COSSERAT MODEL FOR A CIRCULAR HELIX

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1. Introduction

In the discrete Cosserat model, an elastic rod is made up of a connected sequence of linear segments that minimizes the strain energies. In this paper, we will construct the model for the helix and measure the Hooke's constant from the energy function.

2. Helix Cosserat Model

Given the upright[1] helix $r(t) = (R\cos t, R\sin t, ct)$, where R is the radius of the helix and $2\pi c$ is a constant giving the vertical separation of the helix's loops. If s is the arc-length parameter of the helix, then we have:

$$s(t) = \int_0^t |r'(t)|d\tau = \int_0^t \sqrt{R^2+c^2}d\tau = \sqrt{R^2+c^2}t.$$

From this equation, we can reparametrize the center-line of the helix with respect to the arc-length parameter s as follows:

$$r(s) = \left(R\cos\frac{s}{\sqrt{R^2+c^2}}, R\sin\frac{s}{\sqrt{R^2+c^2}}, \frac{cs}{\sqrt{R^2+c^2}}\right). \tag{1}$$

Now that we have had a formula for the center-line, let us calculate the directors, the Euler parameters, and the strain parameters.

2.1. **Directors.** First, assuming inextensibility, we require d_3 to be tangent to the center-line:

$$d_3(s) = r'(s) = \left(-\frac{R\sin\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{\sqrt{c^2+R^2}}, \frac{R\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{\sqrt{c^2+R^2}}, \frac{c}{\sqrt{c^2+R^2}}\right). \tag{2}$$

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[1]For simplicity, our helix will be upright and have starting point at $(0, 1, 0)$.

Now, since $\{d_1, d_2\}$ spans the plane orthogonal to the center-line, we can first choose d_1 to be a vector on the plane, then compute $d_2 = d_3 \times d_1$:

$$d_1(s) = \left(-\cos\frac{s}{\sqrt{R^2+c^2}}, -\sin\frac{s}{\sqrt{R^2+c^2}}, 0\right) \tag{3}$$

$$d_2(s) = \left(\frac{c\sin\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{\sqrt{c^2+R^2}}, -\frac{c\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{\sqrt{c^2+R^2}}, \frac{R}{\sqrt{c^2+R^2}}\right). \tag{4}$$

2.2. **Strain parameters.**

Given the directors, we can compute the strain parameters as follows:

$$\begin{aligned} u_1(s) &= -d'3(s)\cdot d_2(s) = 0 \\ u_2(s) &= d'3(s)\cdot d_1(s) = \frac{R}{c^2+R^2} \\ u_3(s) &= d'1(s)\cdot d_2(s) = \frac{c}{c^2+R^2}. \end{aligned}$$

As a reminder, u_1, u_2 and u_3 represent strain with respect to bending for $j = 1, 2$, and twisting, for $j = 3$. In our discrete model of the rod, we re-scale these strain parameters to get $\theta_i = u_i\frac{s}{N}$, where s is the arc length of the rod and N is the number of segments in our discrete model [4].

2.3. **Euler parameters q_i.**

From the master thesis, we know that the directors and Euler parameters at a point s are related through the equations:

$$d_1 = \frac{1}{\|\boldsymbol{q}\|^2}\begin{pmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 \\ 2(q_1q_2 + q_3q_4) \\ 2(q_1q_3 - q_2q_4) \end{pmatrix} \tag{5}$$

$$d_2 = \frac{1}{\|\boldsymbol{q}\|^2}\begin{pmatrix} 2(q_1q_2 - q_3q_4) \\ -q_1^2 + q_2^2 - q_3^2 + q_4^2 \\ 2(q_1q_4 + q_2q_3) \end{pmatrix} \tag{6}$$

$$d_3 = \frac{1}{\|\boldsymbol{q}\|^2}\begin{pmatrix} 2(q_1q_3 + q_2q_4) \\ 2(-q_1q_4 + q_2q_3) \\ -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix}. \tag{7}$$

With the additional requirement of $\|\boldsymbol{q}\|^2 = 1$, we can compute $\boldsymbol{q}(s)$ and get the following solutions (see Appendix A for the full `Mathematica` code):

$$q_1(s) = -\frac{R\sin\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{2\sqrt{c^2+R^2}\sqrt{\frac{\left(\sqrt{c^2+R^2}+c\right)\left(\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)+1\right)}{\sqrt{c^2+R^2}}}},$$

$$q_2(s) = \frac{1}{2}\sqrt{\frac{\left(\sqrt{c^2+R^2}-c\right)\left(\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)+1\right)}{\sqrt{c^2+R^2}}},$$

$$q_3(s) = \frac{1}{2}\sqrt{\frac{\left(\sqrt{c^2+R^2}+c\right)\left(\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)+1\right)}{\sqrt{c^2+R^2}}},$$

$$q_4(s) = -\frac{R\sin\left(\frac{s}{\sqrt{c^2+R^2}}\right)}{2\sqrt{c^2+R^2}\sqrt{\frac{\left(\sqrt{c^2+R^2}-c\right)\left(\cos\left(\frac{s}{\sqrt{c^2+R^2}}\right)+1\right)}{\sqrt{c^2+R^2}}}}.$$

We have officially finished the Cosserat model for the helix; the code in `helix_energy.m` is updated accordingly.

3. Experimental result

In this section, we will explore the energy of the helix under stretching strains and its relationship to the Hooke's constant.

3.1. **Default helix.** The default parameters for the MATLAB code are as follows (cf. Figure 1):

- `stretch_param=0`, with its range being (-1,1) representing the amount of stretch/shrink relative to the total height,
- `contact_strength=0`, representing the contact strength,
- `nseg=64` representing the number of segments in the discrete model[2],
- `R=1`, the radius of the helix,
- `c=0.1`, the vertical separation parameter of the helix,
- `tmax=6*pi`, which makes sure we have 3 loops in the helix.

With the default strain parameters, we calculate the total energy with respect to the number of segments (cf. Figure 2). From this figure, we can see that `nseg=256` best approximates the energy of default rod, which should be 0. Hence, all calculations of energies from now on will use `nseg=256`.

[2]We choose `nseg=64` out of computation time concerns; it is not necessarily the best `nseg` to approximate the energy of the rod.

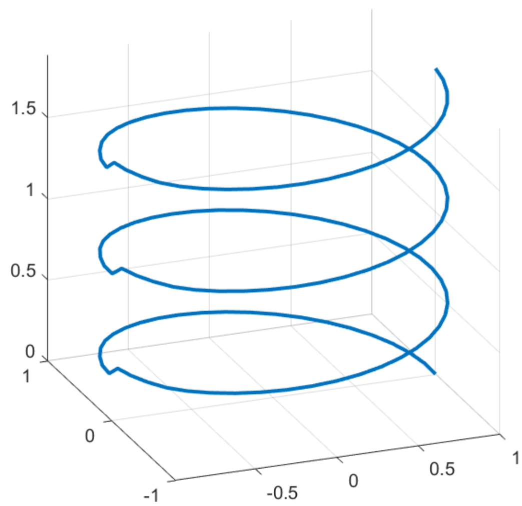


FIGURE 1. Default helix with `nseg=64`. Note the jump from one loop to the other; as we increase the number of segments, the jump gradually disappears.

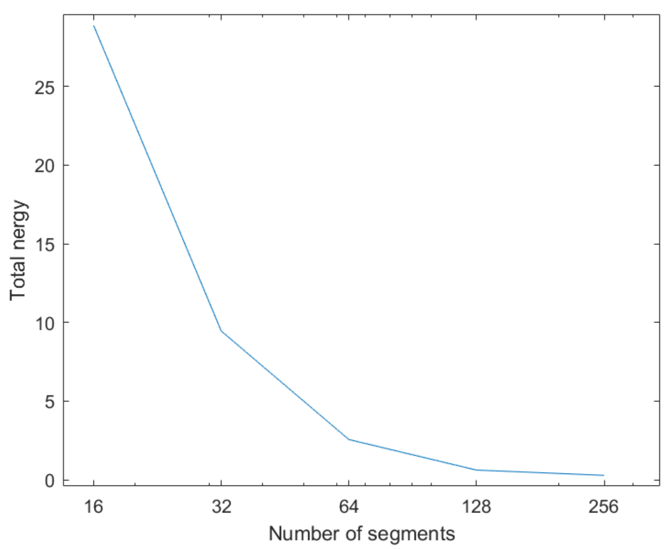


FIGURE 2. Convergence of total energy with respect to `nseg`

3.2. **Stretch/shrink energies.** I then ran the code to calculate the energies of rods with different stretching and contact parameters[3]. We then obtain Figure 3.

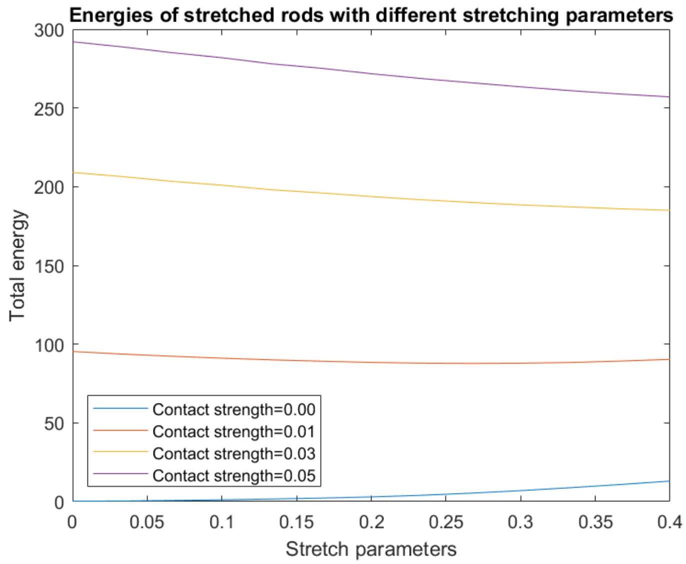


FIGURE 3. Total stretch energy with different stretching parameters and different contact strength Q.

From this figure, we noticed that as we increase the contact strength, the energy increase (which resulted in different line heights), which makes sense due to the increase in potential energy. What's interesting is that there is no clear pattern of the energy when we increase the stretching parameters. Take the purple line for example; since the contact strength is large, the energy of the un-stretched rod is very high; however, as we stretch it out, it kinda "evens out" the contact energy, making the total energy decrease[4]

Now, I also compute the rod energy with negative stretching parameters, i.e. "shrinking parameters" (cf. Figure 4). As we shrink the rod and increase the contact strength, the energy increases, which I think is intuitive.

[3]In the `MATLAB` code, note that the contact strength Q is scaled down by `nseg^2`.

[4]Sorry this part is a bit informal. I don't know how to explain it otherwise.

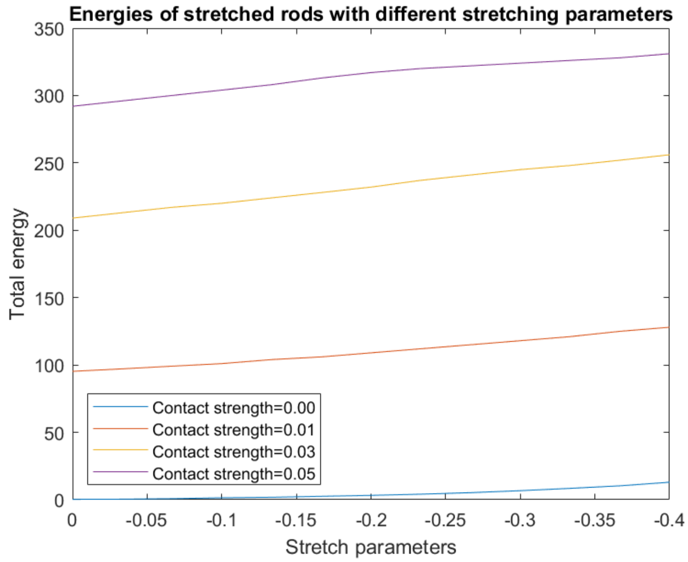


FIGURE 4. Total stretch energy with different stretching parameters and different contact strength Q.

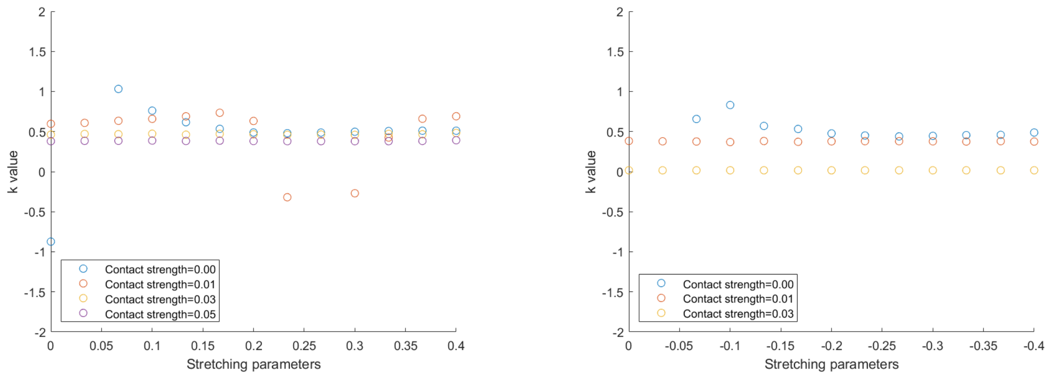
3.3. **Hooke's constant calculation.** Now, let us calculate the Hooke's constant k. From Physics,

$$\mathbb{E} - \mathbb{E}_0 = \frac{1}{2}k(x - x_0)^2,$$

where $\mathbb{E}_0, x_0$ represent the intrinsic energy and displacement of the spring. Now, we know that at $\{x_0, \mathbb{E}_{\nvdash}\}$, the potential energy of the rod is minimized[5]. Therefore, to find $\{x_0, \mathbb{E}_0\}$, we will fit a quadratic curve along our data points. Then, we calculate the Hooke's constant k based on the formula (cf. Figure 5).

From Figure 5, we can see that the Hooke's constant lies in the range $(0.48, 0.5)$. It is important to note that for shrunk rods, we are missing the data when `contact_strength=0.05` because the energy plot for this curve concaves down instead of concaving up like all other lines; for this reason, `MATLAB` wasn't able to find the minimum point $\{x_0, \mathbb{E}_0\}$.

[5]The energy should not be 0 since there is still contact energy.



(A) Stretched rods (B) Shrunk rods

FIGURE 5. Hooke's constant, calculated from energies of stretched/shrunk rods

4. Acknowledgement

This summer, I got the opportunity to learn about the Cosserat model for helix, about rotations with quaternions, about `MATLAB` implementation of the model, all of which are super cool things! I want to thank Rob for being such a great advisor. Thank you for being so clear and helpful in explaining the math concepts to me; and so patient when I felt unproductive.

Appendix A. Euler Parameter Calculations with Mathematica

The following code calculates the Euler parameters by equating the two formulas for the directors. First, let's set up the variables in `Mathematica`.

```
In[]:= ClearAll[R, s, c, θ];
r[s_] := {R Cos[s/Sqrt[R^2 + c^2]], R Sin[s/Sqrt[R^2 + c^2]], c s/Sqrt[R^2 + c^2]};
d3 = D[r[s], s];
d1 = {-Cos[s/Sqrt[R^2 + c^2]], -Sin[s/Sqrt[R^2 + c^2]], 0};
d2 = FullSimplify[Cross[d3, d1]];
u1 = Dot[-D[d3, s], d2];
u2 = FullSimplify[Dot[D[d3, s], d1]];
u3 = FullSimplify[Dot[D[d1, s], d2]];
```

Then, we can relate the two director equations and solve them:

```
In[]:= ClearAll[q1q2, q3q4, q1q3, q2q4, q1q4, q2q3];
       roots1 = FullSimplify[Solve[{2 (q1q2 + q3q4) == d1[[2]], 2 (q1q2 - q3q4) == d2[[1]]}, {q1q2, q3q4}]];
       roots2 = Solve[{2 (q1q3 + q2q4) == d3[[1]], 2 (q1q3 - q2q4) == d1[[3]]}, {q1q3, q2q4}];
       roots3 = Solve[{2 (q1q4 + q2q3) == d2[[3]], 2 (-q1q4 + q2q3) == d3[[2]]}, {q1q4, q2q3}];
       Set @@@ roots1[[1]];
       Set @@@ roots2[[1]];
       Set @@@ roots3[[1]];
In[]:= q2 = FullSimplify[Sqrt[q1q2 * q2q3 / q1q3]];
       q3 = FullSimplify[q2q3 / q2];
       q1 = FullSimplify[q1q2 / q2];
       q4 = FullSimplify[q2q4 / q2];
```

Finally, we can test if the solutions give the same values for the two formulas for the directors. The output for this block of code should be `True` for all four statements.

```
In[]:= d1q = FullSimplify[( q1^2 - q2^2 - q3^2 + q4^2
                             2 (q1 * q2 + q3 * q4)
                             2 (q1 * q3 - q2 * q4) )]; d1q == ArrayReshape[d1, {3, 1}]

       d2q = FullSimplify[( 2 (q1 * q2 - q3 * q4)
                            -q1^2 + q2^2 - q3^2 + q4^2
                            2 (q1 * q4 + q2 * q3) )]; d2q == ArrayReshape[d2, {3, 1}]

       d3q = FullSimplify[( 2 (q1 * q3 + q2 * q4)
                            2 (-q1 * q4 + q2 * q3)
                            -q1^2 - q2^2 + q3^2 + q4^2 )]; d3q == ArrayReshape[d3, {3, 1}]

       FullSimplify[q1^2 + q2^2 + q3^2 + q4^2] == 1
```

Here, the answers you get might be different from the q_i's in Section 2.3 potentially because of the `FullSimplify` function. As long as the q_i's pass the 4 tests, we will consider those as solutions to the Euler parameters.

References

[1] Frank Battaglino. "Self-Contact of Rods via Unconstrained Energy Minimization Techniques". PhD thesis. University of Maryland, Baltimore County, 2018.

[2] Donald J. Dichmann, Yiwei Li, and John H. Maddocks. "Hamiltonian formulations and symmetries in rod mechanics". In: *Mathematical approaches to biomolecular structure and dynamics*. Springer, 1996, pp. 71–113.

[3] Robert S. Manning, John H. Maddocks, and Jason D. Kahn. "A continuum rod model of sequence-dependent DNA structure". In: *The Journal of chemical physics* 105.13 (1996). ISBN: 0021-9606 Publisher: American Institute of Physics, pp. 5626–5646.

[4] Michael Merkle. "A Scaling Analysis for Discrete Elastic Rod Models". PhD thesis. University of Maryland, Baltimore County, May 10, 2020.

[5] Wikipedia contributors. *Quaternions and spatial rotation — Wikipedia, The Free Encyclopedia*. [Online; accessed 7-September-2020]. 2020. URL: https://en.wikipedia.org/w/index.php?title=Quaternions_and_spatial_rotation&oldid=976580469.