

A Theory of Rods with Microstructure as a Model for Double Stranded Rods

Maher Moakher

Ecole Nationale d'Ingénieurs de Tunis

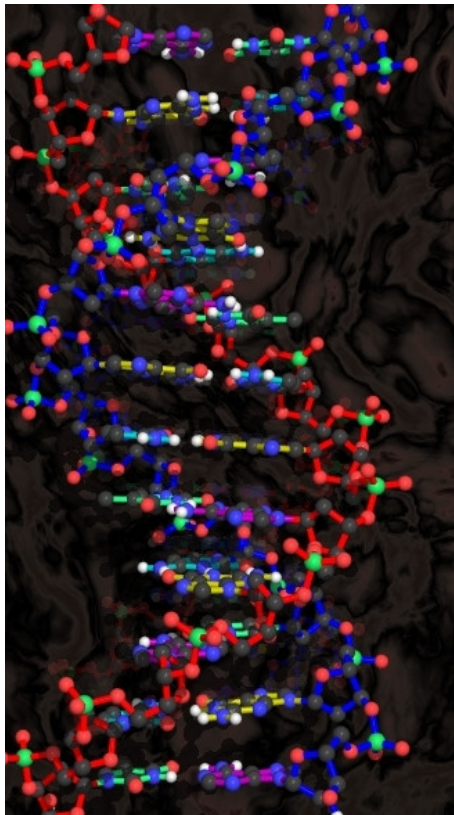
John H. Maddocks

Ecole Polytechnique Fédérale de Lausanne

Fields Institute, Toronto, 2003

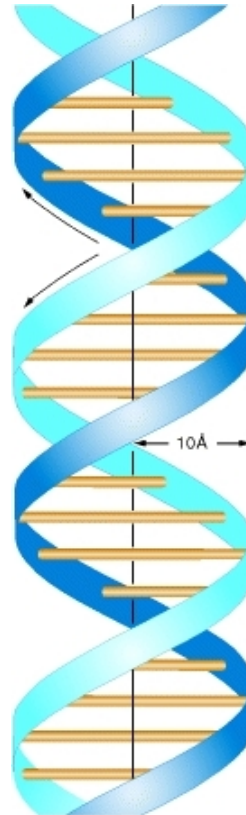
MOTIVATION: DNA MODELING

All Atoms



Primary Structure

Watson-Crick



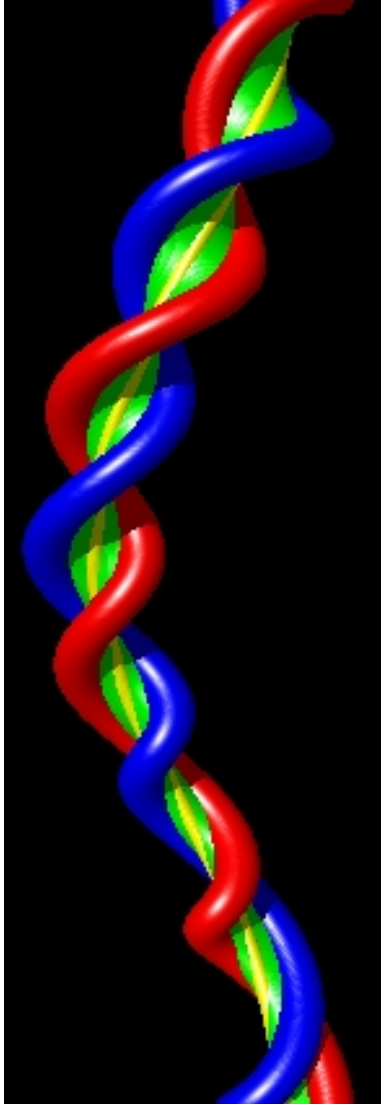
Secondary Structure

Elastic Rod



Tertiary Structure

CONFIGURATION



We consider a ribbon \mathcal{R} composed of two special Cosserat rods \mathcal{R}^+ and \mathcal{R}^- , which we call strands, that are bound together elastically.

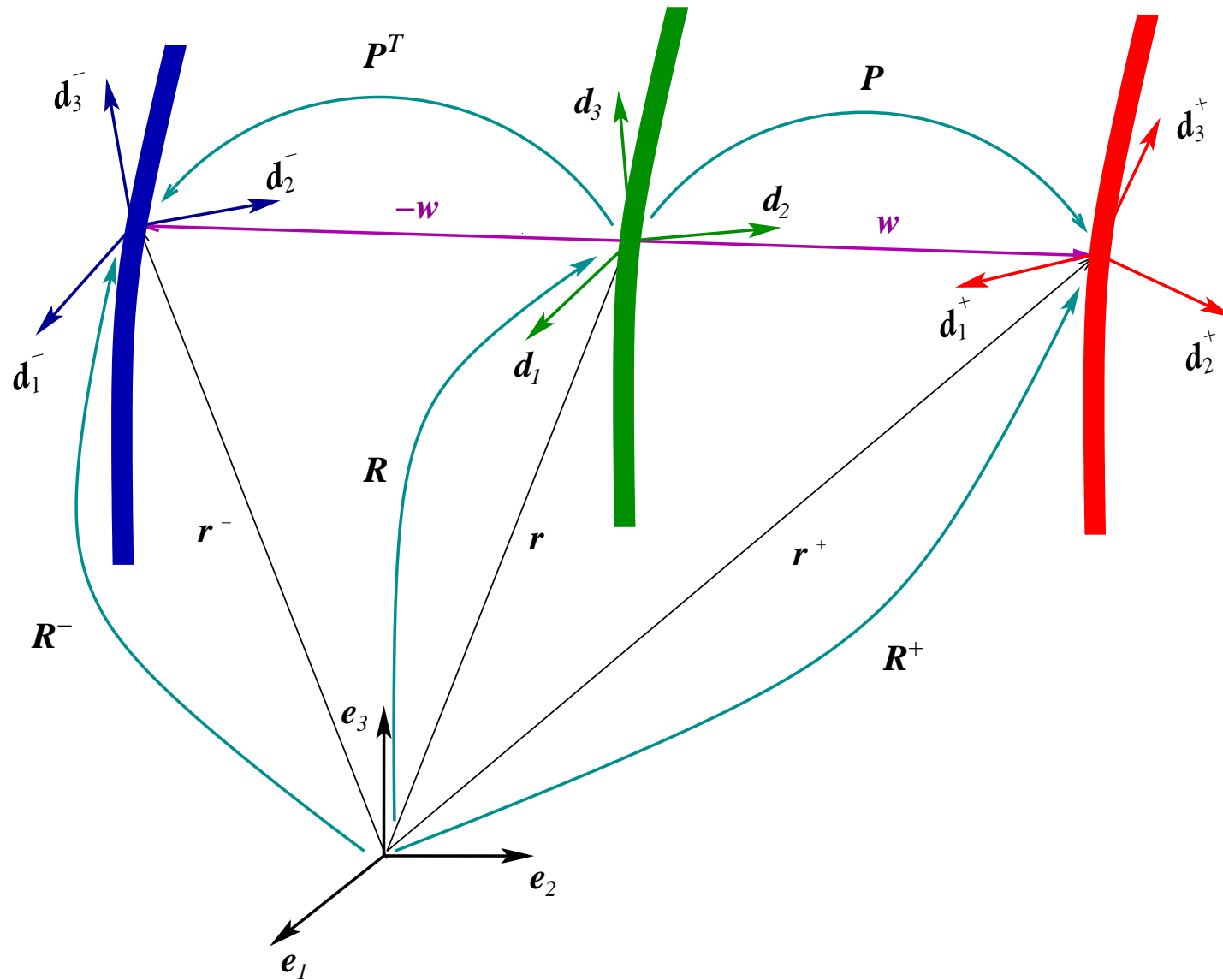
Each strand is completely described by

- a position vector $\mathbf{r}^\pm(s, t)$,
- a frame of directors $\{\mathbf{d}_i^\pm(s, t)\}$.

The curves $\mathcal{C}^\pm(t) \equiv \{\mathbf{r}^\pm(s, t), s \in [0, L]\}$ represent the lines of centroids, in the current configuration, of \mathcal{R}^\pm .

The triads $\{\mathbf{d}_i^\pm(s, t)\}$ give the orientation of the material cross section at s of \mathcal{R}^\pm .

CONFIGURATION: SCHEMATIC



KINEMATICS: Strains associated with the centerlines

We define the strain vectors v and v^\pm by

$$v := r_s,$$

$$v^+ := r_s^+,$$

$$v^- := r_s^-.$$

Then we have the following relations

$$v^+ = v + w_s,$$

$$v^- = v - w_s.$$

KINEMATICS: Strains associated with the directors

Let \boldsymbol{u} and \boldsymbol{u}^\pm be the (Darboux) vectors for \boldsymbol{R} and \boldsymbol{R}^\pm , i.e., such that

$$\boldsymbol{R}_s \boldsymbol{R}^T = \boldsymbol{u}^\times,$$

$$\boldsymbol{R}_s^+ \boldsymbol{R}^{+T} = (\boldsymbol{u}^+)^\times,$$

$$\boldsymbol{R}_s^- \boldsymbol{R}^{-T} = (\boldsymbol{u}^-)^\times.$$

Given a vector \boldsymbol{a} , we denote by \boldsymbol{a}^\times the second order skew-symmetric tensor such that, for any vector \boldsymbol{b} ,

$$\boldsymbol{a}^\times \boldsymbol{b} = \boldsymbol{a} \times \boldsymbol{b}.$$

We have the following relations

$$\begin{aligned} \mathbf{u}^+ &= \mathbf{u} + \alpha \mathbf{A} \boldsymbol{\eta}^\nabla, \\ \mathbf{u}^- &= \mathbf{u} - \alpha \mathbf{A}^T \boldsymbol{\eta}^\nabla, \end{aligned}$$

where

$\boldsymbol{\eta}$ is the Gibbs rotation vector of \mathbf{P} ,

$$\mathbf{A} = \mathbf{I} + \boldsymbol{\eta}^\times,$$

$$\alpha = 2/(1 + \boldsymbol{\eta} \cdot \boldsymbol{\eta}),$$

$$\boldsymbol{\eta}^\nabla = \boldsymbol{\eta}_s - \mathbf{u} \times \boldsymbol{\eta}.$$

$$\mathbf{P} = \mathbf{I} + \alpha[\boldsymbol{\eta}^\times + (\boldsymbol{\eta}^\times)^2].$$

KINEMATICS: Linear velocities

We define the vectors γ and γ^\pm by

$$\gamma := \mathbf{r}_t,$$

$$\gamma^+ := \mathbf{r}_t^+,$$

$$\gamma^- := \mathbf{r}_t^-.$$

Then we have the following relations

$$\gamma^+ = \gamma + \mathbf{w}_t,$$

$$\gamma^- = \gamma - \mathbf{w}_t.$$

KINEMATICS: Angular velocities

Let ω and ω^\pm be the angular velocities for R and R^\pm , i.e., such that

$$R_t R^T = \omega^\times,$$

$$R_t^+ R^{+T} = (\omega^+)^\times,$$

$$R_t^- R^{-T} = (\omega^-)^\times.$$

We then have the following relations

$$\omega^+ = \omega + \alpha A \overset{\circ}{\eta},$$

$$\omega^- = \omega - \alpha A^T \overset{\circ}{\eta},$$

where

$$\overset{\circ}{\eta} = \eta_t - \omega \times \eta.$$

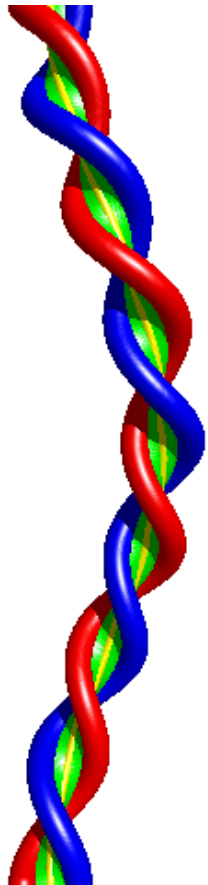
TWO PARADIGMS

Configuration Variables

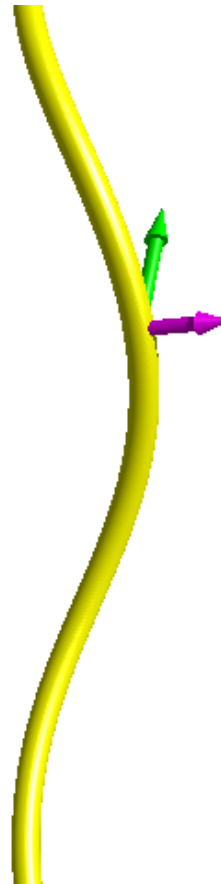
$$\{(\mathbf{r}^+, \mathbf{R}^+), (\mathbf{r}^-, \mathbf{R}^-)\}$$

Configuration Space

$$\{\mathbb{R}^3 \times SO(3)\}^2$$



Double-Stranded Rod
(Bi-rod)



Rod with Microstructure

Configuration Variables

$$(\mathbf{r}, \mathbf{R}, \mathbf{w}, \mathbf{P})$$

Configuration Space

$$\mathbb{R}^3 \times SO(3) \times \mathbb{R}^3 \times SO(3)$$

ACTION DENSITY FOR A ROD WITH MICROSTRUCTURES

We consider a special Cosserat rod \mathcal{R} endowed with two microstructure variables:

- a vector w
- a rotation tensor P .

Let \mathcal{P} be a part of \mathcal{R} which is defined by $s_1 \leq s \leq s_2$ and let \mathcal{I} be the time interval $t_1 \leq t \leq t_2$.

To every set of events $\mathcal{P} \times \mathcal{I}$ we associate the action \mathcal{A} given by

$$\mathcal{A}(\mathcal{P} \times \mathcal{I}) = \int_{t_1}^{t_2} \int_{s_1}^{s_2} \tilde{\mathcal{L}}(s, t, \mathbf{r}, \mathbf{r}_s, \mathbf{r}_t, \mathbf{R}, \mathbf{R}_s, \mathbf{R}_t, \mathbf{w}, \mathbf{w}_s, \mathbf{w}_t, \mathbf{P}, \mathbf{P}_s, \mathbf{P}_t) ds dt.$$

The density of action $\tilde{\mathcal{L}}$ is function of s, t and the macro- and micro-kinematical variables as well as their spatial and time derivatives.

MODIFIED FORM OF THE ACTION DENSITY

It is more convenient to work with w^∇ and $\overset{\circ}{w}$ instead of w_s and w_t and with η , $\alpha\eta^\nabla$ and $\alpha\overset{\circ}{\eta}$ instead of P , P_s and P_t .

We therefore introduce the variables

$$\begin{aligned} v^c &= w^\nabla, & \gamma^c &= \overset{\circ}{w}, \\ u^c &= \alpha\eta^\nabla, & \omega^c &= \alpha\overset{\circ}{\eta}, \end{aligned}$$

where $\alpha = 2/(1 + \eta \cdot \eta)$, and for any vector a we have

$$a^\nabla = a_s - R_s R a, \quad \overset{\circ}{a} = a_t - R_t R a.$$

Accordingly, we define a new density of action \mathcal{L} by

$$\begin{aligned} \mathcal{L}(s, t, r, r_s, r_t, R, R_s, R_t, w, v^c, \gamma^c, \eta, u^c, \omega^c) := \\ \widetilde{\mathcal{L}}(s, t, r, r_s, r_t, R, R_s, R_t, w, w_s, w_t, P, P_s, P_t). \end{aligned}$$

EUCLIDEAN INVARIANCE

We require \mathcal{L} be invariant under the group of Euclidean displacements:

- \mathcal{L} must be independent of t and r .
- \mathcal{L} depends on R only through the reduced variables

$$\begin{array}{lll} \mathbf{v} = R^T \mathbf{r}', & \boldsymbol{\gamma} = R^T \dot{\mathbf{r}}, \\ \mathbf{u}^\times = R^T R', & \boldsymbol{\omega}^\times = R^T \dot{R}, \\ \mathbf{w} = R^T \mathbf{w}, & \mathbf{v}^c = R^T \mathbf{v}^c, & \boldsymbol{\gamma}^c = R^T \boldsymbol{\gamma}^c, \\ \boldsymbol{\eta} = R^T \boldsymbol{\eta}, & \mathbf{u}^c = R^T \mathbf{u}^c, & \boldsymbol{\omega}^c = R^T \boldsymbol{\omega}^c, \end{array}$$

We therefore obtain the following reduced form of the action density

$$\begin{aligned} \mathcal{L}(s, \mathbf{v}, \boldsymbol{\gamma}, \mathbf{u}, \boldsymbol{\omega}, \mathbf{w}, \mathbf{v}^c, \boldsymbol{\gamma}^c, \boldsymbol{\eta}, \mathbf{u}^c, \boldsymbol{\omega}^c) := \\ \mathcal{L}(s, R^T \mathbf{r}_s, R^T \mathbf{r}_t, R^T R_s, R^T R_t, R^T \mathbf{w}, R^T \mathbf{v}^c, R^T \boldsymbol{\gamma}^c, R^T \boldsymbol{\eta}, R^T \mathbf{u}^c, R^T \boldsymbol{\omega}^c). \end{aligned}$$

Further, we assume that \mathcal{L} has the separated form

$$\mathcal{L}(s, \mathbf{v}, \boldsymbol{\gamma}, \mathbf{u}, \boldsymbol{\omega}, \mathbf{w}, \mathbf{v}^c, \boldsymbol{\gamma}^c, \boldsymbol{\eta}, \mathbf{u}^c, \boldsymbol{\omega}^c) = \mathcal{K}(s, \boldsymbol{\gamma}, \boldsymbol{\omega}, \mathbf{w}, \boldsymbol{\gamma}^c, \boldsymbol{\eta}, \boldsymbol{\omega}^c) - \mathcal{W}(s, \mathbf{v}, \mathbf{u}, \mathbf{w}, \mathbf{v}^c, \boldsymbol{\eta}, \mathbf{u}^c).$$

HAMILTON'S PRINCIPLE

According to Hamilton's principle, the equations of motion are given by Euler-Poincaré equations of the variational equation

$$\delta \mathcal{A}(\mathcal{P} \times \mathcal{I}) = 0.$$

We obtain

$$\left(R \frac{\partial \mathcal{W}}{\partial \mathbf{v}} \right)_s - \left(R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\gamma}} \right)_t = \mathbf{0},$$

$$\left(R \frac{\partial \mathcal{W}}{\partial \mathbf{u}} \right)_s + \mathbf{r}_s \times R \frac{\partial \mathcal{W}}{\partial \mathbf{v}} - \left(R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\omega}} \right)_t - \mathbf{r}_t \times R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\gamma}} = \mathbf{0},$$

$$R \left[\frac{\partial \mathcal{W}}{\partial \mathbf{w}} - \left(\frac{\partial \mathcal{W}}{\partial \mathbf{v}^c} \right)_s - \frac{\partial \mathcal{K}}{\partial \mathbf{w}} + \left(\frac{\partial \mathcal{K}}{\partial \boldsymbol{\gamma}^c} \right)_t \right] = \mathbf{0},$$

$$R \left[\frac{\partial \mathcal{W}}{\partial \boldsymbol{\eta}} - \left(\alpha \frac{\partial \mathcal{W}}{\partial \mathbf{u}^c} \right)_s - \frac{\partial \mathcal{K}}{\partial \boldsymbol{\eta}} + \left(\alpha \frac{\partial \mathcal{K}}{\partial \boldsymbol{\omega}^c} \right)_t \right] + \alpha \left(\boldsymbol{\omega}^c \cdot R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\omega}^c} - \mathbf{u}^c \cdot R \frac{\partial \mathcal{W}}{\partial \mathbf{u}^c} \right) \boldsymbol{\eta} = 0.$$

Constitutive Equations

$$\mathbf{p} = R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\gamma}},$$

$$\boldsymbol{\pi} = R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\omega}},$$

$$\mathbf{p}^c = R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\gamma}^c},$$

$$\boldsymbol{\pi}^c = R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\omega}^c} + \mathbf{w} \times \mathbf{p} - \boldsymbol{\eta} \times (\boldsymbol{\pi} - \mathbf{w} \times \mathbf{p}^c),$$

$$2\boldsymbol{\sigma} = R \frac{\partial \mathcal{K}}{\partial \mathbf{w}} + \boldsymbol{\omega} \times \mathbf{p}^c,$$

$$2\boldsymbol{\tau} = \frac{1}{\alpha} R \frac{\partial \mathcal{K}}{\partial \boldsymbol{\eta}} + \boldsymbol{\omega} \times \boldsymbol{\pi}^c - \boldsymbol{\omega}^c \times (\boldsymbol{\eta} \times \boldsymbol{\pi}^c) + \dots$$

$$\mathbf{n} = R \frac{\partial \mathcal{W}}{\partial \mathbf{v}},$$

$$\mathbf{m} = R \frac{\partial \mathcal{W}}{\partial \mathbf{u}},$$

$$\mathbf{n}^c = R \frac{\partial \mathcal{W}}{\partial \mathbf{v}^c},$$

$$\mathbf{m}^c = R \frac{\partial \mathcal{W}}{\partial \mathbf{u}^c} + \mathbf{w} \times \mathbf{n} - \boldsymbol{\eta} \times (\mathbf{m} - \mathbf{w} \times \mathbf{n}^c),$$

$$2\mathbf{f} = R \frac{\partial \mathcal{W}}{\partial \mathbf{w}} + \mathbf{u} \times \mathbf{n}^c,$$

$$2\mathbf{c} = \frac{1}{\alpha} R \frac{\partial \mathcal{W}}{\partial \boldsymbol{\eta}} + \mathbf{u} \times \mathbf{m}^c - \mathbf{u}^c \times (\boldsymbol{\eta} \times \mathbf{m}^c) + \dots$$

Equations of Motion

$$\mathbf{n}_s = \mathbf{p}_t,$$

$$\mathbf{m}_s + \mathbf{r}_s \times \mathbf{n} = \boldsymbol{\pi}_t + \mathbf{r}_t \times \mathbf{p},$$

$$\mathbf{n}_s^c - 2\mathbf{f} = \mathbf{p}_t^c - 2\boldsymbol{\sigma},$$

$$\mathbf{m}_s^c + \mathbf{r}_s \times \mathbf{n}^c - 2\mathbf{c} = \boldsymbol{\pi}_t^c + \mathbf{r}_t \times \mathbf{p}^c - 2\boldsymbol{\tau}.$$

SPECIALIZATION TO DOUBLE-STRANDED RODS

When

$$\mathcal{W}(s; \mathbf{v}, \mathbf{u}, \mathbf{w}, \mathbf{v}^c, \boldsymbol{\eta}, \mathbf{u}^c) = \widetilde{\mathcal{W}}(s; \mathbf{v}^+, \mathbf{v}^-, \mathbf{u}^+, \mathbf{u}^-, \mathbf{w}, \boldsymbol{\eta}),$$

$$\mathcal{K}(s; \boldsymbol{\gamma}, \boldsymbol{\omega}, \mathbf{w}, \boldsymbol{\gamma}^c, \boldsymbol{\eta}, \boldsymbol{\omega}^c) = \widetilde{\mathcal{K}}(s; \boldsymbol{\gamma}^+, \boldsymbol{\gamma}^-, \boldsymbol{\omega}^+, \boldsymbol{\omega}^-, \mathbf{w}, \boldsymbol{\eta}),$$

we obtain

$$\mathbf{p} = \mathbf{p}^+ + \mathbf{p}^-,$$

$$\boldsymbol{\pi} = \boldsymbol{\pi}^+ + \boldsymbol{\pi}^- + \mathbf{w} \times (\mathbf{p}^+ - \mathbf{p}^-),$$

$$\mathbf{p}^c = \mathbf{p}^+ - \mathbf{p}^-,$$

$$\boldsymbol{\pi}^c = \boldsymbol{\pi}^+ - \boldsymbol{\pi}^- + \mathbf{w} \times (\mathbf{p}^+ + \mathbf{p}^-),$$

$$2\boldsymbol{\sigma} = \mathbf{R} \frac{\partial \widetilde{\mathcal{K}}}{\partial \mathbf{w}},$$

$$2\boldsymbol{\tau} = \frac{1}{\alpha} \mathbf{R} \frac{\partial \widetilde{\mathcal{K}}}{\partial \boldsymbol{\eta}} - \boldsymbol{\eta} \times (\mathbf{w} \times \boldsymbol{\sigma}),$$

$$\mathbf{n} = \mathbf{n}^+ + \mathbf{n}^-,$$

$$\mathbf{m} = \mathbf{m}^+ + \mathbf{m}^- + \mathbf{w} \times (\mathbf{n}^+ - \mathbf{n}^-),$$

$$\mathbf{n}^c = \mathbf{n}^+ - \mathbf{n}^-,$$

$$\mathbf{m}^c = \mathbf{m}^+ - \mathbf{m}^- + \mathbf{w} \times (\mathbf{n}^+ + \mathbf{n}^-),$$

$$2\mathbf{f} = \mathbf{R} \frac{\partial \widetilde{\mathcal{W}}}{\partial \mathbf{w}},$$

$$2\mathbf{c} = \frac{1}{\alpha} \mathbf{R} \frac{\partial \widetilde{\mathcal{W}}}{\partial \boldsymbol{\eta}} - \boldsymbol{\eta} \times (\mathbf{w} \times \mathbf{f}),$$

where

$$\begin{aligned} p^+ &= PR \frac{\partial \tilde{\mathcal{K}}}{\partial \boldsymbol{\gamma}^+}, & p^- &= P^T R \frac{\partial \tilde{\mathcal{K}}}{\partial \boldsymbol{\gamma}^-}, \\ \pi^+ &= PR \frac{\partial \tilde{\mathcal{K}}}{\partial \omega^+}, & \pi^- &= P^T R \frac{\partial \tilde{\mathcal{K}}}{\partial \omega^-}, \\ n^+ &= PR \frac{\partial \tilde{\mathcal{W}}}{\partial \mathbf{v}^+}, & n^- &= P^T R \frac{\partial \tilde{\mathcal{W}}}{\partial \mathbf{v}^-}, \\ m^+ &= PR \frac{\partial \tilde{\mathcal{W}}}{\partial \mathbf{u}^+}, & m^- &= P^T R \frac{\partial \tilde{\mathcal{W}}}{\partial \mathbf{u}^-}, \end{aligned}$$

LINEARLY-ELASTIC STRANDS

$$\begin{aligned}
 \begin{pmatrix} \mathbf{p} \\ \mathbf{p}^c \end{pmatrix} &= \rho \begin{pmatrix} \mathbf{r}_t \\ \mathbf{w}_t \end{pmatrix}, \\
 \begin{pmatrix} \boldsymbol{\pi} \\ \boldsymbol{\pi}^c \end{pmatrix} &= \begin{pmatrix} \mathbb{J} & \mathbb{J}^c \\ \mathbb{J}^c & \mathbb{J} \end{pmatrix} \begin{pmatrix} \boldsymbol{\omega} + \boldsymbol{\eta} \times \boldsymbol{\omega}^c \\ \boldsymbol{\omega}^c \end{pmatrix} + \begin{pmatrix} \mathbf{w} \times \mathbf{p}^c \\ \mathbf{w} \times \mathbf{p} \end{pmatrix}, \\
 \begin{pmatrix} \mathbf{n} \\ \mathbf{n}^c \end{pmatrix} &= \begin{pmatrix} \mathbb{L} & \mathbb{L}^c \\ \mathbb{L}^c & \mathbb{L} \end{pmatrix} \left\{ \begin{pmatrix} \mathbf{v} \\ \mathbf{v}^c + \mathbf{w} \times \mathbf{u} \end{pmatrix} - \begin{pmatrix} \mathbf{E} & \mathbf{E}^c \\ \mathbf{E}^c & \mathbf{E} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{v}} \\ \tilde{\mathbf{v}}^c + \tilde{\mathbf{w}} \times \tilde{\mathbf{u}} \end{pmatrix} \right\}, \\
 \begin{pmatrix} \mathbf{m} \\ \mathbf{m}^c \end{pmatrix} &= \begin{pmatrix} \mathbb{K} & \mathbb{K}^c \\ \mathbb{K}^c & \mathbb{K} \end{pmatrix} \left\{ \begin{pmatrix} \mathbf{u} + \boldsymbol{\eta} \times \mathbf{u}^c \\ \mathbf{u}^c \end{pmatrix} - \begin{pmatrix} \mathbf{E} & \mathbf{E}^c \\ \mathbf{E}^c & \mathbf{E} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{u}} + \tilde{\boldsymbol{\eta}} \times \tilde{\mathbf{u}}^c \\ \tilde{\mathbf{u}}^c \end{pmatrix} \right\} + \begin{pmatrix} \mathbf{w} \times \mathbf{n}^c \\ \mathbf{w} \times \mathbf{n} \end{pmatrix},
 \end{aligned}$$

where

$$\rho = \rho^+ + \rho^-$$

$$\mathbb{M} = \mathbb{M}^+ + \mathbb{M}^-,$$

$$\mathbb{M}^+ = \mathbf{P} \mathbf{R} \mathbb{M}^+ \mathbf{R}^T \mathbf{P}^T,$$

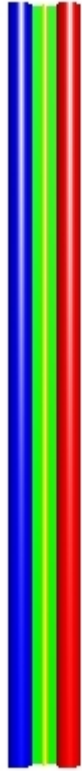
$$\mathbb{M}^c = \mathbb{M}^+ - \mathbb{M}^-,$$

$$\mathbb{M}^- = \mathbf{P}^T \mathbf{R} \mathbb{M}^- \mathbf{R}^T \mathbf{P},$$

$$\mathbf{E} = (\mathbf{P} \mathbf{R} \tilde{\mathbf{R}}^T \tilde{\mathbf{P}}^T + \mathbf{P}^T \mathbf{R} \tilde{\mathbf{R}}^T \tilde{\mathbf{P}})/2, \quad \mathbf{E}^c = (\mathbf{P} \mathbf{R} \tilde{\mathbf{R}}^T \tilde{\mathbf{P}}^T - \mathbf{P}^T \mathbf{R} \tilde{\mathbf{R}}^T \tilde{\mathbf{P}})/2.$$

EXAMPLE: A DOUBLE RING

Reference
configuration
(unstressed)



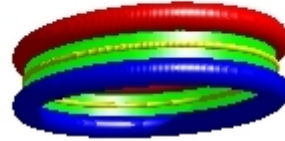
$$\hat{\mathbf{r}} = s\mathbf{e}_3$$

$$\hat{\mathbf{w}} = \hat{h}\mathbf{e}_2$$

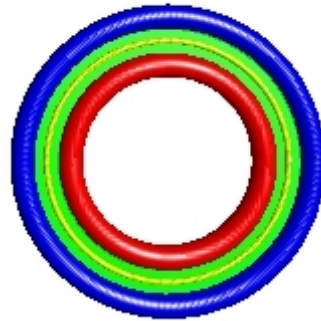
$$s \in [0, L]$$

$$L = 2\pi R$$

Low strain
energy bi-ring



$$\left\{ \begin{array}{l} \mathbf{r} = R(\cos \frac{s}{R}\mathbf{e}_1 + \sin \frac{s}{R}\mathbf{e}_3) \\ \mathbf{w} = \hat{h}\mathbf{e}_2 \\ \mathbf{n} = \mathbf{0}, \quad \mathbf{n}^c = \mathbf{0} \\ \mathbf{m} = \frac{2K}{R}\mathbf{e}_2, \quad \mathbf{m}^c = \mathbf{0} \end{array} \right.$$



High strain
energy bi-ring

$$\left\{ \begin{array}{l} \mathbf{r} = R(\cos \frac{s}{R}\mathbf{e}_2 + \sin \frac{s}{R}\mathbf{e}_3) \\ \mathbf{w} = h(\cos \frac{s}{R}\mathbf{e}_2 + \sin \frac{s}{R}\mathbf{e}_3) \\ h = \frac{G\hat{h}}{A/R^2 + G} \\ \mathbf{n} = \mathbf{0}, \quad \mathbf{n}^c = \frac{2Ah}{R}\mathbf{r}' \\ \mathbf{m} = \frac{2(K + Ah^2)}{R}\mathbf{e}_1, \quad \mathbf{m}^c = \mathbf{0} \end{array} \right.$$