Optimal kinematics of supercoiled filaments

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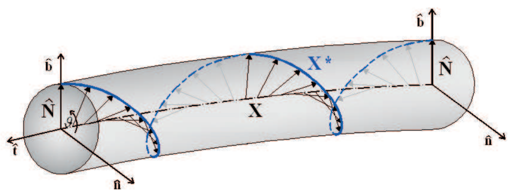
ABSTRACT

In this poster we propose kinematics of writhing and coiling of closed filaments as numerical solutions of the elastic deformation energy minimization. Preliminary work [1] [2] is here extended to require a monotonically decreasing behaviour of the deformation energy of the system, favoring coils formation for given initial and final conditions. The analysis is performed by using a simple thin filament model of circular cross-section under conservation of self-linking number with elastic energy evaluated by means of bending and torsional influence. Time evolution parameters are described by means piecewise polynomial transformations based on cubic spline. Proper constraints are imposed so that the transformation is globally C^2 and the value of the parameters at grids points are the unknowns in a large-scale optimization problem. These results may find useful applications in modelling natural phenomena, from magnetic field dynamos in astrophysical flows to DNA packing in cell biology [3].

1 The filament model

The filament $\mathcal{F}$ is modelled by a thin inextensible rod of length $L = 2\pi$ and of uniform circular cross–section of area $A = \pi a^2$ ($a \ll L$).



The axis $\mathscr{C}$ is a simple, smooth space curve $\mathbf{X} = \mathbf{X}(\xi)$ where $\xi \in [0, 2\pi]$.

2 Measures of filament coiling

2.1 Measures of coiling ($\mathcal{K}$), folding (Wr) and twist (Tw)

Let $\mathscr{C}$ be a closed, smooth, simple curve in $\mathbb{R}^3$ given by $\mathbf{X}(\xi) : [0, L] \longrightarrow \mathbb{R}^3$, with curvature $c(\xi)$ and torsion $\tau(\xi)$ where ξ is a parameter along the curve and $\hat{\mathbf{t}}(\xi) \equiv \mathbf{X}'(\xi)/\|\mathbf{X}'(\xi)\|$ is the unit tangent to $\mathcal{C}$ at ξ.

We consider the following quantities:

- **normalized total curvature**

$$\mathcal{K} := \frac{1}{2\pi}\oint_{\mathscr{C}} c(\xi)\,\|\mathbf{X}'(\xi)\|\,\mathrm{d}\xi\,; \tag{1}$$

- **writhing number** (Fuller 1971)

$$Wr := \frac{1}{4\pi}\oint_{\mathscr{C}}\oint_{\mathscr{C}} \frac{\hat{\mathbf{t}}(\xi)\times\hat{\mathbf{t}}(\xi^*)\cdot[\mathbf{X}(\xi)-\mathbf{X}(\xi^*)]}{|\mathbf{X}(\xi)-\mathbf{X}(\xi^*)|^3}\|\mathbf{X}'(\xi)\|\|\mathbf{X}'(\xi^*)\|\,\mathrm{d}\xi\mathrm{d}\xi^*\,; \tag{2}$$

- **total twist number**

$$Tw := \frac{1}{2\pi}\oint_{\mathscr{C}} \tau(\xi)\|\mathbf{X}'(\xi)\|\,\mathrm{d}\xi + \frac{1}{2\pi}[\Theta]_{\mathcal{F}} = \mathcal{T} + \mathcal{N}\,, \tag{3}$$

  where $\mathcal{T}$ is the normalized total torsion and $\mathcal{N}$ the normalized intrinsic twist of the fibers of $\mathcal{F}$ around $\mathscr{C}$.

2.2 Călugăreanu–White formula

In the case of a closed filament $\mathcal{F}$ in isolation the sum of Wr and Tw is a topological invariant according to the well-known formula:

$$Lk = Wr + Tw\,, \tag{4}$$

where Lk is the linking number of the filament $\mathcal{F}$.

3 Kinematic equations for folding mechanism

We consider a family of time-dependent curves $\mathbf{X} = \mathbf{X}(\xi, t, n)$ (where t is a kinematical time, see [1] and [2]), a sub-class of **Fourier knots**, given by:

$$\mathbf{X} = \mathbf{X}(\xi, t, n)\;:\; \begin{cases} x = [a(t)\cos(\xi) + b(t)\cos(n\xi)]\,/l(t) \\ y = [c(t)\sin(\xi) + d(t)\sin(n\xi)]\,/l(t) \\ z = [e(t)\sin(\xi)]\,/l(t) \end{cases}, \tag{5}$$

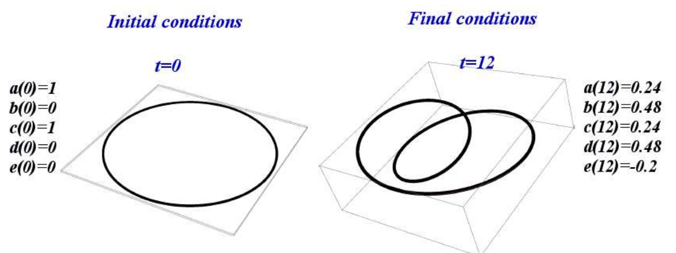
where:

- The integer n controls the number $N = n - 1$ of coils produced.
- $a(t), b(t), c(t), d(t), e(t)$ are **time-dependent functions**. Notice than in [1], time t was merely a kinematic parameter, while an appropriate time-dependence prescription should be dictated by the particular physical process considered. See **Section 5** for the model adopted to determine $a(t), b(t), c(t), d(t), e(t)$.
- In order to ensure the inextenisibility we have normalized by the *length function*

$$l(t) = \frac{1}{2\pi}\int_0^{2\pi}\left[\left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2\right]^{1/2}\mathrm{d}\xi\,. \tag{6}$$

  This rescaling ensures that the total length is kept fixed at $L = L(0) = 2\pi$.
- Eqs. (5) describe the time evolution of closed curves with initial condition $t = 0$ chosen in orden to originate from a plane circle and to evolve to form singly or multiply coiled configurations ($t_{fin} = 12$) as follows:

Reidemeister type I move



Case of one coil formation (n=2)

4 Energetics of folding

Let us consider the **linear elastic theory** for a uniformly homogeneous and isotropic filament ($\chi = K_b/K_t = 1$ with K_b *bending rigidity* and K_t *torsional rigidity*).

- The **deformation energy** is given (to first order) by

$$\tilde{E} = \tilde{E}_b + \tilde{E}_t + \ldots\text{(higher-order terms)} \tag{7}$$

  where

$$\tilde{E}_b(t) = \frac{E_b(t)}{E_0} = \frac{1}{2\pi}\oint_{\mathscr{C}}(c(\xi,t))^2\|\mathbf{X}'(\xi)\|\,\mathrm{d}\xi \quad \textbf{norm. bending energy}$$

$$\tilde{E}_{tw}(t) = E_t|_{\Omega_0} = (Lk - Wr\,(t))^2 \quad \textbf{norm. mean twist energy}$$

$$E_0 = \frac{K_b}{2}\oint_{\mathscr{C}} c_0^2\,\mathrm{d}s \quad \textbf{reference energy} = \pi K_{\mathrm{b}}\,.$$

- According to Michell–Zajac instability (1889-1962) we set $Lk = 3$. The energy that is going to be relaxed in coiling is:

$$\tilde{E}(0) = \tilde{E}_0 = 1 + Lk^2 = 10\,,$$
$$\tilde{E}(t_{fin}) = \tilde{E}_{fin} = 8.5\,.$$

5 Coiling under elastic energy minimization

Kinematics functions $a(t), b(t), c(t), d(t), e(t)$ from curves (5) for single coil formation ($n = 2$) are obtained as solutions of the following problem:

$$\begin{aligned} \min_{a(t),b(t),c(t),d(t),e(t)} \quad & \int_0^{t_{fin}} \tilde{E}(a(t), b(t), c(t), d(t), e(t))\mathrm{d}t \\ s.t. \quad & \tilde{E}(a(0), b(0), c(0), d(0), e(0)) = \tilde{E}_0 \\ & \tilde{E}(a(t_{fin}), b(t_{fin}), c(t_{fin}), d(t_{fin}), e(t_{fin})) = \tilde{E}_{fin} \\ & l(a(t), b(t), c(t), d(t), e(t)) = 2\pi \qquad t \in [0, t_{fin}] \\ & \frac{\mathrm{d}\tilde{E}(a(t), b(t), c(t), d(t), e(t))}{\mathrm{d}t} \le 0 \end{aligned} \tag{8}$$

where the initial ($t = 0$) and final ($t = t_{fin} = 12$) conditions on the total energy $\tilde{E}$ (7) are chosen s.t. $\tilde{E}_0 \geq \tilde{E}_{fin}$.

- Problem (8) is *approximated* by dividing the time period $[t_0, t_{fin}]$ (with $t_0 = 0$) into F equidistant intervals and considering:

$$\begin{aligned} \min \sum_{f=0}^{F}\left[\tilde{E}(a(t_f), b(t_f), c(t_f), d(t_f), e(t_f)) + \gamma p(t_f)\right] + \mu \sum_{f=1}^{F-1} h(t_f) \\ s.t. \quad \tilde{E}(a(0), b(0), c(0), d(0), e(0)) = \tilde{E}_0 \\ \tilde{E}(a(t_{fin}), b(t_{fin}), c(t_{fin}), d(t_{fin}), e(t_{fin})) = \tilde{E}_{fin} \\ l(a(t_f), b(t_f), c(t_f), d(t_f), e(t_f)) = 2\pi \qquad f \in [0, F] \\ \tilde{E}(a(t_f), b(t_f), c(t_f), d(t_f), e(t_f)) \geq \tilde{E}(a(t_{f+1}), b(t_{f+1}), c(t_{f+1}), d(t_{f+1}), e(t_{f+1})) \end{aligned} \tag{9}$$

where the objective function includes **penalizations** on:

- **distance** of $a(t_f), b(t_f), c(t_f), d(t_f), e(t_f)$ from zero with *cost* γ through:

$$p(t_f) = a^2(t_f) + b^2(t_f) + c^2(t_f) + d^2(t_f) + e^2(t_f)\,, \qquad f \in [0, F] \tag{10}$$

- **curvature** by means of the *central difference approximation* of the second derivative with *cost* μ as follows:

$$k(a(t_f)) = \frac{\frac{a(t_{f+1})-a(t_f)}{t_{f+1}-t_f} - \frac{a(t_f)-a(t_{f-1})}{t_f-t_{f-1}}}{t_{f+1}-t_{f-1}}\,,\; f \in [1, F-1] \tag{11}$$

  and

$$h(t_f) = k(a(t_f))^2 + k(b(t_f))^2 + k(c(t_f))^2 + k(d(t_f))^2 + k(e(t_f))^2\,.$$

6 Kinematics by cubic spline interpolation

- Time evolution function $a(t)$ is approximated by **spline function** $a_s^3(t)$, a piecewise-polynomial real function of **order** 3 obtained by interpolating between all pairs of "knots" $(t_{f-1}, a(t_{f-1}))$ and $(t_f, a(t_f))$, $f \in [1, F]$, where $a(t_f)$ are solutions of problem (9).
  The restriction of $a_s^3(t)$ to an f–interval is a polynomial continuously differentiable to order 2 at the interior points t_f, $f = 1, \ldots, F-1$.
- Altermative approach: **cubic Hermite spline interpolation**, a third-degree spline with each polynomial as follows:

$$a_h^{f,3}(t) = a_{00}^{(f)}h_{00}(t) + a_{01}^{(f)}h_{01}(t) + a_{10}^{(f)}h_{10}(t) + a_{11}^{(f)}h_{11}(t)\,, \quad f = 1, \ldots, F$$

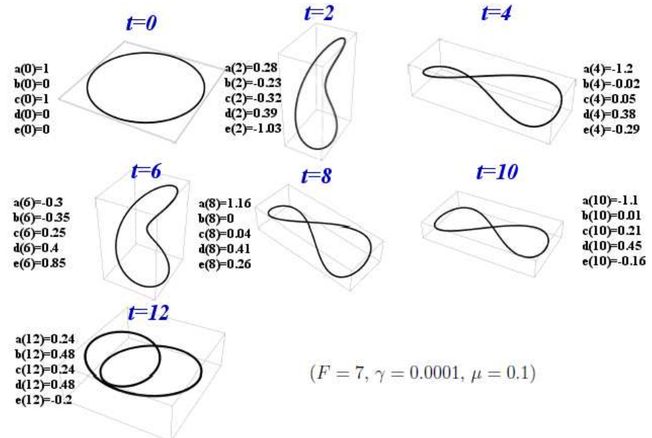
  where

$$\begin{cases} h_{00}(t) = 2t^3 - 3t^2 + 1 \\ h_{01}(t) = -2t^3 + 3t^2 \\ h_{10}(t) = t^3 - 2t^2 + t \\ h_{11}(t) = t^3 - t^2 \end{cases}$$

  are Hermite basis functions and $a_{00}^{(f)}$ and $a_{11}^{(f)}$ respectively the stating and final point with their derivatives $a_{10}^{(f)}$ and $a_{01}^{(f)}$ in the f – interval ($f = 1\ldots, F$).
  Similarly for $b(t), c(t), d(t), e(t)$.

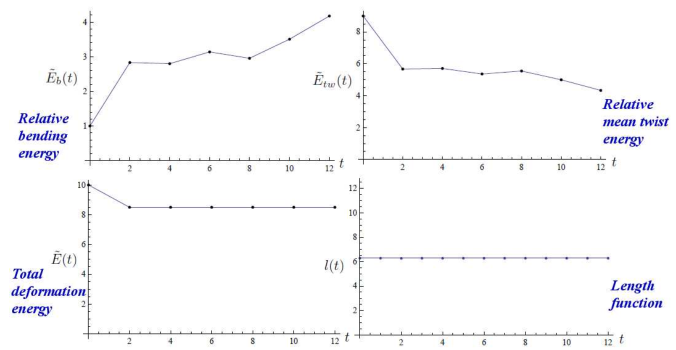
7 Preliminary numerical results

7.1 Kinematics solution for folding mechanism



Solution in case of one coil formation (n=2)

7.2 Energetics $\tilde{E} = \tilde{E}_b + \tilde{E}_{tw}$



- Convergence with respct to penalization costs μ, γ and number of intervals F has been tested.

8 Conclusions and future directions

- Kinematics of coil formation as solution of the elastic energy minimization problem (9) are proposed.
- By an alternating folding mechanism, the model considered can produce *high degree of coiling by keeping the writhing number bounded*.
- We plan to extend the numerical investigation to kinematics of multiple coils formation ($N > 1$) and to Fourier knots.

References

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