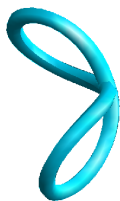
where

$$\boldsymbol{\Gamma}^{(v,e)}(s) = \begin{bmatrix} \boldsymbol{\Gamma}_{11}^{(v,e)}(s) & \boldsymbol{\Gamma}_{12}^{(v,e)}(s) \\ \boldsymbol{\Gamma}_{21}^{(v,e)}(s) & \boldsymbol{\Gamma}_{22}^{(v,e)}(s) \end{bmatrix}, \quad \boldsymbol{\Sigma}^{(v,e)}(s) = \begin{bmatrix} \boldsymbol{\Phi}^v(s) & -\boldsymbol{\Phi}^e(\bar{s}) \\ \mathbf{0} & \boldsymbol{\Phi}^{e'}(\bar{s}) \end{bmatrix}.$$

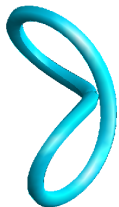
# Planar configurations with self contact



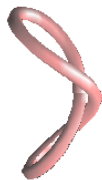
## 3D configurations with self contact



(I)



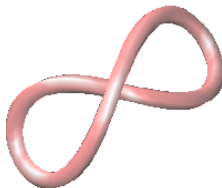
(II)



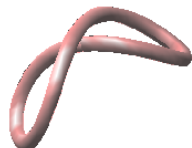
(I)



(II)



(III)



(IV)