

Tissue Biomechanics UE 317.523

Solutions due: 21.04.2025

Tutorial 1: Protein mechanics and entropic elasticity

Total points: 10

Problem 1: Linear versus nonlinear change in distributions

A polypeptide chain is composed of 251 stiff amino acids and the peptide bond length is 0.15 nm.

- How many peptide bonds does the polypeptide chain have? (0.25 pt)
- Plot the stretching force to account for (1) linear and (2) non-linear change in distributions. For point (2) use the Pade approximation. (0.5 pt)
- At which stretch, $x=r/L$, is the Langevin force 1.1 times greater than the force estimated by the freely joint model? (0.25 pt)

Problem 2: FJC (linear) and worm-like chain

Present in a graph the force in **piconewtons** (or pN) **as a function of stretch (r/L)** needed to extend:

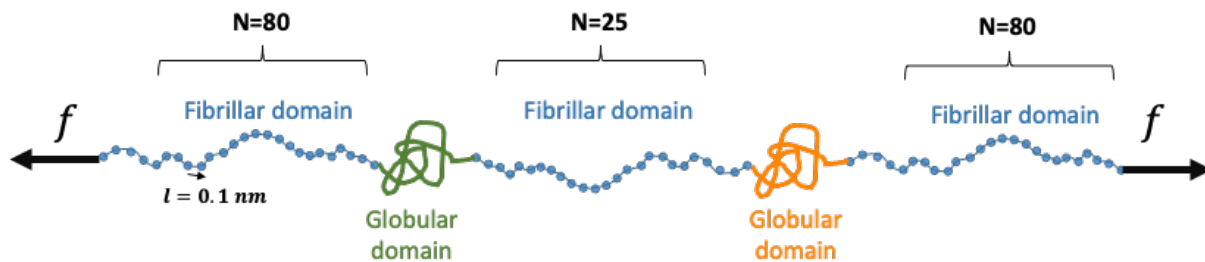
- A chain composed of 50 freely jointed domains, with 1 nm to be the distance between the domains, up to a stretch of 0.8. (1.0 pt).
- A worm-like chain of 1000 domains, each of which is a single amino acid and the peptide bond length (segment length) is 0.5 nm. (2.0 pt)

For the above problem, plot the force as a function of the ratio of the end-to-end distance (r) over the length (L) of the chain. The ratio r/L is also known as *stretch* ($0 \leq r \leq L \Rightarrow 0 \leq r/L \leq 1$). For point (b) plot the force vs. stretch x , i.e. r/L , for the cases the persistence length is 0.5 nm, 5 nm and 10 nm in one graph to compare the plots.

Problem 3: A macromolecule with "smart" dissipative mechanisms

A worm-like chain is composed of two globular domains and three fibrillar domains (see figure below). As shown in the figure, two of the fibrillar domains on the sides, of this so-called macromolecule, are composed of 80 segments each and the fibrillar domain in the middle is composed of 25 segments. The bond length, l , between successive segments in the fibrillar domains is 0.1 nm for all fibrillar domains. The globular domains will unfold once a certain

threshold force is reached. One globular domain unfolds at a lower force than the other. This force is generated by the pulling of the fibrillar domains assumed to behave as worm-like chains of persistence length 0.5 nm. The **unfolded** globular domains are assumed to have the same persistence length with the fibrillar domains.



- Calculate the force in piconewtons (pN) needed to unfold the globular domains during stretching of this worm-like-chain given that the unfolding of the left globular domain occurs at $r_{u_left} = 12$ nm (r_u stands for the unfolding distance) and that of the right globular domain occurs at $r_{u_right} = 20$ nm. Consider here that once unfolded, the globular domains are composed of 50 segments each and the distance between two segments, l , is also 0.1 nm. (2.0 pt)
- Plot a graph of the force, f (pN) against the end-to-end distance, r , in nanometers (nm) in the range for $0 \leq r \leq 20$ nm. Point in your graph where the unfolding events occur and discuss which globular domain will unfold first. (2.0 pt)
- Once globular domains are unfolded
 - How many bonds are present once the globular domains are unfolded? (0.25 pt)
 - Considering that the chain breaks at $r_{break} = 25$ nm, plot a graph of the force against the end-to-end distance (r), i.e., for $(0 \leq r \leq 25)$ nm. (1.5 pt)
 - What is the maximum force experienced at an end-to-end distance r_{break} when the chain breaks? (0.25 pt)

It is recommended that you use an Excel spreadsheet, Matlab, Mathematica or some means of computer calculations to plot and solve the above problems.

The Boltzmann's constant is $k_b = 1.38 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$.

The temperature is assumed to be (37°C). Note that the temperature in the calculations corresponds to the absolute temperature in Kelvin!

1 nm = 10^{-9} m, 1 pN = 10^{-12} N.