8 Adapted Framing of a Curve

Given a curve $\mathbf{r}(s)$ and a local frame, $(\mathbf{d_1}(s), \mathbf{d_2}(s), \mathbf{d_3}(s))$, an adapted frame is a right handed frame $(\mathbf{D_1}(s), \mathbf{D_2}(s), \mathbf{D_3}(s))$, determined by a 3-dimensional rotation of the local frame about the vector $\mathbf{d_3}$ by an angle $\varphi(s)$.

$\mathbf{D} = \mathbf{dQ}$ where

$$\mathbf{D} = \begin{bmatrix} \mathbf{D_1} & \mathbf{D_2} & \mathbf{D_3} \end{bmatrix}, \mathbf{d} = \begin{bmatrix} \mathbf{d_1} & \mathbf{d_2} & \mathbf{d_3} \end{bmatrix}$$

and

$$\mathbf{Q} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

We want to determine how the strains transform with the new frame.
We have a strain vector $\mathbf{u}$ which is defined by

$$\mathbf{d}_i' = \mathbf{u} \times \mathbf{d}_i,$$

and we want to relate it to $\mathbf{U}$ which is defined by

$$\mathbf{D}_i' = \mathbf{U} \times \mathbf{D}_i.$$

A straightfoward computation yields

$$\begin{aligned} \mathbf{D_1'} &= \cos\varphi\ \mathbf{d_1'} + \sin\varphi\ \mathbf{d_2'} + (-\sin\varphi\ \mathbf{d_1} + \cos\varphi\ \mathbf{d_2})\varphi' \\ \mathbf{D_2'} &= -\sin\varphi\ \mathbf{d_1'} + \cos\varphi\ \mathbf{d_2'} + (-\cos\varphi\ \mathbf{d_1} - \sin\varphi\ \mathbf{d_2})\varphi' \\ \mathbf{D_3'} &= \mathbf{d_3'} \end{aligned} \tag{8.163}$$

which yields

$$\begin{aligned} \mathbf{D_1'} &= \left(\mathbf{u} \times \mathbf{D_1} + \varphi'\mathbf{D_2}\right) = (\mathbf{u} + \varphi'\mathbf{D_3}) \times \mathbf{D_1} \\ \mathbf{D_2'} &= \left(\mathbf{u} \times \mathbf{D_2} - \varphi'\mathbf{D_1}\right) = (\mathbf{u} + \varphi'\mathbf{D_3}) \times \mathbf{D_2} \\ \mathbf{D_3'} &= (\mathbf{u} \times \mathbf{D_3}) = (\mathbf{u} + \varphi'\mathbf{D_3}) \times \mathbf{D_3} \end{aligned} \tag{8.164}$$

Hence, we deduce that

$$\mathbf{U} = (\mathbf{u} + \varphi'\mathbf{D_3}) = (\mathbf{u} + \varphi'\mathbf{d_3}). \tag{8.165}$$

The relations between the components of $\mathbf{U}$ and those of $\mathbf{u}$ are

$$\begin{aligned} U_1 &= \cos\varphi u_1 + \sin\varphi u_2 \\ U_2 &= -\sin\varphi u_1 + \cos\varphi u_2 \\ U_3 &= u_3 + \varphi' \end{aligned} \tag{8.166}$$

Note that $U_i = \mathbf{U} \cdot \mathbf{D}_i$ and $u_i = \mathbf{u} \cdot \mathbf{d}_i$.

Remarks

- φ' does not enter in the expression for U_1 and U_2
- ${u_1}^2 + {u_2}^2 = {U_1}^2 + {U_2}^2$
- $u_3 = U_3 - \varphi'$ wich implies that
$$\varphi(s) - \varphi(s_0) = \int_{s_0}^{s} (U_3 - u_3) ds \tag{8.167}$$
- The freedom in changing from one adapted framing to another is one scalar function $\varphi(s)$

Next, we want to know how the Hamiltonian transforms when a different adapted framing is chosen as the reference state. Recall that the expression for the Hamiltonian:

$$H(\mathrm{r}, \mathrm{q}, \mathrm{n}, \nu) = \sum_{i=1}^{3} \left(\frac{m_i^2}{2\,K_i} + \hat{u}_i m_i \right) + \mathbf{n} \cdot \mathbf{d}_3. \tag{8.168}$$

The $\hat{\mathbf{u}}$ transform to $\hat{\mathbf{U}}$ and

$$\begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \text{ is transformed to the vector } \begin{bmatrix} \cos\varphi m_1 + \sin\varphi m_2 \\ \cos\varphi m_2 - \sin\varphi m_1 \\ m_3 \end{bmatrix}.$$

The first term in the Hamiltonian, i.e.,

transforms to

$$\frac{1}{2} \begin{bmatrix} M_1 & M_2 & M_3 \end{bmatrix} \begin{bmatrix} \frac{\cos\varphi^2}{K_1} + \frac{\sin\varphi^2}{K_2} & \sin\varphi\cos\varphi(\frac{1}{K_1} - \frac{1}{K_2}) & 0 \\ \sin\varphi\cos\varphi(\frac{1}{K_1} - \frac{1}{k_2}) & \frac{\cos\varphi^2}{K_2} + \frac{\sin\varphi^2}{K_1} & 0 \\ 0 & 0 & \frac{1}{K_3} \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \end{bmatrix} \tag{8.169}$$

Note that for the isotropic case, i.e., when $K_1 = K_2$, the transformed matrix remains diagonal.

8.1 Frenet-Serret Frame

The Frenet-Serret frame is a particular adapted frame where $(\mathbf{D_1}, \mathbf{D_2}, \mathbf{D_3})$ is usually denoted $(\mathbf{n},\mathbf{b},\mathbf{t})$, and

$$\mathbf{t}(s) = \mathbf{r}'(s),$$

$$\mathbf{t}'(s) = \kappa(s)\mathbf{n}(s).$$

The vector $\mathbf{n(s)}$ is the principal normal and $\kappa(s)$ is the curvature. Note that this frame is well defined provided that $\mathbf{t}'(s)$ does not vanish at any s. The binormal vector $\mathbf{b} = \mathbf{t} \times \mathbf{n}$ satisfies $\mathbf{b}' = -\tau(s)\mathbf{n}$, where the function $\tau(s)$ is the ***geometrical*** torsion of the axial curve.
Therefore, for the Frenet-Serret frame we get

$$\begin{aligned} \mathbf{n}'(s) &= -\kappa(s)\mathbf{t}(s) + \tau(s)\mathbf{b} \\ \mathbf{b}'(s) &= -\tau(s)\mathbf{n}(s) \\ \mathbf{t}'(s) &= \kappa(s)\mathbf{n}(s) \end{aligned} \tag{8.170}$$

or

$$\begin{bmatrix} \mathbf{n} \\ \mathbf{b} \\ \mathbf{t} \end{bmatrix}' = \begin{bmatrix} 0 & \tau & -\kappa \\ -\tau & 0 & 0 \\ \kappa & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{n} \\ \mathbf{b} \\ \mathbf{t} \end{bmatrix}.$$

The Frenet-Serret frame is an adaptive frame with $U_1 = 0, U_2 = \kappa$ and $U_3 = \tau$.
Remark
A rotation by $\frac{\pi}{2}$ of the Frenet-Serret frame is another adapted frame with $U_2 = 0$, $U_1 = \kappa$ and $U_3 = \tau$.

8.2 Natural Frame

An important case for the adapted framing is the parallel or natural transport frame. This frame is defined by imposing U_3 to be zero so that

$$\begin{bmatrix} \mathbf{D_1} \\ \mathbf{D_2} \\ \mathbf{D_3} \end{bmatrix}' = \begin{bmatrix} 0 & 0 & -U_2 \\ 0 & 0 & U_1 \\ U_2 & -U_1 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{D_1} \\ \mathbf{D_2} \\ \mathbf{D_3} \end{bmatrix}$$

This frame is well defined on all curves, including straight segments, and it is uniquely defined up to an arbitrary choice of $\mathbf{D_1(0)}$ with $\mathbf{D_1(0)} \cdot \mathbf{r'(0)} = \mathbf{0}$.

Remark

If we consider a closed loop with no inflection point, then the ribbon formed by the normal vector is always closed in the Frenet-Serret frame, because the principal normal has a local definition. For the natual frame, the ribbon is closed only if the angle $\varphi(s)$ between the natural and Frenet-Serret frame satisfies $\varphi(L) = \varphi(0)$ modulo $2k\pi$. We can see from (8.167) with $U_3 = 0$, for the natural frame, that $\varphi(L) = \varphi(0)$ modulo 2π if and only if $\int \tau = 2k\pi$ for some integer k.

8.3 Why work with adapted frames?

The crucial difficulty when working with the local frame in the DNA application is that the normal vector rotates rapidly about the centerline, making a full revolution approximately every 10.5 base-pairs. Furthermore, when the centerline is curved with a slowly varying curvature and torsion and with the normal vector $\mathbf{d_1}$ spins rapidly, there will be rapid oscillations in u_1 and u_2 because of the high twist. Consider, for example, a centerline $\mathbf{r}(s) = \langle R\cos(s/R), R\sin(s/R), 0\rangle$ with the corresponding tangent vectors $\mathbf{d_3}(s) = \langle -\sin(s/R), \cos(s/R), 0\rangle$, and choose normal vector $\mathbf{d_1}(s) = \langle \cos(s/R)\cos(\gamma s/R), \sin(s/R)\cos(\gamma s/R), -\sin(\gamma s/R)\rangle$. We can then compute $u_2(s) = \mathbf{d}_3'(s) \cdot \mathbf{d_1}(s) = -\cos(\gamma s/R)/R$, which oscillates rapidly for γ large. In the DNA context, we have exactly this problem, a slowly varying reference centerline with a rapidly varying material reference frame $\{\hat{\mathbf{d}}_i(s)\}$. Because $u_1(s)$ and $u_2(s)$ vary rapidly in s, it is desirable to avoid computing with the local DNA frames. Fortunately, we can compute on a different set of frames which are not rapidly rotating, and then recover the true DNA results analytically from the transformed results. It is possible to transform the natural frame for the reference state, and to compute how this frame deforms when the rod is bent and twisted. At any stage it is possible to recover the material frame because the angle $\varphi(s)$ between it and the deformed image of the natural frame in the reference state is constant, independant of the deformation.