DNA Modelling Course
Exercise Session 3
Summer 2006 Part 1

SOLUTIONS

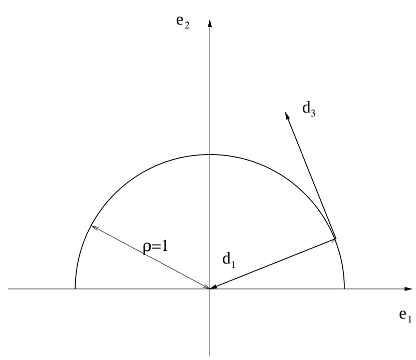
1 Configurations and Equilibria of an Extensible Shearable Rod

Kinematics

1.(a) Either by direct calculation, or by observation from the sketch of the configuration, one has

$$\left\{ \begin{array}{c} v_1 \\ v_2 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \\ 1+\epsilon \end{array} \right\} \quad \text{and} \quad \left\{ \begin{array}{c} u_1 \\ u_2 \\ u_3 \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 1 \\ 0 \end{array} \right\} \tag{1.1}$$

where $v_i = \boldsymbol{v} \cdot \boldsymbol{d}_i$ and $u_i = \boldsymbol{u} \cdot \boldsymbol{d}_i$.



(b) In this case there are essentially two possibilities to compute the Euler parameters. For the direct computation we refer to the solution of Exercise 2 (Helical curves)(d). We will then obtain the result in exactly the same way as carried out there, where $\boldsymbol{Q}$ is now given by

$\boldsymbol{Q} = [\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3]$: For $(q_1, q_2, q_3)^T \in \ker(\boldsymbol{Q} - \boldsymbol{Q}^T) = \mathrm{span}\{((\cos(s) - 1)/\sin(s), 1, 1)^T\}$ we get

$$\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = C \begin{pmatrix} \cos(s) - 1 \\ \sin(s) \\ \sin(s) \end{pmatrix}, \tag{1.2}$$

$$C^2 = \frac{3 + \cos(s)}{4(3 - 2\cos(s) - \cos^2(s))},$$

and for q_4 we have the relation

$$q_4^2 = \frac{1 - \cos(s)}{4}.$$

We now have determined q_4 and (q_1, q_2, q_3) up to the signs. The sign of q_4 can be chosen free but the choice will then fix the sign of (q_1, q_2, q_3) due to $\boldsymbol{d}_i(\boldsymbol{q}) = \boldsymbol{d}_i(-\boldsymbol{q})$.

We could equivalently compute a unit axis of rotation $\boldsymbol{k} = (k_1, k_2, k_3)^T$ and the corresponding rotation angle ϕ in order to express $\boldsymbol{q}$ which is then given by

$$q_i = k_i \sin(\phi/2), \qquad i = 1, 2, 3, \qquad q_4 = \cos(\phi/2).$$

But $\boldsymbol{k}$ is given by normalizing the vector on the RHS of (1.2). Therefore

$$\boldsymbol{k} = \frac{1}{\sqrt{(1 - \cos(s))^2 + 2\sin^2(s)}} \begin{pmatrix} \cos(s) - 1 \\ \sin(s) \\ \sin(s) \end{pmatrix}. \tag{1.3}$$

The angle ϕ is computed by using the identity $1 + 2\cos\phi = \mathrm{tr}(\boldsymbol{Q})$ which immediately provides us with

$$\phi = \pm \arccos(-1/2(1 + \cos(s))).$$

The correct sign is simply obtained by verifying the results. In so doing, we take $s = \pi/2$ and verify the result for the third component of $\boldsymbol{d}_2(\boldsymbol{q}(s))$. We then obtain that ϕ must be given by $\phi = -\arccos(-1/2(1 + \cos(s)))$. Note that the wrong sign will provide us with the rotation matrix $\boldsymbol{Q}^{-1}$ instead of $\boldsymbol{Q}$. We could also choose $-\boldsymbol{k}$ for the axis of rotation where the corresponding angle then is $-\phi$. This is due to

$$\begin{aligned} q_i &= -k_i \sin(-\phi/2) = k_i \sin(\phi/2), \qquad i = 1, 2, 3, \\ q_4 &= \cos(-\phi/2) = \cos(\phi/2). \end{aligned}$$

Second possibility: Composition of Rotation Matrices We only sketch the idea of the method which is based on the following: Suppose that the rotation matrix $\boldsymbol{Q} = [\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3]$ with rotation axis $\boldsymbol{k}$ and rotation angle ϕ is composed by two rotation matrices $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$, that is,

$$\boldsymbol{Q}(\boldsymbol{k}, \phi) = \boldsymbol{Q}_2(\boldsymbol{k}_2, \phi_2)\, \boldsymbol{Q}_1(\boldsymbol{k}_1, \phi_1), \tag{1.4}$$

where the expression in the brackets denote the corresponding (unique) rotation axis and rotation angle, i.e., $\boldsymbol{Q}_i$, $i = 1, 2$ represents rotation around the axis $\boldsymbol{k}_i$ with angle ϕ_i. It is shown in a paper of DICHMANN[1] that a straightforward calculation then leads to expressions for $\boldsymbol{k}$ and ϕ if $\boldsymbol{k}_i, \phi_i$ for $i = 1, 2$ are known.

We restrict to the computation of $\boldsymbol{Q}_i$ and $\boldsymbol{k}_i$, ϕ_i for $i = 1, 2$ here. For the computation of $\boldsymbol{k}$ and ϕ by means of $\boldsymbol{k}_i, i = 1, 2$ and $\phi_i, i = 1, 2$ we refer to the article of DICHMANN. A careful inspection of the directors frame $\{\boldsymbol{d}_i(s)\}$ reveals that we basically have two reasonable possibilities to define a composition of rotation matrices. The key step is the definition of a rotation matrix $\boldsymbol{P}$ that gives a permutation of the fixed basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ such that $\boldsymbol{e}_2$ is mapped to $\boldsymbol{e}_3$. These assumptions immediately lead to

$$\boldsymbol{P} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Now, we can either choose $\boldsymbol{P} = \boldsymbol{Q}_1$ or $\boldsymbol{P} = \boldsymbol{Q}_2$ in order to obtain the decomposition (1.4), for $\boldsymbol{Q}\boldsymbol{P}^{-1}$ as well as $\boldsymbol{P}^{-1}\boldsymbol{Q}$ are rotation matrices. Explicitly:

$$\boldsymbol{Q}(\boldsymbol{k}, \phi) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -\sin(s) & 0 & \cos(s) \\ 0 & 1 & 0 \\ -\cos(s) & 0 & -\sin(s) \end{pmatrix}, \tag{1.5}$$

$$\boldsymbol{Q}(\boldsymbol{k}, \phi) = \underbrace{\begin{pmatrix} -\sin(s) & -\cos(s) & 0 \\ \cos(s) & -\sin(s) & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{=\boldsymbol{Q}\boldsymbol{P}^{-1} =: \boldsymbol{R}(\boldsymbol{k}_1, \phi_1)} \underbrace{\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}}_{\boldsymbol{P}(\boldsymbol{k}_2, \phi_2)}. \tag{1.6}$$

[1] Donald J. Dichmann, Notes on the Mecjanics of Rigid Body Rotations, Quaternions and some Associated Mathematics

We will restrict to the second equality (1.6) and state the rotation axes $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ as well as the rotation angles ϕ_1 and ϕ_2 corresponding to $\boldsymbol{R} = \boldsymbol{Q}\boldsymbol{P}^{-1}$ and $\boldsymbol{P}$.

Rotation axis and angle of $\boldsymbol{P}$: It is easy to see that $\boldsymbol{P}\mathbf{1} = \mathbf{1}$ where $\mathbf{1}$ denotes the vector where every component is 1. Therefore, we have

$$\boldsymbol{k}_1 = \frac{1}{\sqrt{3}}\mathbf{1}.$$

The angle of rotation will then be given by

$$\mathrm{tr}(\boldsymbol{P}) = 1 + 2\cos\phi_1 = 0 \qquad \Rightarrow \qquad \phi_1 = \pm\arccos(-1/2).$$

Verifying the results we easily obtain $\phi_1 = \arccos(-1/2)$.

Rotation axis and angle of $\boldsymbol{R}$: We immediately obtain $\boldsymbol{R}(0,0,1)^T = (0,0,1)^T$ such that

$$\boldsymbol{k}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and the angle ϕ_2 is given by

$$\mathrm{tr}(\boldsymbol{R}) = 1+2\cos\phi_2 = 1-2\sin(s) \qquad \Rightarrow \qquad \phi_2 = \pm\arccos(-\sin(s)).$$

Verifying the results we easily obtain $\phi_2 = \arccos(-\sin(s))$.

Balance laws

2.(a) For the natural configuration $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{d}}_i\}$ we find

$$\begin{pmatrix} \hat{v}_1 \\ \hat{v}_2 \\ \hat{v}_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \hat{u}_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

where $\hat{v}_i = \hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{d}}_i$ and $\hat{u}_i = \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{d}}_i$. Using the results from 1.(a) we then obtain

$$\begin{aligned} \boldsymbol{n}(s) &= \epsilon G_3 \boldsymbol{d}_3(s), \\ \boldsymbol{m}(s) &= K_2 \boldsymbol{d}_2(s). \end{aligned}$$

(b) Assuming $\boldsymbol{\tau} \equiv \mathbf{0}$, a configuration $\{\boldsymbol{r}, \boldsymbol{d}_i\}$ is an equilibrium (with $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{d}}_i\}$ serving as the reference) if

$$\boldsymbol{n}' = -\boldsymbol{f} \quad \text{and} \quad \boldsymbol{m}' + \boldsymbol{r}' \times \boldsymbol{n} = 0, \qquad \text{for all } s \in (0, \pi).$$

One can easily verify that the configuration is an equilibrium for the radial force

$$\boldsymbol{f}(s) \;=\; -\epsilon\, G_3 \boldsymbol{d}_1(s).$$

Moreover, the endforce $\boldsymbol{g}$ and the end moment $\boldsymbol{h}$ at $s = 0, \pi$ required to maintain this equilibrium are

$$\begin{aligned} \boldsymbol{g}(0) &= -\boldsymbol{n}(0) = -\epsilon\, G_3 \boldsymbol{e}_2, &\quad \boldsymbol{g}(\pi) &= \boldsymbol{n}(\pi) = -\epsilon\, G_3 \boldsymbol{e}_2 \\ \boldsymbol{h}(0) &= -\boldsymbol{m}(0) = -K_2 \boldsymbol{e}_3, &\quad \boldsymbol{h}(\pi) &= \boldsymbol{m}(\pi) = -K_2 \boldsymbol{e}_3. \end{aligned}$$

2 Helical curves

(a) By definition arclength s is such that

$$\left| \frac{d\boldsymbol{r}(s)}{ds} \right| = 1 \tag{2.1}$$

so clearly the parameter t is not arc-length, as

$$\left| \frac{d\boldsymbol{r}(t)}{dt} \right| = \sqrt{R^2 + P^2}. \tag{2.2}$$

Using the chain rule

$$\frac{d\boldsymbol{r}}{dt} = \frac{d\boldsymbol{r}}{ds}\frac{ds}{dt}, \tag{2.3}$$

and solving the resulting differential equation

$$\left| \frac{ds}{dt} \right| = \sqrt{R^2 + P^2}, \tag{2.4}$$

we easily get that s arc-length is

$$s = \sqrt{R^2 + P^2}\, t, \tag{2.5}$$

where the constant of integration is chosen such that $s = 0$ corresponds to $t = 0$. Finally we then have the new arclength parametrization which reads

$$\boldsymbol{r}(s) = \left(R\, \cos \frac{s}{\alpha}, R\, \sin \frac{s}{\alpha}, P\, \frac{s}{\alpha} \right) \tag{2.6}$$

where $\alpha = \sqrt{R^2 + P^2}$. Note that in general,

$$s(t) = \int_0^t \frac{dr}{dt}(\tau)\, d\tau, \tag{2.7}$$

but that in this example the quadrature can be carried out explicitly to obtain (2.5) because $\sqrt{R^2 + P^2}$ is a constant along the helix.

(b) The Frenet-Serret frame is an intrinsic framing, given by the tangent $\boldsymbol{T}(s)$ to the curveline $\boldsymbol{r}(s)$, the principal normal $\boldsymbol{N}(s)$ defined via $\boldsymbol{T}'(s)$, and the binormal $\boldsymbol{B}(s)$. The following equivalences hold

$$\boldsymbol{T}(s) = \frac{d\boldsymbol{r}}{ds} \tag{2.8}$$

$$\boldsymbol{T}'(s) = \frac{d\boldsymbol{T}(s)}{ds} = \kappa(s)\boldsymbol{N}(s) \tag{2.9}$$

where the curvature $\kappa(s)$ is a non negative scalar, and $\boldsymbol{N}(s)$ is the principal normal, which is well defined as soon as $\boldsymbol{T}'(s)$ does not vanish at any s. Then $\boldsymbol{B}(s)$ is found as $\boldsymbol{T}(s)\times\boldsymbol{N}(s)$. The (geometrical) torsion can be extracted from the equations

$$[\boldsymbol{NBT}]' = [\boldsymbol{NBT}]\begin{pmatrix} 0 & -\tau & \kappa \\ \tau & 0 & 0 \\ -\kappa & 0 & 0 \end{pmatrix} \tag{2.10}$$

It is then easy to check that on a helix

$$\boldsymbol{T}(s) = \left(-\frac{R}{\alpha}\sin\frac{s}{\alpha}, \frac{R}{\alpha}\cos\frac{s}{\alpha}, \frac{P}{\alpha}\right) \tag{2.11}$$

$$\boldsymbol{N}(s) = \left(-\cos\frac{s}{\alpha}, -\sin\frac{s}{\alpha}, 0\right) \tag{2.12}$$

$$\boldsymbol{B}(s) = \left(\frac{P}{\alpha}\sin\frac{s}{\alpha}, -\frac{P}{\alpha}\cos\frac{s}{\alpha}, \frac{R}{\alpha}\right), \tag{2.13}$$

and that

$$\kappa = \frac{R}{\alpha^2} \tag{2.14}$$

$$\tau = \frac{P}{\alpha^2} \tag{2.15}$$

(c) By construction of the Frenet equations (2.10), it should be clear that the curvature and the torsion are the only non-vanishing components of the Darboux vector $\boldsymbol{u}$ expressed in the Frenet frame $\{\boldsymbol{N}, \boldsymbol{B}, \boldsymbol{T}\}$, specifically $\boldsymbol{u} = \kappa\boldsymbol{B} + \tau\boldsymbol{t}$, which is true for any curve whatsoever. For the helix after substitution of the previously computed specific forms of κ, $\boldsymbol{B}$, τ, and $\boldsymbol{T}$ we find that $\boldsymbol{u} = \frac{1}{\alpha}\boldsymbol{e}_z$, which is a very special property of the helix resulting from symmetry of rotation about the z-axis.

(d) We first make some remarks.

- The Darboux vector $\boldsymbol{u}$ is the axial vector of a skew matrix $\boldsymbol{S}$, given by
$$\boldsymbol{S} = \boldsymbol{Q}'(s)\boldsymbol{Q}^T(s). \tag{2.16}$$
It represents the infinitesimal change, or 'angular velocity' of the rotation matrix $\boldsymbol{Q}(s)$ along the one-parameter family of rotation matrices parametrized by s. The Darboux vector $\boldsymbol{u}$ has no relation with the axial vector of the skew matrix $\tilde{\mathbf{S}}$
$$\tilde{\mathbf{S}} = \boldsymbol{Q}(s) - \boldsymbol{Q}^T(s), \tag{2.17}$$
defined at each fixed value of s. At each s, $\tilde{\mathbf{S}}(s)$ determines the Euler axis of rotation of the given rotation matrix $\boldsymbol{Q}(s)$ as described in Session 1.
- The quaternion parametrization is particular in the fact it gives immediately the axis of rotation, as the first three components (q_1, q_2, q_3) define this axis up to a constant, i.e. $\boldsymbol{Qk} = \boldsymbol{k}$ if $\boldsymbol{k} = (q_1, q_2, q_3)^T$[2], and the angle of rotation up to a sign as $q_4^2 = \cos^2\theta/2$.

Having said this, we can proceed in finding the quaternion parametrization for $t = \pi$ (note that t is not arc-length!). Bearing in mind that in the Frenet frame $\boldsymbol{Q} = [NBT]$, for $t = \pi$ we have

$$\boldsymbol{Q} - \boldsymbol{Q}^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2R/\alpha \\ 0 & 2R/\alpha & 0 \end{pmatrix} \tag{2.18}$$

Therefore the axial vector of $\boldsymbol{Q} - \boldsymbol{Q}^T$ is some $\boldsymbol{z} = (2R/\alpha, 0, 0)^T$, and since the axis of rotation is a unit vector parallel to $\boldsymbol{z}$, we have that

$$\text{axis of rotation} = \boldsymbol{w} = (1, 0, 0)^T \tag{2.19}$$

so that

$$\boldsymbol{k} = (q_1, q_2, q_3)^T = C\boldsymbol{w} \tag{2.20}$$

where C is a constant. Moreover, still in $t = \pi$,

$$\text{tr}[\boldsymbol{Q}] = 1 + 2\cos\theta = 1 + 2\frac{P}{\alpha} \tag{2.21}$$

[2]The axis of rotation is a unit vector wheras $\boldsymbol{k}$ in general has the norm fixed by the condition $\boldsymbol{q} \cdot \boldsymbol{q} = 1$, so typically it will be $\boldsymbol{k} = \pm \sin\theta/2\boldsymbol{w}$ where $\boldsymbol{w}$ is the axis of rotation, i.e. $||\boldsymbol{w}|| = 1$

which in turn implies

$$q_4^2 = \frac{1 + \frac{P}{\alpha}}{2}. \tag{2.22}$$

Finally then from the normalization condition on $\boldsymbol{q}$, we get

$$C^2 = 1 - q_4^2 = \frac{1 - \frac{P}{\alpha}}{2}. \tag{2.23}$$

Now, we have determined q_4 and $\boldsymbol{k} = (q_1, q_2, q_3)^T$ up to the signs. Recalling that $\boldsymbol{q} = (q_1, q_2, q_3, q_4)^T$ and $-\boldsymbol{q}$ define the same rotation matrix we can choose q_4 to be

$$q_4 = \sqrt{\frac{1 + \frac{P}{\alpha}}{2}} \qquad \text{or} \qquad q_4 = -\sqrt{\frac{1 + \frac{P}{\alpha}}{2}},$$

but the choice of the sign of q_4 will determine the sign of $\boldsymbol{k}$. Thus, let us choose

$$q_4 = \sqrt{\frac{1 + \frac{P}{\alpha}}{2}}.$$

Then, we find that

$$C = -\sqrt{\frac{1 - \frac{P}{\alpha}}{2}},$$

which can be verified by calculating $B(s = \alpha\pi)$ in terms of $\boldsymbol{q}$ and comparing the result[3]to (2.13).

3 Transformation of Cross Products

(a) Consider a vector $\boldsymbol{v} \in^3$. Then we have for any two vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$

$$\boldsymbol{v} \cdot (\boldsymbol{a} \times \boldsymbol{b}) = \det([\boldsymbol{v}, \boldsymbol{a}, \boldsymbol{b}]).$$

[3]For

$$C = \sqrt{\frac{1 - \frac{P}{\alpha}}{2}}$$

we obtain for the third component B_3 of B the expression $B_3 = \frac{-R}{\alpha}$ which contradicts (2.13).

Therefore,

$$\begin{aligned}
\boldsymbol{v} \cdot (\boldsymbol{A}\boldsymbol{a} \times \boldsymbol{A}\boldsymbol{b}) &= \det([\boldsymbol{v}, \boldsymbol{A}\boldsymbol{a}, \boldsymbol{A}\boldsymbol{b}]) \\
&= \det(\boldsymbol{A}[\boldsymbol{A}^{-1}\boldsymbol{v}, \boldsymbol{a}, \boldsymbol{b}]) \\
&= \det(\boldsymbol{A}) \det([\boldsymbol{A}^{-1}\boldsymbol{v}, \boldsymbol{a}, \boldsymbol{b}]) \\
&= \det(\boldsymbol{A}) \, (\boldsymbol{A}^{-1}\boldsymbol{v} \cdot (\boldsymbol{a} \times \boldsymbol{b})) \\
&= \det(\boldsymbol{A})(\boldsymbol{v}\boldsymbol{A}^{-T}(\boldsymbol{a} \times \boldsymbol{b})) \\
&= \boldsymbol{v} \cdot (\det(A)\boldsymbol{A}^{-T}(\boldsymbol{a} \times \boldsymbol{b})).
\end{aligned}$$

This is true for any $\boldsymbol{v} \in I\!R^3$. Therefore,

$$\boldsymbol{A}\boldsymbol{a} \times \boldsymbol{A}\boldsymbol{b} = \det(\boldsymbol{A})\boldsymbol{A}^{-T}(\boldsymbol{a} \times \boldsymbol{b}).$$

(b) For an orthogonal matrix $\boldsymbol{Q} \in \mathrm{SO}(3), \det(\boldsymbol{Q}) = 1$ and $\boldsymbol{Q} = \boldsymbol{Q}^{-T}$.