

Geometry of the DNA Double Helix

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Abstract. DNA base stacking is modeled by using three local rotation angles and a three-dimensional local translation for each dinucleotide. Together the six degrees of freedom completely specify the spacial position of base pair $n + 1$ calculated relative to the local coordinate frame of base pair n and can be used to reconstruct an arbitrary DNA conformation in global Cartesian coordinates.

$N + 1$ DNA base pairs are modeled as rigid bodies to which local coordinate frames are attached (Figure 1). The position of base pair $n + 1$ calculated relative to the coordinate frame of base pair n is uniquely specified by six geometric parameters (Figure 2).

- Three angles define the axes of base pair $n + 1$ calculated relative to the coordinate frame of base pair n .
 - $\tau(n)$ is the rotation of base pair $n + 1$ about the x axis of base pair n (the tilt). Positive tilt opens the angle between base pairs toward strand I.
 - $\rho(n)$ is the rotation of base pair $n + 1$ about the y axis of base pair n (the roll). Positive roll opens the angle between base pairs towards the minor groove.
 - $\Omega(n)$ is the rotation of base pair $n + 1$ about the z axis of base pair n (the twist). Positive twist is defined by the right-hand rule.
- The local translation $\mathbf{L}(n)$ gives the origin of base pair $n + 1$ calculated relative to the coordinate frame of base pair n .
 - $L_1(n)$ is the shift.
 - $L_2(n)$ is the slide.
 - $L_3(n)$ is the rise.

The global rotation matrix $R(n)$ gives the axes of base pair n calculated relative to the coordinate frame of base pair 1, the “global coordinate frame”. The six geometric parameters can be used to construct the global rotation matrix of each base pair recursively.

$$\begin{cases} R(1) \leftarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ R(n+1) \leftarrow R(n)T(n) \quad (n = 1, \dots, N) \end{cases} \quad (1)$$

where each $T(n)$ matrix is a product of three rotations.

$$T(n) = Z\left(-\frac{\Omega(n)}{2} + \phi(n)\right) Y(\Gamma(n)) Z\left(-\frac{\Omega(n)}{2} - \phi(n)\right) \quad (2)$$

Here, $Y(\theta)$ and $Z(\theta)$ are the rotation matrices around the local y and z axes, respectively. $Y(\Gamma(n))$ introduces both roll and tilt with a single rotation through $\Gamma(n)$.

$$Y(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix} \quad (3)$$

$$Z(\theta) = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (4)$$

$$\Gamma(n) = \left((\rho(n))^2 + (\tau(n))^2\right)^{1/2} \quad (5)$$

$$\phi(n) = \arg(\rho(n) + \tau(n)i) \quad (6)$$

The global translation $\mathbf{G}(n)$ gives the origin of base pair n calculated relative to the global coordinate frame. The six geometric parameters can be used to construct the global translation of each base pair recursively.

$$\begin{cases} \mathbf{G}(1) \leftarrow \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\ \mathbf{G}(n+1) \leftarrow \mathbf{G}(n) + R_M(n) \mathbf{L}(n) \quad (n = 1, \dots, N) \end{cases} \quad (7)$$

where

$$R_M(n) = R(n) T_M(n) \quad (8)$$

$$T_M(n) = Z\left(-\frac{\Omega(n)}{2} + \phi(n)\right) Y\left(\frac{\Gamma(n)}{2}\right) Z(-\phi(n)) \quad (9)$$

References

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- [3] Morozov, A., Fortney, K., Gaykalova, D., Studitsky, V., Widom, J., and Siggia, E. Using DNA mechanics to predict *in vitro* nucleosome positions and formation energies. *Nucleic Acids Research* 37, 4704-4722, 2009.

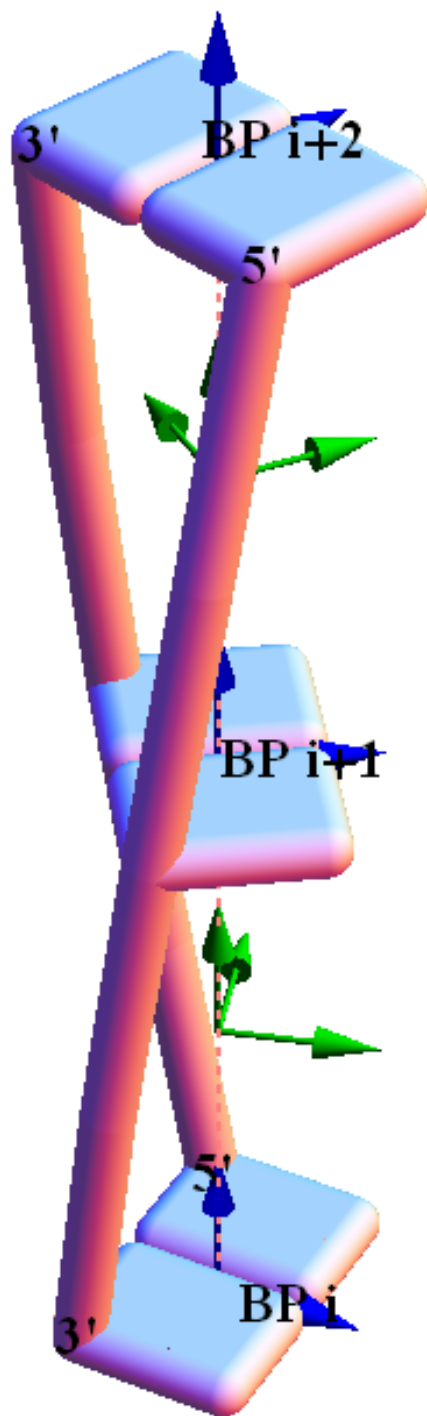


Figure 1: Schematic illustration of three dinucleotides.

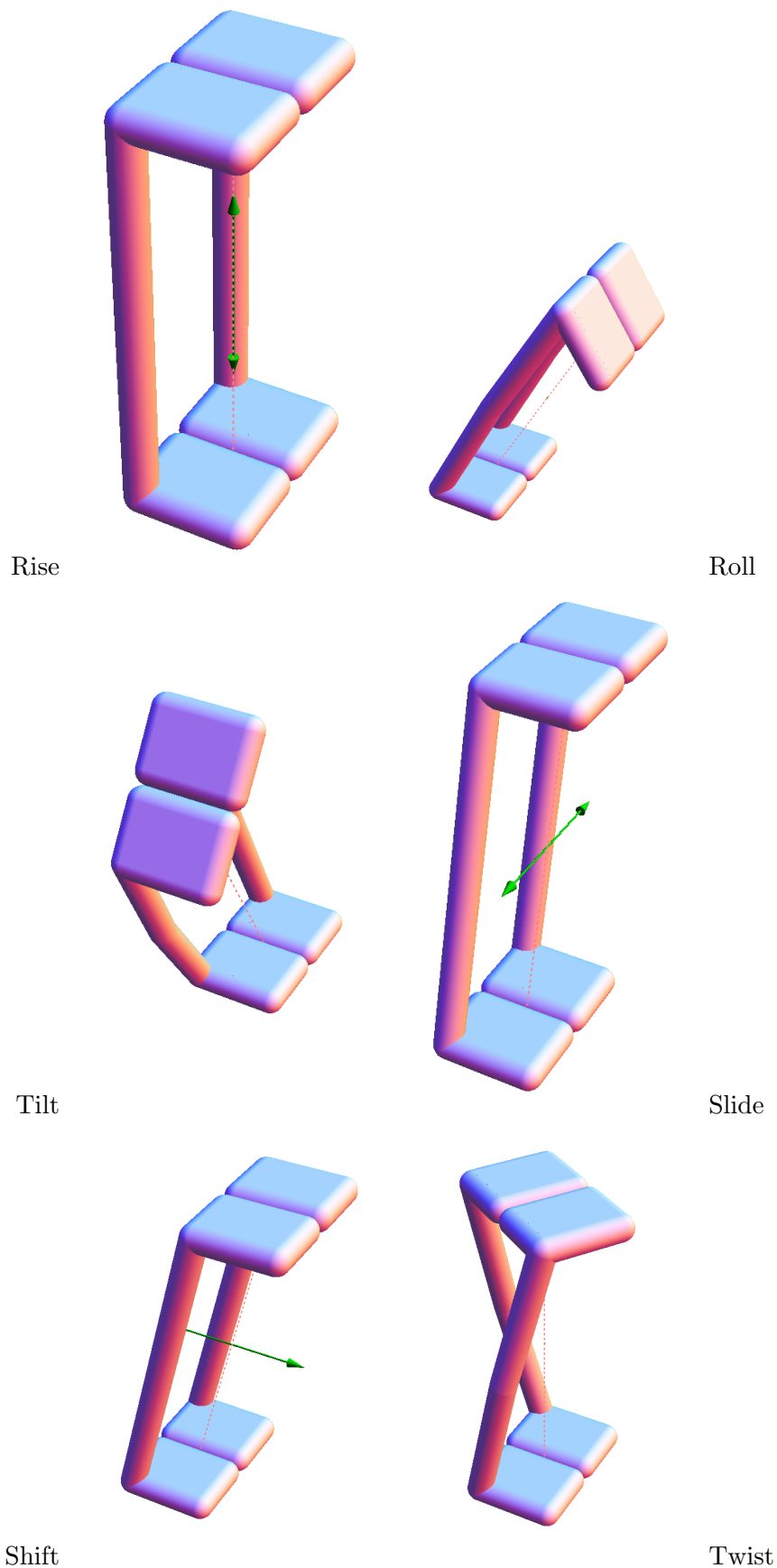


Figure 2: Conformation of a single DNA basestep is described by six geometric degrees of freedom: rise, shift, slide, twist, roll, and tilt.