Written by Ilya M. Beskin.

Worm-Like Chain Model Simulation: Working Principle

Introduction:

In order to compare the standard deviation of the transverse displacement from the average position of a collagen fibril in solution (henceforth referred to as fluctuation amplitude) to a model, we need to model this exact collagen fibril with the same boundary conditions and the identical radius profile. We assume that our fibers are clamped at one end and free to fluctuate at the other end. Mores specifically, at one end, the position and the tangent vector of the fibril is fixed while on the free end, the force and torque are 0. If $f(s)$ is the transverse displacement of the fibril as a function of its arclength parametrization s with $s = 0$ at the clamped end and $s = L$ at the free end, these boundary can be written more mathematically as:

Clamped End	Free End
$f(0) = 0$	$\frac{\partial^2 f}{\partial s^2}\Big\|_{s=L} = 0$
$\frac{\partial f}{\partial s}\Big\|_{s=0} = 0$	$\frac{\partial^3 f}{\partial s^3}\Big\|_{s=L} = 0$

The differential equation governing the motion of the worm-like chain balances the elastic force and the drag force. It reads:

$$\kappa \frac{\partial^4 f}{\partial s^4} = -\varsigma \frac{\partial f}{\partial t}$$

where ς is the drag coefficient and κ is the bending stiffness. For a filament with fixed bending stiffness along its length and a known drag coefficient, the solutions to this equation given our boundary conditions is known [*Macromolecules*, **18**(10):1868-1875 (1985) , *Biophys J*, **74**(2):1043-1060 (1998), *Phys Rev E*, **55**(3):3092-3101 (1997)]. However, we have found that collagen fibrils can change radii and therefore change their bending stiffness along their length. In order to simulate our measured collagen fibril fluctuations, we write the following code:

Procedure:

- Give simulation a radius profile.
- Give simulation an elastic modulus.

- Compute the bending stiffness profile given the radius profile and elastic modulus.
- Set first chain link at transverse position 0 and at an angle of 0 to the x-axis.

↷ **Loop 1 starts here!**

↷ **Loop 2 starts here!**

- Given the temperature $T = 300K$ and the local bending stiffness at the end of the first chain link, use the Boltzmann factor to construct a probability distribution of deflection angles for the next chain link.
- Take a random angle from that probability distribution and attach the next chain link at that angle.

↻ **Repeat loop until the chain reaches the desired number of chain links.**

↻ **Repeat for desired number of worm-like chains.**

- Compute the fluctuation amplitude as a function of distance along filament.
- Check that the fluctuation amplitude behaves like a power law and fit a power law to the data.

We then can perform this for different values of Young's modulus and observe how the behavior of our model changes. Comparing to our data, we can now extract a Young's modulus for collagen from our measurements.