3 Biopolymers

3.1 Motivation

3.2 Energy

3.2.1 The Euler Bernoulli theory

In the introduction to mechanics, we have discussed that several kinematic assumptions could be made to reduce the set of governing equations. The simplest theory for one dimensional structures is the Euler Bernoulli beam theory. Its kinematic assumptions are referred to as the Euler Bernoulli hypothesis in the mechanics literature. In particular, they consist of three kinematic assumptions for the normal to the cross section under applied loads:

- normals remain straight (they do not bend)
- normals remain unstretched (they keep the same length)
- normals remain normal (they remain orthogonal to the beam axis)

Based on these assumptions, the total displacement of a beam can be expressed in the following form.

$$u^{\text{tot}}(x,z) = u(x) - z\,w(x)_{,x} \tag{3.2.1}$$

It consists of an axial stretch $u(x)$ which is parameterized in the axial direction x and component $-z\,w(x)_{,x}$ which is introduced through the rotation of the normal of the beam axis $w(x)_{,x}$. The latter contribution varies linearly across the beam thickness z. Recall that we will use what some of you refer to as the European notation for the derivative, which is $w(x)_{,x} = \mathrm{d}w \,/\, \mathrm{d}x$. According to its definition, the strain ε_{xx} follows as $\varepsilon_{xx} = u^{\text{tot}}_{,x}$.

$$\varepsilon = u^{\text{tot}}_{,x} = u_{,x} - z\,w_{,xx} \tag{3.2.2}$$

Since we required the normal to be inextensible, there are no strain components in the out of plane direction, i.e. $\varepsilon_{xz} = \varepsilon_{zz} = 0$. For the sake of simplicity, we have droped the indices $_{xx}$ on the only relevant strain component implying that $\varepsilon = \varepsilon_{xx}$. Take a closer look at the strains! They consist of a contribution $\varepsilon^{\text{con}} = u_{,x}$ which is independent of the z-coordinate and thus constant over the thickness and a contribution $\varepsilon^{\text{lin}} + -z\,w_{,xx}$ that varies linearly over the thickness. The former is related to the axial deformation in the form of tension and similar to the one we have analyzed for the one dimensional truss. The latter is related to the transverse deformation in the form of bending. The overall deformation of beams can thus be understood as the superposition of two basic deformation modes, axial stretching and bending. These two modes will be addressed independently in the following subsections.

3.2.2 Axial deformation - Tension

Let us first take a look at the axial deformation, and thereby repeat the equations we have discussed in the motivation section for the one dimensional bar. We restrict our-

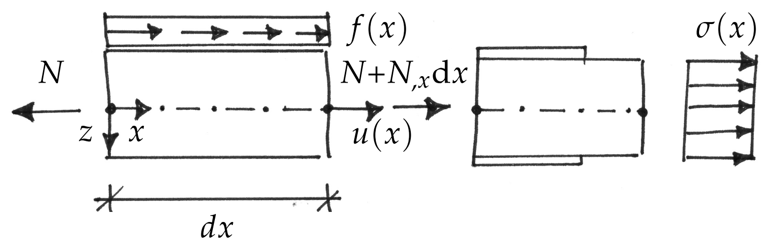

Figure 3.1: Axial loading of one dimensional structure ∘ Stresses σ are constant across the cross section

selves to the strain contribution that is constant across the thickness $\varepsilon = \varepsilon^{\text{con}} = u_{,x}$ assuming that the linear contribution is negligibly small $\varepsilon^{\text{lin}} = -z\, w_{,xx} \approx 0$. This situation is depicted in figure 3.1. The axial strains are the simply given as follows.

$$\varepsilon = u_{,x} \tag{3.2.3}$$

For a linear elastic material, the axial stresses then simply follow as

$$\sigma = E\,\varepsilon = E\,u_{,x} \tag{3.2.4}$$

where E is young's modulus. The stress resultant N, i.e., the normal force in axial direction simply follows from the integration over the total height h.

$$N = \int_{-h/2}^{+h/2} \sigma\,\mathrm{d}z = \sigma\,h = E\,h\,\varepsilon \tag{3.2.5}$$

The equilibrium equation follows straightforwardly from summing all the forces in figure 3.1.

$$\sum f_x \doteq 0 \qquad N_{,x} + f = 0 \tag{3.2.6}$$

The combination of the above equations renderns the Laplace equation

$$EA\,u_{,xx} + f = 0 \qquad \text{with} \qquad EA \;\; \text{... axial stiffness} \tag{3.2.7}$$

which is often expressed in terms of the Laplace operator $\Delta(\circ) = (\circ)_{xx} = \mathrm{d}(\circ)\,/\,\mathrm{d}x^2$ as $EA\,\Delta u + f = 0$. It relates the axial deformation u to the axial force f. Herein, EA

	r	A	E	EA
microtubule	12.5 nm	491 nm^2	$1.9{\cdot}10^9$ N/m^2	$93{\cdot}10^{-8}$ N
intermediate filament	5.0 nm	79 nm^2	$2.0{\cdot}10^9$ N/m^2	$15{\cdot}10^{-8}$ N
actin filament	3.5 nm	39 nm^2	$1.9{\cdot}10^9$ N/m^2	$7{\cdot}10^{-8}$ N

Table 3.1: Axial stiffness EA of major consituents of cytoskeleton: microtubules, intermediate filaments and actin filaments

is the axial stiffness. It characterizes the resistance of the structure with respect to an axial deformation or stretch. Given the radius r of the cross section of microtubules, intermediate filaments and actin filaments and Young's modulus E, you can calculate the cross section area $A = \pi\, r^2$ and the axial stiffness EA.

Example Determine the elongation of an active muscle with Young's modulus $E =$ 40MPa= $4 \cdot 10^7$N/m^2, a cross section of $A =$ 1000mm^2 =10^{-3}m^2 and a total length $l =$ 10mm= 0.01m! Assume that the muscle is loaded by a weight of $m =$ 10kg. What is its elongation Δl and its its strain ε? ∘ The force acting on the muscle is $N = m\, g$ with the acceleration due to gravity $g =$ 10m/s^2 = 10N/kg, thus $N =$ 10kg·10N/kg = 100N. The elongation Δl then follows as $\Delta l = \varepsilon\, l = \sigma\, l \,/\, E = N\, l \,/\, [EA] =$ 100N · 0.01m / [$4 \cdot 10^7$N/m^2 · 10^{-3}m^2] = $2.5 \cdot 10^{-2}$mm. The strain simply follows as $\varepsilon = \Delta l \,/\, l =$ 2.5 · 10mm / 10 mm = 0.0025 = 0.25%.

3.2.3 Transverse deformation - Bending

We have seen that the axial deformation can be described in terms of a second order partial differential equation. What about the transverse deformation? How is the out of plane deformation related to the out of plane forces? Let us elaborate

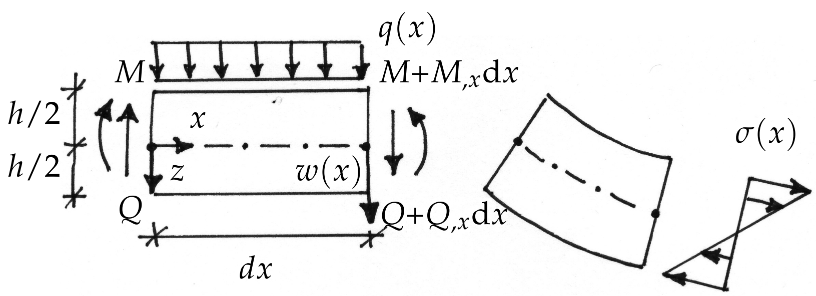

Figure 3.2: Transverse loading of one dimensional structure ∘ stresses σ vary linearly across the cross section

the component of the strain that contribution that varies linearly across the thickness $\varepsilon^{\text{lin}} = -z\, w_{,xx}$ and for now assume that the constant strain contribution is negligibly small $\varepsilon = \varepsilon^{\text{con}} = u_{,x} \approx 0$. This situation which depicted in figure 3.2 is characterized through the following strain displacement relation.

$$\varepsilon = -w_{,xx}\, z = \kappa\, z \tag{3.2.8}$$

Here, we have introduced the curvature κ. If you think of an arc, $\kappa = 1/r$ would be the inverse of the underlying circle's radius, κ has thus the unit of 1/length. Again, the stresses just simply follow through Hooke's law of linear elasticity.

$$\sigma = E\,\varepsilon = -E\,w_{,xx}\,z = E\,\kappa\,z \tag{3.2.9}$$

For a moment, think of bending a beam. At the inner side, the beam will be compressed to a shorter total length while at the outer side, the beam will be stretched. The stress in a beam thus varies linearly across the cross section. At the inner side, it the stress in negative or compressive while at the outer side, it is positive or tensile. The dash dotted line in figure 3.2 is called the neutral axis. As you can see in the figure, this is the axis in which the normal stresses vanish. The stress resultant of this linearly varying stress is the bending moment M which is simply given by integrating the stress times the distance to the neutral axis z over the cross section height.

$$M = \int_{-h/2}^{+h/2} \sigma\,z\,\mathrm{d}z = \int_{-h/2}^{+h/2} E\,\kappa\,z^2\,\mathrm{d}z = EI\,\kappa \tag{3.2.10}$$

We have introduced the abbreviation $I = \int_{-h/2}^{+h/2} z^2\,\mathrm{d}z = h^3\,/\,12$ for the integral of z^2 over the height, assuming a unit width of the cross section. This geometric property of the cross section is called the geometrical moment of inertia. It is a geometric measure of the resistance of the cross section to bending. In combination with Young's modulus E, the moment of inertia I defines the bending stiffness EI. For beding problems, we typically analyze two equilibrium equations, i.e., the equilibrium of forces in the transverse direction and the equilibrium of bending moments.

$$\begin{array}{llll} \sum f_z \doteq 0 & Q_{,x} & + \; q & = 0 \\ \sum m \doteq 0 & M_{,x} & - \; Q & = 0 \end{array} \tag{3.2.11}$$

A combination of ($3.2.11_1$) and ($3.2.11_2$) yields the following simple second order equation.

$$M_{,xx} + q = 0 \tag{3.2.12}$$

By making use of the constitutive equation $M = EI\,\kappa$ and the kinematics $\kappa = -w_{,xx}$ we obtain the classical fourth order differential equation for thin beams, the Euler-Bernoulli beam equation.

$$q = EI\,w_{,xxxx} \qquad \text{with} \qquad EI \;\text{... bending stiffness} \tag{3.2.13}$$

It relates the transverse force q to the fourth gradient of the transverse displacements w in terms of the bending stiffness EI. Mathematicians would typically rewrite the plate equation in compact notation in terms of the Laplace differential operator $\Delta(\circ) = \mathrm{div}(\nabla(\circ)) = \mathrm{d}^2(\circ)/\mathrm{d}x^2 = (\circ)_{,xx}$ as $q = EI\;\Delta^2 w$. Given the radius r of the cross section of microtubules, intermediate filaments and actin filaments and Young's modulus E, you can calculate the moment of inertia for circular cross sections $I = \pi\,r^4\,/\,4$ and the bending stiffness EI.

	r	I	E	EI
microtubule	12.5 nm	19,175 nm^4	$1.9{\cdot}10^9 N/m^2$	$364{\cdot}10^{-25} Nm^2$
intermediate filament	5.0 nm	491 nm^4	$2{\cdot}10^9 N/m^2$	$10{\cdot}10^{-25} Nm^2$
actin filament	3.5 nm	118 nm^4	$1.9{\cdot}10^9 N/m^2$	$2{\cdot}10^{-25} Nm^2$

Table 3.2: Bending stiffness of major consituents of cytoskeleton: microtubules, intermediate filaments and actin filaments

3.3 Entropy

Example: Persistence length of spaghetti Try to guess the persistence length A of spaghetti at room temperature. Would it be smaller than the spaghetti length, approximately the same or larger? Assume spaghetti have a diameter of $d = 2$mm and a Young's modulus of $E = 1 \cdot 10^8 \text{J/m}^3 = 1 \cdot 10^8 \text{N/m}^2$. The temperature and the Boltzmann constant are $T = 300$K and $k = 1.38 \cdot 10^{-23}$J/K. The persistence length of spaghetti is $A = [EI] \,/\, [kT]$, with the moment of inertia $I = [\pi\, r^4] \,/\, 4$ with r=1mm. Accordingly, $A = [1 \cdot 10^8 \,\text{N/m}^2\, \pi \,\text{mm}^4] \,/\, [4 \cdot 1.38 \cdot 10^{-23}\, \text{J/K} \cdot 300\,\text{K}] = 1.8 \cdot 10^{18}$m. An uncooked spaghetti changes its direction at length scales of the order of $A = 1.8 \cdot 10^{15}$km. Is that a lot? Well, yes, that's quite stiff if you consider that the distance from the earth to the moon is about $3.8 \cdot 10^5$km!

Example: Persistence length of flagella Flagella are tail-like structures that project from the cell body of certain prokaryotic and eukaryotic cells. Flagella are hollow cylinders, of the order of 10μm long, used for locomotion. Calculate the persistence length A of flagella at room temperature $T = 300$K. Assume an inner and outer radius of $r^{\text{int}} = 0.07\,\mu$m and $r^{\text{out}} = 0.10\,\mu$m, respectively, and a Young's modulus of $E = 1 \cdot 10^8 \,\text{J/m}^3 = 1 \cdot 10^8 \,\text{N/m}^2$. For hollow cylinders, $I = \pi\, [\, r^{\text{out}\,4} - r^{\text{int}\,4}\,] \,/\, 4$. Accordinlgy, $A = [EI] \,/\, [kT] = [1 \cdot 10^8 \,\text{J/m}^3\, \pi\, [0.10^4 - 0.07^4]\, \mu\text{m}^4] \,/\, [4 \cdot 1.38 \cdot 10^{-23} \cdot \text{J/K}\, 300\,\text{K}] = 1.44$ m. The persistence length of flagella is $A = 1.44$m. As expected, they are relatively stiff to support cell locomotion.

3.4 Summary

3.5 Problems

Problem 3.1 - Polymerization kinetics

A polymer starts to grows in a monomer solution of initial concentration C_0. Assume the rate equation for the number of monomers in the filament is governed by the kinetics of assembly as discussed in class.

$$\frac{\mathrm{d}n}{\mathrm{d}t} = k_{on}\,C - k_{off}$$

In class, we have assumed that the free monomer concentration C does not change in time. Assume now, that no new monomer is added to the solution as the filament grows.

- Sketch the evolution of the free monomer concentration C as a function of time t.
- Determine the equation for the free monomer evolution, i.e., the equation for this plot, at $t \to 0$.
- Determine the asymptotic value for the concentration C as $t \to \infty$.

Problem 3.2 - Polymerization kinetics

To get a better feeling for stresses that the cytoskeleton induces on the cell membrane, this problem deals with determining membrane pressure resulting from microtubules. Consider a representative cell of radius 10μm with a tubulin (heterodimer) concentration C of 1μM.

- Calculate the total length of microtubules that could be made from this amount of protein if each dimer is approximately 8 nm long.
- Assume all microtubules connect the center of the cell with its membrane. What is the average membrane area per microtubule?
- Assume each microtubule generates a force of 5 pN. What is the total pressure exerted on the cell membrane?

Problem 3.3 - Solid vs hollow structures

In class, we have assumed microtubules to be solid cylinders with a Young's modulus of $E = 1.9 \cdot 10^9\mathrm{N/m}^2$ and a radius of approximately r^{solid} =12.5nm. We have calculated their cross section area $A^{\mathrm{solid}} = \pi\, r^{\mathrm{solid}\,2}$ to $A^{\mathrm{solid}} = \pi\,(12.5\mathrm{nm})^2$ = 491 nm^2 and their moment of inertia $I^{\mathrm{solid}} = 1/4\,\pi\, r^4$ to $I^{\mathrm{solid}} = 1/4\,\pi\,(12.5\text{ nm})^4$ = 19,175 nm^4. Actually this was an oversimplification! In reality, microtubules are hollow cylinders. The outer and inner radii have been determined to r^{outer} =14.0 nm and r^{inner} =11.0 nm.

- Calculate the cross section area $A^{\mathrm{hollow}} = [\, r^{\mathrm{outer}\,2} - r^{\mathrm{inner}\,2}\,]$ of microtubules when considered as a hollow cylinders.
- Calculate the moment of inertia $I^{\mathrm{hollow}} = 1/4\pi[\, r^{\mathrm{outer}\,4} - r^{\mathrm{inner}\,4}\,]$ of microtubules when considered as a hollow cylinders.

- Calculate the radius r^{solid} of an imaginary solid cylinder which would have the same cross section area as microtubules.
- Calculate the moment of inertia of I^{solid} of this imaginary solid cylinder of equal cross section area.

Problem 3.4 - Bending stiffness

To gain a better understanding of the bending stiffness of microtubules, consider microtubules as cantiliver beams of length $L = 10\mu$m, clamped on one side and loaded by a point load F on the other. We are interested in the transverse force F that creates a beam deflection of $w = 1\mu$m on the free end.

- Compare the forces needed to deform microtubulues when considered as hollow cylinders (use the moment of inertia I^{hollow} calculated in the previous problem) with the forces needed to deform an imaginary solid cylinder of equal volume (use the value I^{solid} calculated at the end of the previous problem).
- Discuss the results! Why, do you think, nature prefers hollow structures over solid strucutres?

Hints: To solve this problem, you might need the equation for the Euler Bernoulli beam $EI\, w_{,xx} - M = 0$ as derived in class. In addition, you need to know that the bending moment for a cantiliver beam is $M = [L - x]F$. Combine this equation with the beam equation. You then need to integrate the beam equation twice. To determine the integration constants, you need to use the boundary conditions of a cantiliver $w(0) = 0$ and $w'(0) = 0$. Solve the final equation for the force F for the different moments of inertia I^{hollow} and I^{solid}!

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