Mathematical Mechanical Biology

Module 1: Bio-Filaments

Lecture Notes for C5.9

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Based on previous notes of Eamonn Gaffney and Alain Goriely

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HEALTH WARNING:

The following lecture notes are meant as a rough guide to the lectures. They are not meant to replace the lectures. You should expect that some material in these notes will not be covered in class and that extra material will be covered during the lectures (especially longer proofs, examples, and applications). Nevertheless, I will try to follow the notation and the overall structure of the notes as much as possible.

1 Chain models

■ Overview

We consider the statistical mechanics of different chains of increasing complexity to describe the geometry and physical response of chains in a thermal bath. Past the entropic regime, many bio-filaments behave as an elastic material and we will then use classical rod mechanics to characterise their behaviour.

1.1 FJC: Freely jointed chain models

1.1.1 Without external force

This model is also known as Random Flight Model (as we will see it is closely related to the problem of diffusion/Brownian motion). We consider a chain of links that are free to rotate with respect to one another. We have the following assumptions.

1) The chain has N links

2) Each link has a fixed length b (b for bond length)

3) The orientation of the tangent $\mathbf{t}_i$ at node $(i-1)$ is independent from the orientation of the other tangents.

4) There are no excluded volume effects.

The nodes have position $\mathbf{R}_i \in \mathbb{R}^3$ for $i = 0, \dots, N$ and the vector from node $i-1$ to i is denoted by $\mathbf{r}_i = b\mathbf{t}_i$. We define the average $< . >$ of a quantity $\mathbf{a}$ as

$$< \mathbf{a} >= \int_{(\mathbb{R}^3)^N} \mathbf{a}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) p(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) dV, \tag{1}$$

where dV is the volume element of $(\mathbb{R}^3)^N$ and $p(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the probability distribution for the configuration vector $(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. In our case $p = \prod_{i=1}^N \psi(\mathbf{r}_i)$ with

$$\psi(\mathbf{r}) = \frac{1}{4\pi b^2} \delta(|\mathbf{r}| - b). \tag{2}$$

We define the end-to-end vector as

$$\mathbf{R} \equiv \mathbf{R}_N - \mathbf{R}_0, \tag{3}$$

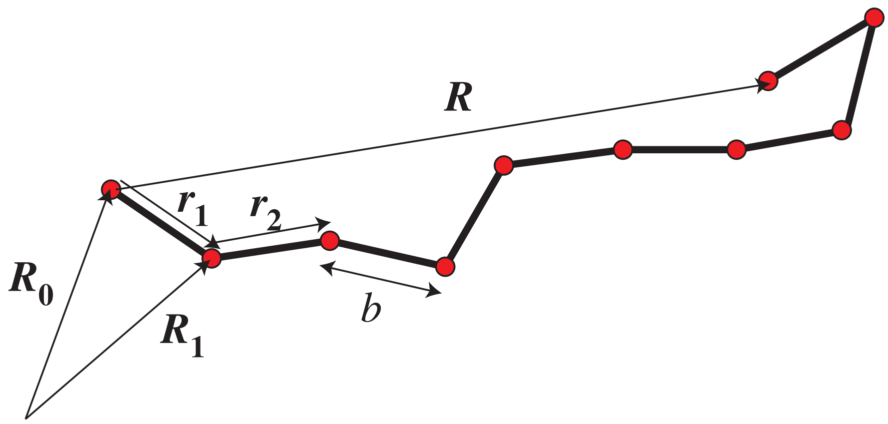

Figure 1: The freely jointed chain. Each segment has constant length with independent orientation.

and compute its average

$$<\mathbf{R}>=0$$

Therefore, we introduce $<\mathbf{R}^2>$ to find a characteristic length.

$< \mathbf{R}^2 >= Nb^2$

We define the typical *end-to-end distance* as

$$\bar{R} = \sqrt{< \mathbf{R}^2 >} = \sqrt{N}b. \tag{4}$$

1.1.2 Gyration radius

The gyration radius is closely related to the *end-to-end distance*. It is defined as the root-mean-square distance of a collection of points with respects to their centre of gravity. Defining $\mathbf{s}_i$ the vector from the centre of gravity to the node at position $\mathbf{R}_i$, the *gyration radius* is

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \mathbf{s_i} \cdot \mathbf{s_i}. \tag{5}$$

By a theorem due to Lagrange, we also have

$$s^2 = \frac{1}{(N+1)^2} \sum_{0 \le i < j \le N} r_{ij}^2, \tag{6}$$

where $r_{ij} = \mathbf{R}_j - \mathbf{R}_i$, the vector from node i to node j.

We can now compute the gyration radius for the freely jointed chain.

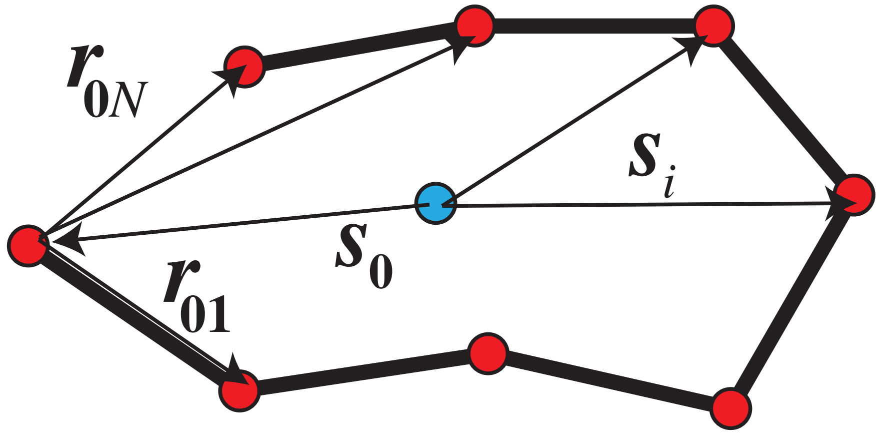

Figure 2: The gyration radius is an average distance with respect to the centre of mass of the system.

gyration radius for FJC

and we conclude that

$$< s^2 >= \frac{b^2}{6} N \frac{N+2}{N+1}. \tag{7}$$

For $N \to \infty$, we find (Debye, 1946)

$$< R^2 >= 6 < s^2 > . \tag{8}$$

The radius of gyration is an important notion as it can be measured by light scattering or sedimentation experiments.

1.1.3 With external force: force-extension behaviour

Next, we fix one end of the chain and apply a constant force $\mathbf{F} = F_z \mathbf{e}_z$ at the other end. We have the following assumptions

1) The chain is a FJC (with fixed bond length).
2) It is fixed at one end and under a constant force at the other end.
3) The chain is in an infinite heat bath.

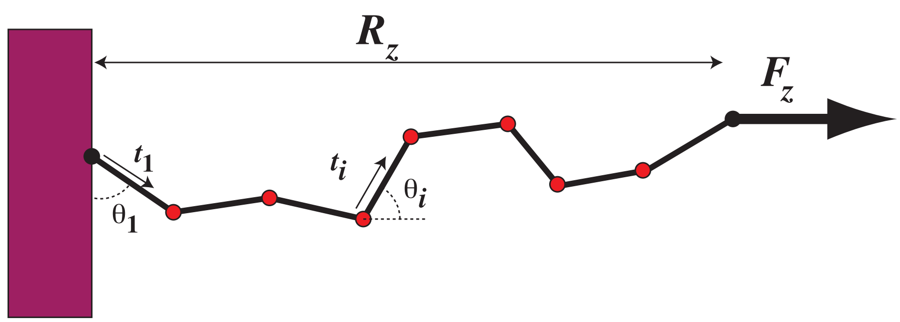

Figure 3: The freely jointed chain with external force. One end is fixed, the other one is pulled (both with free joints) with a constant force. The problem is now to find the distance along the force direction as a function of the force.

The question is then to find the force-displacement relationship that is $< R_z >$ as a function of F_z.

When the chain is pulled, the number of possible configurations decreases (to one when the chain is fully extended). Therefore, the entropy decreases and it takes energy to do so. The resistance of the chain to extend is an entropic response, i.e. it is an *emergent phenomenon* resulting from the entire system's statistical tendency to increase its entropy, as opposed to a particular underlying force; hence the name of **entropic spring** for such structures that owe their mechanical response to entropy.

The work to extend the chain is $W = \mathbf{F} \cdot \mathbf{R}$, which gives the total internal energy

$$E = -W = -\mathbf{F} \cdot \mathbf{R} = -F_z b \sum_{i=1}^{N} \cos\theta_i \tag{9}$$

where θ_i is the angle between $\mathbf{e}_z$ and $\mathbf{t}_i$.

The probability of finding the chain in a given orientation $\Theta = \{\theta_1, \theta_2, \ldots, \theta_N\}$ is given by the Boltzmann distribution for the canonical ensemble.

$$p(\Theta) = \frac{1}{\mathcal{Z}} e^{-\beta E(\Theta)} \tag{10}$$

where $\beta = (k_b T)^{-1}$, with k_b denoting Boltzmann's constant, and $\mathcal{Z}$ is the partition function

$$\mathcal{Z} = \int_{(S^2)^N} e^{-\beta E(\Theta)} dS := \int_{(S^2)^N} d\Omega_1 \ldots d\Omega_N \; e^{-\beta E(\Theta)} \tag{11}$$

where $(S^2)^N$ is the direct product of N spheres and $d\Omega_i = d\theta_i d\phi_i \sin\theta_i$ is the solid angle increment for the i^{th} sphere. Note that we integrate each θ from 0 to π and each angle φ from 0 to 2π.

The partition function: $\mathcal{Z} = z^N$

and we conclude that

$$\mathcal{Z} = z^N \quad \text{with} \quad z = 4\pi \frac{\sinh \alpha}{\alpha}. \tag{12}$$

where $\alpha = \beta b F_z$.

Now, we compute the average distance

$$< R_z >= \int_{(S^2)^N} p(\Theta) R_z dS. \tag{13}$$

The average distance

Finally, we have

$$< R_z >= bN \left[\coth(\alpha) - \frac{1}{\alpha}\right] \equiv bN\mathcal{L}(\alpha).$$

In the last expression, we have introduced the *Langevin function* $\mathcal{L}(\cdot)$. Note also that bN is the *contour length*, that is the maximal length of the chain.

For small forces

1.2 WLC: Worm-like chain models

The freely-jointed chain does not take into account that for short lengths, polymers are stiff. Therefore, we need to include the bending stiffness of the chain in order to penalise bending. We first consider the discrete model of Kratky and Porod (1949).

1.2.1 Without external force

We first consider the problem in the absence of an external force. We have the following assumptions.

1) The chain has $N + 1$ links.
2) Each link has a fixed length b (b for bond length).
3) The internal energy to bend two links is proportional to the scalar product between their tangents.
4) There are no excluded volume effects.

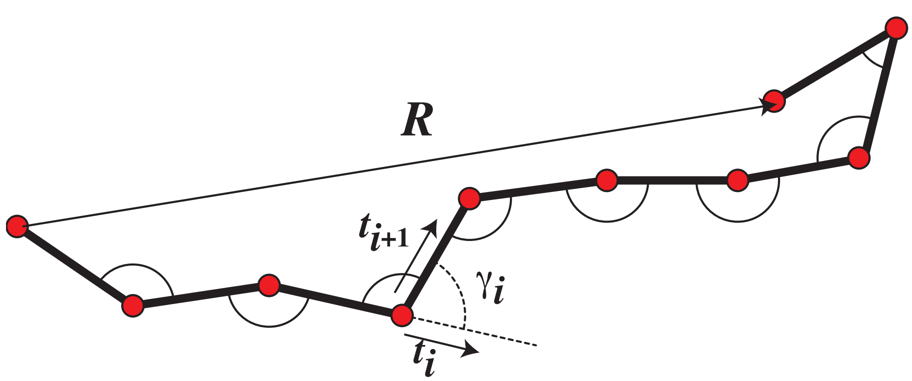

Figure 4: The worm-like chain model. We assume that the chain has a bending stiffness represented by a spring

That is, the internal energy is now

$$Q = -K \sum_{i=1}^{N} \mathbf{t}_i \cdot \mathbf{t}_{i+1} = -K \sum_{i=1}^{N} \cos \gamma_i \tag{14}$$

Note the similarity between this form of the internal energy and the the internal energy for the FJC with external force. Accordingly, following the same steps we have

$$\mathcal{Z} = z^N \quad \text{with} \quad z = 4\pi \frac{\sinh \lambda}{\lambda} \tag{15}$$

where $\lambda = \beta K$.

1.2.2 Root mean square distance

Next, we would like to compute the distance

$$< \mathbf{R}^2 >= b^2 < (\sum \mathbf{t}_i)^2 >= b^2 < \sum_{i,j} \mathbf{t}_i \cdot \mathbf{t}_j > . \tag{16}$$

We define the correlation between neighbours separated by n nodes as

$$\omega_n =< \mathbf{t}_i \cdot \mathbf{t}_{i+n} > . \tag{17}$$

We first evaluate the nearest neighbour correlation

Nearest neighbour correlation: $\omega =< \mathbf{t}_i \cdot \mathbf{t}_{i+1}) >$

and we conclude that

$$\omega_1 = \mathcal{L}(\lambda) \tag{18}$$

Second, we show that

$\omega_n = \omega\omega_{n-1}$

$$\Rightarrow \omega_n = \omega^{|n|} = [\mathcal{L}(\lambda)]^{|n|}\,. \tag{19}$$

We can now return to the computation of the mean square end-to-end distance, $< \mathbf{R}^2 >$

Mean square of the end-to-end distance

and conclude that for large N, we have

$$< \mathbf{R}^2 > \approx b^2 \frac{1+\omega_1}{1-\omega_1} N \tag{20}$$

1.2.3 Persistence length

Here we consider the limit of stiff polymers, i.e. $\lambda \gg 1$, and derive a useful approximation for the tangent-tangent correlations.

For stiff polymers, $\lambda \gg 1$:

and we conclude

$$< \mathbf{t}_i \cdot \mathbf{t}_{i+n} > \sim \exp(-|n|\frac{b}{\xi_P}) \tag{21}$$

In the last expression we have defined a fundamental quantity for the mechanics of chains, the *persistence length*

$$\xi_P = \beta b K. \tag{22}$$

The persistence length is the characteristic length for which tangent-tangent correlations decay. If L is the contour length, we have the following possibilities

- $\xi_P \gg L$: The chain is very stiff.
- $\xi_P \ll L$: The chain is very flexible (low bending stiffness or high temperature, well captured by the FJC model).
- $\xi_P \approx L$: The chain is semi-flexible.

Examples from cellular filaments are given in Table 1.

1.2.4 Continuous limit

We would like to relate the discrete problem to a continuous formulation of the curve and the energy. We know from classical elasticity that the elastic energy of an unshearable, inextensible beam is

$$\mathcal{E}_{el} = \frac{EI}{2} \int_0^L \kappa^2(s) ds \tag{23}$$

Table 1: Persistence lengths and other parameters of various biopolymers (Howard 2001; Gittes *et al.* 1993).

Type	Approximate diameter	Persistence length	Contour length
DNA	2 nm	50 nm	$\lesssim$ 1 m
F-actin	7 nm	17 μm	$\lesssim$ 50 μm
Microtubule	25 nm	$\sim$ 1-5 mm	10s of μm

where κ is the *curvature*, s the *arc length* of the curve, E the *Young modulus* and I the *second moment of area* (for a circular cross-section of radius r it is given by $I = \pi r^4/4$). The product $B = EI$ is the *bending stiffness*, that is it takes a moment $M = B\kappa$ to bend a beam to a section of a ring of curvature κ. Note also that

$$|\kappa| = \left|\frac{\partial \mathbf{t}}{\partial s}\right| . \tag{24}$$

In comparing the elastic energy $\mathcal{E}_{el}$ of the continuous curve with the internal energy E of the worm-like chain we notice that the minimum of the discrete chain is at $E = -K$ whereas the minimum energy of the curve is at 0. Therefore, we shift the potential of the discrete chain so that the two minimum values of the energy coincide. That is, we define

$$U = E + E_0 = -K \sum_{i=1}^{N} \left(\mathbf{t}_i \cdot \mathbf{t}_{i+1} - 1\right) . \tag{25}$$

Next, we take the limit $N \to \infty$, $b \to 0$ while keeping the contour length Nb constant.

Continuous limit of the chain

So that we can identify $B = Kb$ and the persistence length is

$$\xi_P = B\beta = B/(k_b T), \tag{26}$$

The last expression can be used to define a bending stiffness for a semi-flexible filament as $B = \xi_P/\beta$.

For the continuous problem, we can write the Hamiltonian

$$H = \frac{B}{2}\int_0^L \left(\frac{\partial \mathbf{t}}{\partial s}\right)^2 ds, \tag{27}$$

for which we can write the (formal) partition function in terms of the functional integral

$$\mathcal{Z} = \int \mathcal{D}[\mathbf{t}(s)] e^{-\beta H[\mathbf{t}(s)]} \delta(|\mathbf{t}(s)| - 1). \tag{28}$$

A proper definition of this integral is out of the scope of these lectures. The interesting aspect of a continuous formulation is that we can compute the tangent-tangent correlation given by

$$< \mathbf{t}(s) \cdot \mathbf{t}(s') > \propto e^{-|s-s'|/\xi_P} \tag{29}$$

As an example, we compute in this context the end-to-end distance

End-to-end distance

and conclude that

$$< \mathbf{R}^2 >= L^2 f_D(L/\xi_P) \tag{30}$$

where $f_D(x) = 2x^{-2}(x - 1 + e^{-x})$ is the Debye function.

2 Continuous filaments

When stochastic motion can be ignored, that is when the elastic energy of the rod is much larger than the typical energy provided by the thermal bath k_bT (low temperature, high bending stiffness, or large forces), a theory of elastic rods can be used to model many different behaviours of bio-filaments (coiling, super-coiling, twisting, buckling,....).

Here we develop a general theory of shearable, extensible, hyperelastic rods. Then, we consider the appropriate reductions that lead to reduced theories (inextensible rods, planar elastica, beam theory).

2.0.1 Frenet frame

We define a dynamical *space curve* $\mathbf{r}(S,T)$ as a smooth function of a material parameter S and the time T, *i.e.* $\mathbf{r} : \mathbb{R}^2 \to \mathbb{R}^3$. At any time t the arc length s is defined as

$$s = \int_0^S d\sigma \left| \frac{\partial \mathbf{r}(\sigma, T)}{\partial \sigma} \right|. \tag{31}$$

The unit tangent vector $\boldsymbol{\tau}$ to the space curve, $\mathbf{r}$, is

$$\boldsymbol{\tau} = \frac{\partial \mathbf{r}}{\partial s}, \tag{32}$$

and we can construct the standard *Frenet frame* (or *Frenet-Serret frame*) of tangent, $\boldsymbol{\tau}$, normal, $\boldsymbol{\nu}$, and binormal, $\boldsymbol{\beta}$, vectors which form a right-handed orthonormal basis on $\mathbf{r}$. Along the curve, this triad moves as a function of arc length according to the *Frenet equations*:

$$\frac{\partial \boldsymbol{\tau}}{\partial s} = \kappa\, \boldsymbol{\nu}, \tag{33}$$

$$\frac{\partial \boldsymbol{\nu}}{\partial s} = \tau\, \boldsymbol{\beta} - \kappa\, \boldsymbol{\tau}, \tag{34}$$

$$\frac{\partial \boldsymbol{\beta}}{\partial s} = -\tau\, \boldsymbol{\nu}. \tag{35}$$

where the *curvature*

$$\kappa = \left| \frac{\partial \boldsymbol{\tau}}{\partial s} \right|, \tag{36}$$

measures the turning rate of the tangent along the curve and is geometrically given by the inverse of the radius of the best fitting circle at a given point. The *torsion* τ measures the rotation of the Frenet triad around the tangent $\boldsymbol{\tau}$ as a function of arc length and is related to the non-planarity of the curve. If the curvature and torsion are known for all s, the triad $(\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau})$ can be obtained as the unique solution of the Frenet-Serret equations up to a translation and rotation of the curve. The space curve $\mathbf{r}$ is obtained by integrating the tangent vector $\mathbf{t}$, using (32).

2.0.2 General frames

In order to study the motion of elastic filamentary structures that can sustain bending and stretching but also twisting and shearing, we need to generalise the notion of space curves to geometric rods. A *general frame* for a given curve is a frame (a set of three linearly independent vectors) defined at each point along the curve that is orthornormal.

A geometric *rod* is defined by its centerline $\mathbf{r}(S, T)$ where T is time and S is a material parameter taken to be the arc length in a stress free configuration ($0 \leq S \leq L$) and two orthonormal vector fields $\mathbf{d}_1(S, T)$, $\mathbf{d}_2(S, T)$ representing the orientation of a material cross section at s. Together $\mathbf{d}_1(S, T)$, $\mathbf{d}_2(S, T)$ and the vector $\mathbf{d}_3(S, T) \equiv \mathbf{d}_1(S, T) \times \mathbf{d}_2(S, T)$ form a general frame. The

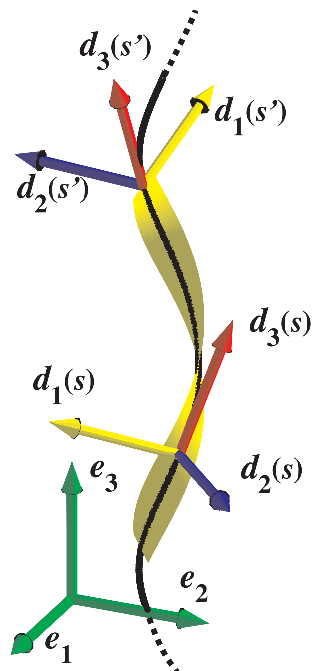

Figure 5: The director basis represents the evolution of a local basis along the rod.

components of a vector $\mathbf{a} = \mathsf{a}_1\mathbf{d_1} + \mathsf{a}_2\mathbf{d_2} + \mathsf{a}_3\mathbf{d_3}$ in the local basis are denoted by $\mathbf{a} = (\mathsf{a}_1, \mathsf{a}_2, \mathsf{a}_3)$.[1] To understand the mathematical structure of the system, it is convenient to introduce a matrix describing the basis

$$\mathbf{D} = \begin{pmatrix} \mathbf{d}_1 & \mathbf{d}_2 & \mathbf{d}_3 \end{pmatrix}, \tag{37}$$

so that $\mathbf{a} = \mathbf{D}\mathsf{a}$. We can now compute the derivative of the frame (w.r.t S or T)

[1] We use the sans-serif fonts to denote the components of a vector in the local basis.

Derivative of the frame

Thus there are antisymmetric matrices (the *twist matrix* $\mathbf{U}(S,T)$ and the *spin matrix* $\mathbf{W}(S,T)$) such that

$$\frac{\partial \mathbf{D}}{\partial S} \equiv \left(\frac{\partial \mathbf{d}_1}{\partial S} \quad \frac{\partial \mathbf{d}_2}{\partial S} \quad \frac{\partial \mathbf{d}_3}{\partial S} \right) = \mathbf{DU}, \tag{38}$$

$$\frac{\partial \mathbf{D}}{\partial T} \equiv \left(\frac{\partial \mathbf{d}_1}{\partial T} \quad \frac{\partial \mathbf{d}_2}{\partial t} \quad \frac{\partial \mathbf{d}_3}{\partial T} \right) = \mathbf{DW}. \tag{39}$$

The entries of $\mathbf{U}$ and $\mathbf{W}$ are not independent. By differentiating (38) with respect to time and (39) with respect to arc length and then equating their cross-derivatives, we obtain a compatibility relation

$$\frac{\partial \mathbf{U}}{\partial T} - \frac{\partial \mathbf{W}}{\partial S} = [\mathbf{U}, \mathbf{W}]\,, \tag{40}$$

These matrices are associated with the axial vectors u and w respectively,

$$\mathbf{U} = \begin{pmatrix} 0 & -\mathsf{u}_3 & \mathsf{u}_2 \\ \mathsf{u}_3 & 0 & -\mathsf{u}_1 \\ -\mathsf{u}_2 & \mathsf{u}_1 & 0 \end{pmatrix}, \quad \mathbf{W} = \begin{pmatrix} 0 & -\mathsf{w}_3 & \mathsf{w}_2 \\ \mathsf{w}_3 & 0 & -\mathsf{w}_1 \\ -\mathsf{w}_2 & \mathsf{w}_1 & 0 \end{pmatrix}. \tag{41}$$

In terms of the vectors $\mathbf{u}$, $\mathbf{w}$, and the basis $\mathbf{d}_i$, $i = 1, 2, 3$, the relations

$$\frac{\partial \mathbf{D}}{\partial S} = \mathbf{D}\mathbf{U}, \quad \frac{\partial \mathbf{D}}{\partial T} = \mathbf{D}\mathbf{W}$$

can be written

$$\frac{\partial \mathbf{d}_i}{\partial S} = \mathbf{u} \times \mathbf{d}_i, \quad \frac{\partial \mathbf{d}_i}{\partial T} = \mathbf{w} \times \mathbf{d}_i, \qquad i = 1, 2, 3,$$

A complete kinematic description is thus given by:

$$\frac{\partial \mathbf{r}}{\partial S} = \mathbf{v}, \tag{42}$$

$$\frac{\partial \mathbf{d}_i}{\partial S} = \mathbf{u} \times \mathbf{d}_i, \qquad i = 1, 2, 3, \tag{43}$$

$$\frac{\partial \mathbf{d}_i}{\partial T} = \mathbf{w} \times \mathbf{d}_i \qquad i = 1, 2, 3, \tag{44}$$

where $\mathbf{u}$, $\mathbf{v}$ are the *strain* vectors and $\mathbf{w}$ is the *spin* vector. Note the orthonormal frame $(\mathbf{d_1}, \mathbf{d_2}, \mathbf{d_3})$ is different from the Frenet-Serret frame (normal,binormal,tangent)=$(\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau})$. While the $(\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau})$ frame is entirely defined by the space curve $\mathbf{r}$, the frame $(\mathbf{d_1}, \mathbf{d_2}, \mathbf{d_3})$ is a *material* frame; it encodes the orientation of the cross-section.

We define the *stretch* by $\alpha = \frac{\partial s}{\partial S}$. The two first components $\mathsf{v}_1, \mathsf{v}_2$ of the *stretch vector* $\mathbf{v}$ represent transverse shearing of the cross-sections while $\mathsf{v}_3 > 0$ is associated with stretching and compression. Since the vectors $\mathbf{d}_i$ are normalized, the norm of $\mathbf{v}$ gives the stretch of the rod during deformation: $\alpha = |\mathbf{v}| = |\mathsf{v}|$. The two first components of the *Darboux vector* are associated with bending while u_3 represents twisting, that is the rotation of the basis (not the curve) around the $\mathbf{d}_3$ vector.

2.0.2.1 The case of inextensible, unshearable rods A particularly important class of rods is obtained by taking $\mathsf{v}_1 = \mathsf{v}_2 = 0,\ \mathsf{v}_3 = 1$. In this case there is no stretch, $s = S$ and $\alpha = 1$, and the possible deformations of rods are restricted so that the vectors spanning the cross sections remain perpendicular to the tangent axis. It will be the geometric constraint used to characterise rods which are both unshearable and inextensible (here we just call *inextensible rods* those rods that are both inextensible and unshearable). Geometrically, the vectors $(\mathbf{d_1}, \mathbf{d_2})$ lie in the normal plane to the tangent axis and are related to the normal and binormal vectors by a rotation through the *register angle* φ,

$$\mathbf{d}_1 = \boldsymbol{\nu} \cos\varphi + \boldsymbol{\beta} \sin\varphi, \tag{45}$$

$$\mathbf{d}_2 = -\boldsymbol{\nu} \sin\varphi + \boldsymbol{\beta} \cos\varphi. \tag{46}$$

This rotation implies that

$$\mathbf{u} = (\kappa \sin\varphi, \kappa \cos\varphi, \tau + \frac{\partial \varphi}{\partial S}) \tag{47}$$

where κ and τ are the usual *Frenet curvature and torsion*. These relations can also be inverted to yield φ, κ and τ as functions of the twist vector components:

$$\cot\varphi = \frac{\mathsf{u}_2}{\mathsf{u}_1}, \tag{48}$$

$$\kappa = \sqrt{\mathsf{u}_1^2 + \mathsf{u}_2^2}, \tag{49}$$

$$\tau = \mathsf{u}_3 + \frac{\mathsf{u}_2'\mathsf{u}_1 - \mathsf{u}_1'\mathsf{u}_2}{\mathsf{u}_1^2 + \mathsf{u}_2^2}. \tag{50}$$

The quantities τ, $\frac{\partial\varphi}{\partial S}$ and u_3 play related but distinct roles. The torsion τ is a property of the curve alone and is a measure of its non-planarity. Hence a curve with null torsion is a plane curve, and any two rods having the same curvature and torsion for all s and t have the same space curve $\mathbf{r}$ as axis, and can only be distinguished by the orientation of the local basis. The quantity $\frac{\partial\varphi}{\partial S}$, *the excess twist*, is a property that is independent of the centreline. It represents the rotation of the local basis with respect to the Frenet frame as the arc length increases. An untwisted rod, characterized by $\frac{\partial\varphi}{\partial S} = 0$ is therefore called a *Frenet rod*. In a Frenet rod, the angle φ between the binormal $\mathbf{b}$ and the vector field $\mathbf{d}_2$ is constant, hence the binormal is representative of the orientation of the local basis $(\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3)$. The twist density, u_3, is a property of both the space curve and the rod, measuring the total rotation (as can be seen from the third component of (47)) of the local basis around the space curve as the arc length increases.

2.0.3 The mechanics of Kirchhoff rods

The stress acting on the cross section at $\mathbf{r}(S)$ from the part of the rod with $S' > S$ gives rise to a resultant force $\mathbf{n}(S,T)$ and resultant moment $\mathbf{m}(S,T)$ attached to the central curve. By applying the balance of linear and angular momenta one obtains

$$\frac{\partial\mathbf{n}}{\partial S} + \mathbf{f} = \rho A \frac{\partial^2\mathbf{r}}{\partial T^2}, \tag{51}$$

$$\frac{\partial\mathbf{m}}{\partial S} + \frac{\partial\mathbf{r}}{\partial S} \times \mathbf{n} + \mathbf{l} = \rho\left(I_2\mathbf{d_1} \times \frac{\partial^2\mathbf{d}_1}{\partial T^2} + I_1\mathbf{d_2} \times \frac{\partial^2\mathbf{d}_2}{\partial T^2}\right), \tag{52}$$

where $\mathbf{f}(S,T)$ and $\mathbf{l}(S,T)$ are the body force and couple per unit reference length applied on the cross section at S. These body forces and couple can be used to model different effects such as short and long range interactions between different parts of the rod or can be the result of active stress, self-contact, or contact with another body. $A(S)$ is the cross-section area (in the reference frame), $\rho(S)$ the mass density (mass per unit reference volume), and $I_{1,2}(S)$ are the second moments of area of the cross section corresponding to the directions $\mathbf{d}_{1,2}$ at a material point S. Explicitly, they read

$$I_1 = \int_{\mathcal{S}} x_2^2 \, dx_1 dx_2 \ , \quad I_2 = \int_{\mathcal{S}} x_1^2 \, dx_1 dx_2. \tag{53}$$

where $\mathcal{S}$ is the section at point S and a point on this section is given by a pair $\{x_1, x_2\}$ and located at $\mathbf{r}(S) + x_1\mathbf{d}_1(S) + x_2\mathbf{d}_2(S)$.

To close the system, we assume that the resultant stresses are related to the strains via given constitutive laws.

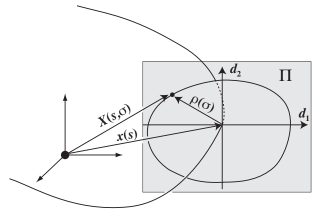

Figure 6: Cross-section of a rod and local coordinates

2.0.4 Constitutive laws

In a shearable rod, the cross-sections are not necessarily orthogonal to the tangent to the centreline. In this course, we will restrict to shearable rods, for which we can align $\mathbf{d}_3 = \boldsymbol{\tau}$.

2.0.4.1 Extensible rods Since the arclength is not fixed in an extensible rod, i.e. the material may be stretched or compressed in the direction of the tangent, we require a constitutive law that relates the degree of stretch, characterised by

$$\alpha = \frac{\partial s}{\partial S}$$

to the axial component of $\mathbf{n}$, i.e. a constitutive law of the form

$$\mathsf{n}_3 = f(\alpha - 1), \tag{54}$$

where the function f should satisfy $f(0) = 0$. In the simplest case of a Hookean law, we would take f to be linear:

$$\mathsf{n}_3 = EA(\alpha - 1),$$

where E is the Youngs modulus, and A the cross-sectional area, so that EA captures the stretching stiffness.

To close the system, we also require a constitutive law relating the moment to the curvature. The most common form, which we will exclusively use in this course, is the linear relation

$$\mathbf{m} = EI_1(\mathsf{u}_1 - \hat{\mathsf{u}}_1)\mathbf{d}_1 + EI_2(\mathsf{u}_2 - \hat{\mathsf{u}}_2)\mathbf{d}_2 + \mu J(\mathsf{u}_3 - \hat{\mathsf{u}}_3)\mathbf{d}_3 \tag{55}$$

where E is the Young's modulus, μ is the shear modulus, J is a parameter that depends on the cross-section shape and and I_1 and I_2 are the second moments of area given by (53). Also, $\hat{\mathbf{u}} = \hat{\mathsf{u}}_1\mathbf{d}_1 + \hat{\mathsf{u}}_2\mathbf{d}_2 + \hat{\mathsf{u}}_3\mathbf{d}_3$ is the *intrinsic curvature*. That is, this defines the reference shape of the rod, in the absence of any loads or boundary constraints. Note that if the rod is straight in its reference shape, we have simply that $\hat{\mathbf{u}} = \mathbf{0}$.

The relation (62) comes from the analysis of bending and twisting of cylinders in the general 3D theory of linear elasticity. Note that for a rod with uniform circular cross section of radius R, the stiffness parameters are:

$$I_1 = I_2 = \frac{J}{2} = \frac{\pi R^4}{4}. \tag{56}$$

The products $EI_1 \equiv K_1$ and $EI_2 \equiv K_2$ are the *principal bending stiffnesses* of the rod, and $\mu J \equiv K_3$ is the *torsional stiffness.*

For our purposes, it is useful to observe that any deviation from the stress free, 'desired' curvature produces a moment, and that this is decomposed into bending components about each of the three axes $\mathbf{d}_i$.

2.0.4.2 Inextensible rods In the case of an inextensible rod, we still require the constitutive relation (62). Except that since stretch along the arclength is not permitted, material parameter $S = s$ becomes the arc length, i.e. $\alpha \equiv 1$ by assumption, and this geometric constraint replaces the constitutive law (54).

2.0.5 The basic Kirchhoff rods

The most commonly used model of rod is obtained by assuming that the rod is unshearable, inextensible as detailed in Section 2.0.4.2 with a circular cross-section ($I_1 = I_2 = I$). In this case, we have the following set of equations provided by

1) Kinematics

$$\mathbf{r}' = \mathbf{d}_3 \tag{57}$$

$$\frac{\partial \mathbf{d}_i}{\partial S} = \mathbf{u} \times \mathbf{d}_i, \tag{58}$$

$$\frac{\partial \mathbf{d}_i}{\partial T} = \mathbf{w} \times \mathbf{d}_i \tag{59}$$

2) Mechanics

$$\frac{\partial \mathbf{n}}{\partial S} + \mathbf{f} = \rho A \frac{\partial^2 \mathbf{r}}{\partial t^2}, \tag{60}$$

$$\frac{\partial \mathbf{m}}{\partial S} + \frac{\partial \mathbf{r}}{\partial S} \times \mathbf{n} + \mathbf{l} = \rho I \left(\mathbf{d_1} \times \frac{\partial^2 \mathbf{d}_1}{\partial t^2} + \mathbf{d_2} \times \frac{\partial^2 \mathbf{d}_2}{\partial t^2} \right), \tag{61}$$

3) Constitutive theory

$$\mathbf{m} = EI\left[\mathsf{u}_1 \mathbf{d}_1 + (\mathsf{u}_2 - \hat{\mathsf{u}}_2)\mathbf{d}_2\right] + \mu J(\mathsf{u}_3 - \hat{\mathsf{u}}_3)\mathbf{d}_3, \qquad I = \frac{J}{2} = \frac{\pi R^4}{4}. \tag{62}$$

A few comments are in order

1) The material is described by its response through two bending and twisting stiffnesses EI and μJ, its density ρ and by its geometry (radius R, stress-free curvature $\hat{\mathsf{u}}_2$ and twist $\hat{\mathsf{u}}_3$, length L).

2) One can always choose the orientation of the director basis so that $\hat{\mathsf{u}}_1 \equiv 0$.

3) The system is characterised by three coordinates $\mathbf{r}$, three curvatures $\mathbf{u}$, three spins $\mathbf{w}$, three resultant forces $\mathbf{n}$, and three resultant moments $\mathbf{m}$. That is, 15 variables. The last 3 sets of equations provide 9 equations. The first one provide another 3. The second and third equations provide only three independent relationships. They are really both a set of 9 equations for the elements of $\mathbf{D}$ but written in a suitable set of coordinates, say the Euler angles, they provide only each three independent relationships. Further, these two sets are not independent as they are connected to each other by the compatibility condition (40).

4) One of the practical problems of rod theory is that the mechanical balance is easily written in terms of an external basis, whereas the constitutive law is written in the local basis.

5) In a given problem, one can usually solve the equations in components of either the local basis or an external fixed basis, then compute the curvatures, then integrate the curvatures to obtain the local basis and the shape of the rod. Doing so, one can often decouple the problem into problems of smaller dimensions.

6) The body force $\mathbf{f}$ and body couple $\mathbf{l}$ are given based on the physics of the problem (gravity, magnetic forces, electrical forces, self-contact,...). Body couples can also occur, for instance for the effect of internal molecular motors on motile filaments such as cilia and flagella.

7) The rotary inertia term (R.H.S. of (61)) is often ignored based on a discussion and analysis of typical time scales.

8) A rod is said to be *initially straight* if the unstressed curvatures vanish identically $\hat{\mathbf{u}} = \mathbf{0}$.

2.0.6 The Planar elastica: Bernoulli-Euler equations

We now consider a reduction of the three-dimensional basic rod above. We assume that the rod is planar, unshearable and inextensible, has a circular cross-section, is naturally straight and that there is no body force or couple. Therefore, it has no torsion. We further assume that it has no twist, so that

$$\mathbf{u} = (0, \kappa, 0). \tag{63}$$

A convenient representation of the rod is obtained by assuming that it lies in the $x - y$ plane and introducing the angle θ between the tangent vector and the x-axis. That is

$$\boldsymbol{\tau} = \mathbf{d}_3 = \cos\theta \mathbf{e}_x + \sin\theta \mathbf{e}_y, \tag{64}$$

Reduction

So that

$$F' = \rho A \ddot{x} \tag{65}$$

$$G' = \rho A \ddot{y} \tag{66}$$

$$EI\theta'' + G\cos\theta - F\sin\theta = \rho I \ddot{\theta} \tag{67}$$

This is now a set of three equations for three unknowns.

2.0.6.1 Static solutions We first consider the static case. Therefore $\ddot{x} = \ddot{y} = 0$ and $\ddot{\theta} = 0$ and we conclude that F and G are constant and therefore $\mathbf{n}$ is a constant vector. WLOG, we choose $\mathbf{e}_x$ to be along this constant force so that $G = 0$ and

$$EI\theta'' - F\sin\theta = 0 \tag{68}$$

or

$$\theta'' + \alpha^2 \sin\theta = 0 \tag{69}$$

where $\alpha^2 = -F/EI$ is positive if $F < 0$, that is if the force is compressive. We recognise at this point the equation for the pendulum (in which $\alpha^2 = g/l$, gravity acceleration divided by length of the bob). Therefore, any solution of the pendulum in time is a solution of the elastica in space (with appropriate boundary value), a fact already known by Euler (see Fig.7).

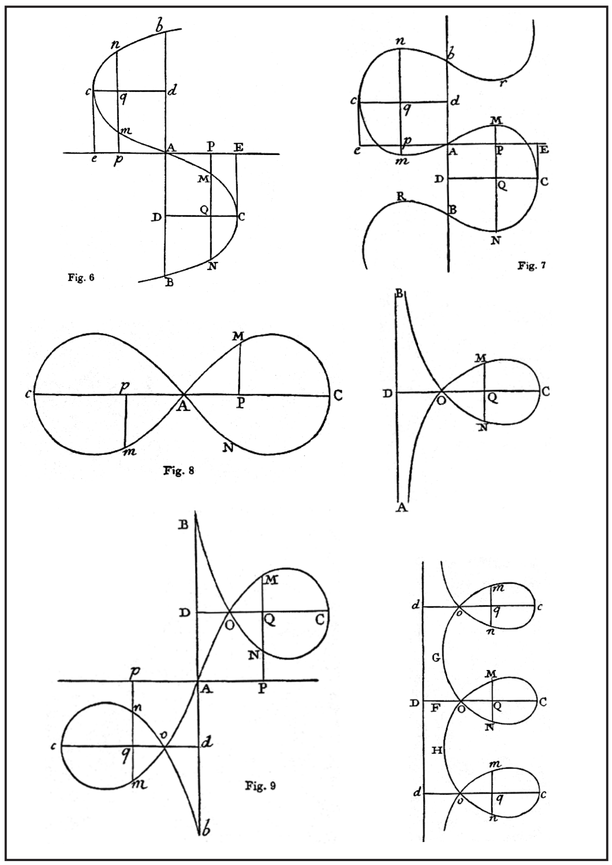

Figure 7: Euler's Drawing of spatial equilibria of the elastica.

Rather than writing the general solution for the problem (in terms of elliptic functions), we can look at appropriate limits. For instance, we can look at the simple case where the rod is compressed and pinned-pinned (see Fig.8) so that there is no curvature at either ends.

Buckling problem

That is, the critical buckling force is

$$F_c = EI\frac{n^2\pi^2}{L^2} \tag{70}$$

For $n = 1$, we recognise the classical Euler buckling criterion, a fundamental concept in many scientific fields.

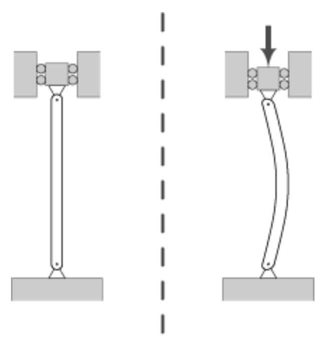

Figure 8: Buckling of a planar compressed pinned-pinned rod.

2.0.7 From elastica to beams

We consider again the elastica

$$EI\theta'' + G\cos\theta - F\sin\theta = \rho I\ddot{\theta} \tag{71}$$

and assume that θ is small so that there is only a small deflection $x \sim s$ and the curve can be written $y = w(x)$ with

$$w'(x) = \theta \tag{72}$$

so that, to first order, we have

$$EIw''' + G - Fw' = \rho I\ddot{w}' \tag{73}$$

an extra x-derivative leads to

$$EIw'''' + \rho A\ddot{w} - Fw'' = \rho I\ddot{w}'' \tag{74}$$

In the static case, we have the classical beam equation

$$EIw'''' - Fw'' = 0 \tag{75}$$

Note that the beam equation that we have derived is slightly different from the classical Timoshenko beam equation obtained under a different asymptotic limit and reads

$$EIw'''' + \rho A\ddot{w} - Fw'' + \rho g = 0 \tag{76}$$

the ρg term is just the added effect of a body force due to gravity (in the y-direction). The difference is in the extra time-derivative that depends on the rotary inertia of the cross-sections (which can be ignored in many applications).