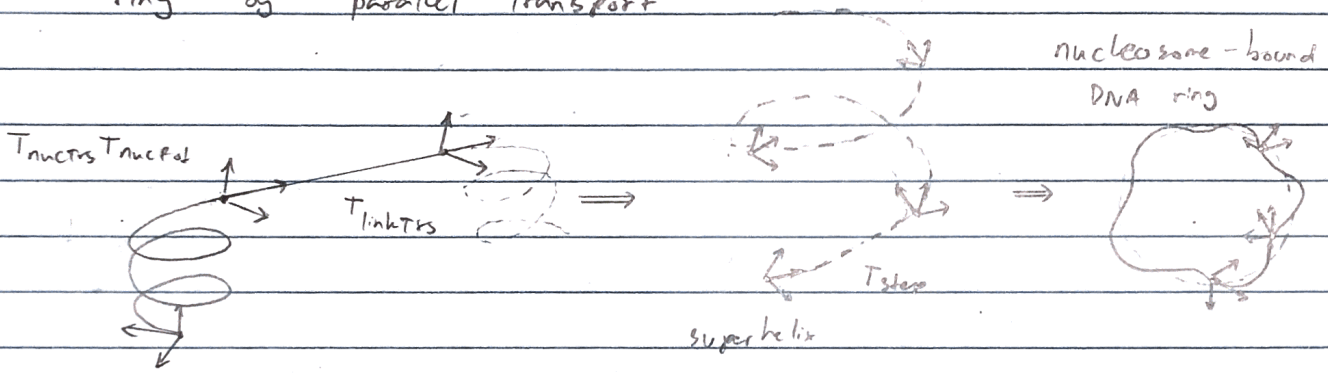
Nucleosome Ring Geometry 7/24/19

Key points

- T_{step} transforms a configuration (position & orientation) as if it moves along the helical wrapping nucleosome-bound DNA and the linker to the next nucleosome.
  $T_{step} = T_{nucTrs}\, T_{nucRot}\, T_{linkTrs}$ is the effective propagator.
- Successive applications of T_{step} result in configurations of points along a nucleosome-bound DNA, which form a "superhelix" according to Chasles theorem.
- The (linear) superhelix can be transformed into a ring by "parallel transport"



Objective: To find configurations of points on nucleosome-bound DNA ring

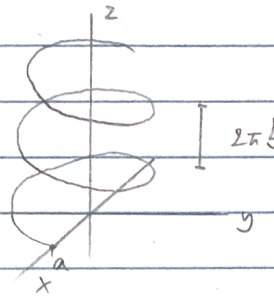
Relevant Curves

Helix (along z-axis, left-handed)

$C(t) = (a\cos t,\ -a\sin t,\ bt)$

$s = \sqrt{a^2+b^2}\, t$

$C(s) = \left(a\cos\frac{s}{m},\ -a\sin\frac{s}{m},\ b\frac{s}{m}\right)$



where $m = \sqrt{a^2+b^2}$

a is the radius

$2\pi b$ is the pitch

For a finite helix having T (rad) turns, the total arc length is

$L = mT$

$$\Omega(s) = (n \quad b \quad u) = \begin{pmatrix} -\cos s/m & -b/m \sin s/m & -a/m \sin s/m \\ \sin s/m & -b/m \cos s/m & -a/m \cos s/m \\ 0 & -a/m & b/m \end{pmatrix}$$

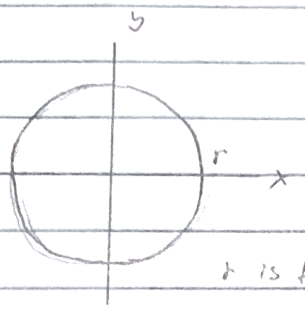
$$\tau(s) = -\frac{b}{m^2}$$

Circle (on xy-plane)

$C(t) = (r\cos t, \; r\sin t, \; 0)$

$s = rt$

$C(s) = \left(r\cos\frac{s}{r}, \; r\sin\frac{s}{r}, \; 0\right)$



r is the radius.

$$\Omega(s) = \begin{pmatrix} -\cos s/r & 0 & -\sin s/r \\ -\sin s/r & 0 & \cos s/r \\ 0 & 1 & 0 \end{pmatrix} \qquad \tau(s) = 0$$

Step Transformation

I want T_{step} to be "relative". In other words, it should transform a configuration to the right amount of displacement and rotation relative to the starting configuration. To apply a transformation with respect to a point's own frame, the operator matrix is post-multiplied.

$$H_{i+1} = H_i \; T_{step}$$

The elementary transformations in Tstep should be post-multiplied so that in each step the configuration transforms in its own intermediate frame.

$$T_{step} = T_{nucTrs} \; T_{nucRot} \; T_{linkTrs}$$

Note that DNA has intrinsic twist, and linker displacement should include this twist. However, I will incorporate this twist into T_{nucRot} for compactness.

Configuration

Configuration of a bead can be represented as follows:

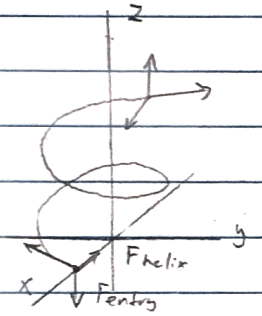
$$H = \begin{pmatrix} | & | & | & | \\ n & b & u & r \\ | & | & | & | \\ -0- & & -1- & \end{pmatrix}$$

n : normal vector
b : binormal vector
u : tangent vector
r : position in lab frame

} normalized

The three entries of each vector are the scalars in x, y, and z direction. For example, $n = (n_x, n_y, n_z)^T$.

Nucleosome Translation



The helical path depends on the initial configuration of the point.

Parameters:

L : wrapping length (nm)
T : # turns (rad)
h : pitch (nm)

$\rightarrow$ $b = h/2\pi$ helix parameters

$a = \left((L/T)^2 - b^2 \right)^{1/2}$

$m = \left(a^2 + b^2 \right)^{1/2} = L/T$

In the frame of the helix, F_{helix}, the displacement is

$$d_{nucTrs}^{F_{helix}} = \begin{pmatrix} a(\cos T - 1) \\ -a \sin T \\ bT \end{pmatrix}$$

The translation operator in F_{helix} is $T_{nucTrs}^{F_{helix}} = \begin{pmatrix} I_{3\times 3} & d_{nucTrs}^{F_{helix}} \\ 0_{1\times 3} & 1 \end{pmatrix}$

I need to describe the transformation in the frame of the entry triad, F_{entry}.

$$d_{F_{helix}}^{F_{entry}} = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} \qquad R_{F_{helix}}^{F_{entry}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -b/m & -a/m \\ 0 & -a/m & b/m \end{pmatrix}$$

Note that $R_{F_{helix}}^{F_{entry}}$ is the initial orientation of the canonical left-handed helix, $\Omega(0)$.

The frame transformation matrix is $H^{F_{entry}}_{F_{helix}} = \begin{pmatrix} R^{F_{entry}}_{F_{helix}} & d^{F_{entry}}_{F_{helix}} \\ 0_{1\times3} & 1 \end{pmatrix}$

∴ The nucleosome translation operator (relative to the entry triad) is

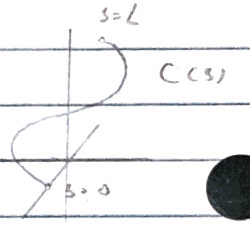
$$T_{nucTrs} = H^{F_{entry}}_{F_{helix}} \; T^{F_{helix}}_{nucTrs} \; \left(H^{F_{entry}}_{F_{helix}}\right)^{-1}$$

Nucleosome Rotation

Refer to the supplementary material of "Geometrical Heterogeneity Dominates Thermal Fluctuations in Determining Chromatin Elasticity".

The rotation matrix that rotates the entry triad to the exit of a helix with intrinsic twist is:

$$R_{nucRot} = \underbrace{\Omega_C^{-1}(0)\,\Omega_C(L)}_{\text{contribution from the geometry of twist-free helix}} \underbrace{R_z\left(\int_0^L \tau\, ds\right)}_{\text{contribution from the intrinsic twist}}$$



$\left(\Omega_{C,s:0\to s:L} = \Omega_C^{-1}(s=0)\,\Omega_C(s=L)\right)$

Note that

$$\Omega_C^{-1}(0) = \Omega_C(0) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -b/m & -a/m \\ 0 & -a/m & b/m \end{pmatrix}$$

$$\Omega_C(L) = \begin{pmatrix} -\cos L/m & -b/m \sin L/m & -a/m \sin L/m \\ \sin L/m & -b/m \cos L/m & -a/m \cos L/m \\ 0 & -a/m & b/m \end{pmatrix}$$

$R_z(\theta)$ is the rotation along z-axis.

$$R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The term $\int_0^L \tau\, ds$ serves 2 purposes:

1. Detwist the inherent twist of the helix geometry

$$\int_0^L (-\tau_{helix})\, ds = -\left(-b/m^2\right) \cdot L = bL/m^2$$

3. Add additional twist (e.g. DNA intrinsic twist and other introduced twist)

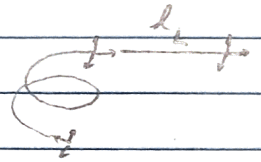
Here, let's assume that the twist is only from the inherent twist of DNA along the linker length (Assume no intrinsic twist when wrapping around nucleosome).

$$\int_0^L (\tau_{DNA})\, ds = \tau_{DNA}\, l_L \quad ; \quad l_L : \text{linker length}$$

Note that the linker twist actually occurs after exiting from the nucleosome helix. However, for compactness, I introduce such twist here, so that we don't need to have "Linker Rotation".

And the nucleosome rotation operator is

$$T_{nucRot} = \begin{pmatrix} R_{nucRot} & 0_{3\times 1} \\ 0_{1\times 3} & 1 \end{pmatrix}$$



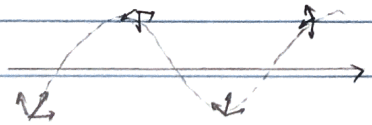
Linker Translation

Linker translation is only translation along the local z-axis (tangent vector of the triad).

$$T_{linkers} = \begin{pmatrix} I_{3\times 3} & d \\ 0_{1\times 3} & 1 \end{pmatrix} \quad ; \quad d = \begin{pmatrix} 0 \\ 0 \\ l_L \end{pmatrix}$$

l_L : linker length

Successive applications of T_{step} to an entry configuration yield a sequence of triads which is said to form an "superhelix". However, in order to transport such superhelix onto a circle, we need to define a "principal" axis of this superhelix. For now, we define this "principal" axis as the axis passing through the center of the helix, as in the z-axis of the canonical helix.



I will transform the superhelix formed by successive applications of T_{step} into the canonical helix — the principal axis is the lab frame's z-axis and the first triad placed on the x-axis at $(r_{screw}, 0, 0)$ where r_{screw} is the radius of the super helix.

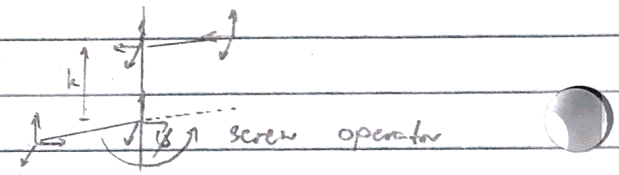
Even though only a_{screw} and θ_{screw} (orientation) are needed, I will describe the full characterization of the superhelix as a reference for screwLeftParam.m in my code.

Superhelix : Screw Axis Characterization

According to Chasles theorem, any rigid body transformation can be described by a screw operator — displacement and rotation.

$$A = \Phi \Lambda \Phi^{-1}$$

- A: any rigid transformation operator
- Φ: frame change
- Λ: screw operator



This screw can be viewed as a segment of a helix.
By evaluating its pitch, h_{screw}, and its radius, a_{screw}, we fully specify the parameters of the superhelix.
Note that in my code (screwLeftParam.m), the number of points is an argument, so that the length of this superhelix can be evaluated.
My calculation regarding Chasles theorem is based on the lecture note "The Theorems of Euler and Chasles" by V. Kumar. There are minor modifications since my fitted superhelix is left-handed. However, they should not change the key results needed for further calculations (r_{screw} and θ_{screw}).
Given the step operator, T_{step}, and the number of steps, I will evaluate the superhelix parameters.

rotation ↑ translation ↗

$$T_{step} = \begin{pmatrix} R_{step} & d_{step} \\ 0_{1\times 3} & 1 \end{pmatrix}$$

According to Rodrigues formula,

$$\phi = \arccos\left(\frac{1}{2}(Tr(R) - 1)\right) \quad \text{sweep angle}$$

$$\hat{u} = \frac{1}{2\sin\phi}(R - R^T)$$

$$= \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}$$

where $u = (u_1, u_2, u_3)^T$ is the axis of rotation.

The displacement along the axis of rotation is

$$k = u \cdot d_{step}$$

Consequently, the pitch is

$$h_{screw} = 2\pi k / (2\pi - \phi)$$

Projection of d_{step} onto a plane perpendicular to u is

$$d_p = d_{step} - ku$$

I am going to determine a vector to a point on the axis of rotation, which is necessary in order to evaluate r_{screw}. In other words, I will evaluate the displacement of Φ.

$$\Phi = \begin{pmatrix} Q & c \\ 0_{1\times 3} & 1 \end{pmatrix} \rightarrow \text{displacement.}$$

Consider

$$\Lambda = \Phi^{-1} T_{step} \Phi = \begin{pmatrix} Q^T & -Q^T c \\ 0 & 1 \end{pmatrix} \begin{pmatrix} R_{step} & d_{step} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} Q & c \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} Q^T R Q & Q^T R c - Q^T c + Q^T d \\ 0 & 1 \end{pmatrix}$$

The translation is

$$Q^T R c - Q^T c + Q^T d = (Q^T R Q - I) Q^T c + Q^T d$$

Note that the rotation of Λ is the canonical rotation about z-axis.

$$Q^T R Q = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Let $c' = Q^T c$ and $d' = Q^T d$.

Hence,

$$(Q^T R Q - I) Q^T c + Q^T d = \begin{pmatrix} \cos\phi - 1 & -\sin\phi & 0 \\ \sin\phi & \cos\phi - 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} c_x' \\ c_y' \\ c_z' \end{pmatrix} + \begin{pmatrix} d_x' \\ d_y' \\ d_z' \end{pmatrix}$$

Note that the translation of Λ is purely along z-axis.

$$\begin{pmatrix} \cos\phi - 1 & -\sin\phi \\ \sin\phi & \cos\phi - 1 \end{pmatrix} \begin{pmatrix} c_x' \\ c_y' \end{pmatrix} = - \begin{pmatrix} d_x' \\ d_y' \end{pmatrix}$$

$$\begin{pmatrix} c_x' \\ c_y' \end{pmatrix} = - \begin{pmatrix} \cos\phi - 1 & -\sin\phi \\ \sin\phi & \cos\phi - 1 \end{pmatrix}^{-1} \begin{pmatrix} v \cdot d \\ w \cdot d \end{pmatrix}$$

where v and w are unit vectors orthogonal to u.

$$v = d_p / \|d_p\|$$

$$w = u \times v$$

$$\begin{pmatrix} c_x' \\ c_y' \end{pmatrix} = \frac{\|d_p\|}{2(1-\cos\phi)} \begin{pmatrix} 1 - \cos\phi \\ \sin\phi \end{pmatrix}$$

$$c' = \frac{\|d_p\|}{2} \begin{pmatrix} 1 \\ \frac{\sin\phi}{1-\cos\phi} \\ 0 \end{pmatrix} ; \qquad c = Q c' = \frac{\|d_p\|}{2} \left(v + \frac{\sin\phi}{1-\cos\phi} w \right)$$

The screw radius is

$$r_{screw} = \| c - (c \cdot u) u \|$$

The orientation vectors of the screw helix is:

$$t_1 = -c / \|c\|$$

$$t_3 = u$$

$$t_2 = t_3 \times t_1$$