# Mathematical Model for Structure and Dynamics of Chromatin

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An explicit formulation of the configuration-dependent potential energy function and the Brownian Dynamics (BD) algorithm used to simulate the chromatin polymer is detailed. For the readers' convenience, this document provides a complete description of our methodology, and thus some of the material is redundant with that found in the Material and Methods section of Beard & Schlick (*Structure with Folding and Design* **??**:??–??, 2000).

## Model Geometry

The model structure is illustrated in Figure 1. Each core particle disk is connected to one or two linker DNA segments (see Figure 1, top panel). In Figure 1, $\mathbf{r}_i$ denotes the position of the center of a core disk, while $\mathbf{r}_{i-1}$, $\mathbf{r}_{i+1}$, and $\mathbf{r}_{i+2}$, denote positions of linker DNA beads. The orientation of the core disk is specified by a local coordinate system $\{\mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i\}$ where the unit vectors $\mathbf{a}_i$ and $\mathbf{b}_i$ lie in the plane of the flat surface of the disk, and $\mathbf{c}_i = \mathbf{a}_i \times \mathbf{b}_i$. The attachment of the linker DNA to the core particle is illustrated in the lower panel of Figure 1. The linker DNA enters the core particle at the position $\mathbf{r}_i - r_o[\mathbf{b}_i \cos\theta_o - \mathbf{a}_i \sin\theta_o] + w_o \mathbf{c}_i$ and exits at position $\mathbf{r}_i - r_o \mathbf{b}_i - w_o \mathbf{c}_i$. The scalar parameters $r_o$, $w_o$, and $\theta_o$ are determined by the geometry of the wrapped DNA supercoil. Based on the crystal structure [1], we set the values of these parameters as follows: $r_o = 4.8$ nm, $w_o = 1.8$ nm, $\theta_o = 90°$ (see Table 1).

A local coordinate system $\{\mathbf{a}_j, \mathbf{b}_j, \mathbf{c}_j\}$ is also associated with each linker bead position, $\mathbf{r}_j$, and is used to calculate the local torsion on the linker beads. We define the sets $I_c$ and $I_l$ to be, respectively, the set of core beads and the set of linker DNA beads. The vectors $\{\mathbf{a}_i\}$ for $i \in I_l$ are directed in the direction of the linker DNA segment:

$$\mathbf{a}_i = \begin{cases} (\mathbf{r}_{i+1} - \mathbf{r}_i)/\|\mathbf{r}_{i+1} - \mathbf{r}_i\| & \text{for } i+1 \in I_l \\ \dfrac{\mathbf{r}_{i+1} - r_o(\mathbf{b}_{i+1}\cos\theta_o - \mathbf{a}_{i+1}\sin\theta_o) + w_o\mathbf{c}_{i+1} - \mathbf{r}_i}{\|\mathbf{r}_{i+1} - r_o(\mathbf{b}_{i+1}\cos\theta_o - \mathbf{a}_{i+1}\sin\theta_o) + w_o\mathbf{c}_{i+1} - \mathbf{r}_i\|} & \text{for } i+1 \in I_c \end{cases} \tag{1}$$

Since the wrapped DNA does not make two full turns around the core disk, the unstressed trajectory of $\mathbf{a}_{i-1}$ is not parallel to $\mathbf{a}_i$ when the $i^{th}$ bead is a disk. The trajectory of the wrapped DNA, is denoted $\mathbf{a}_i^-$ (see Figure 1, bottom panel), and is calculated as $\mathbf{a}_i^- = \mathbf{a}_i \cos\theta_o + \mathbf{b}_i \sin\theta_o$. Similarly, the trajectory of

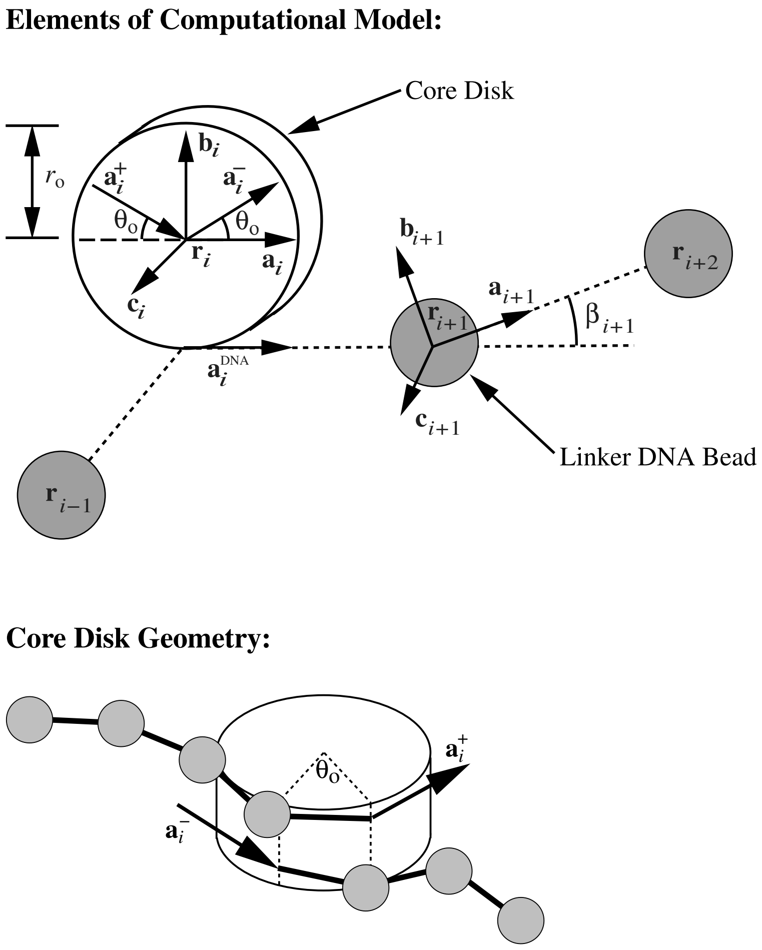


Figure 1: Diagram of the subunits of our chromatin model. The upper panel illustrates the components of the computational model: a core disk is located at position $\mathbf{r}_i$, and linker DNA beads are located at $\mathbf{r}_{i-1}$, $\mathbf{r}_{i+1}$, and $\mathbf{r}_{i+2}$. The lower panel illustrates the core disk geometry.

the wrapped DNA, as it exits the core is denoted by $\mathbf{a}_i^+$. The local coordinate systems of the wrapped DNA entering and exiting the core particle are given by:

$$\begin{aligned}\mathbf{a}_i^- &= \mathbf{a}_i \cos\theta_o + \mathbf{b}_i \sin\theta_o \\ \mathbf{b}_i^- &= -\mathbf{a}_i \sin\theta_o + \mathbf{b}_i \cos\theta_o \\ \mathbf{c}_i^- &= \mathbf{c}_i \end{aligned} \tag{2}$$

and $\{\mathbf{a}_i^+, \mathbf{b}_i^+, \mathbf{c}_i^+\} = \{\mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i\}$. For the core particle, we introduce the vectors $\{\mathbf{a}_i^{\mathrm{DNA}}, \mathbf{b}_i^{\mathrm{DNA}}, \mathbf{c}_i^{\mathrm{DNA}}\}$ (see Figure 1), to represent the local coordinate system associated with the DNA segment connecting the core at $\mathbf{r}_i$ and the linker vertex $\mathbf{r}_{i+1}$. The calculation of $\{\mathbf{a}_i^{\mathrm{DNA}}, \mathbf{b}_i^{\mathrm{DNA}}, \mathbf{c}_i^{\mathrm{DNA}}\}$ is outlined next.

## Euler Angles

The bending and twisting terms in the potential energy function are expressed in terms of the Euler angles [2], $\{\alpha_i, \beta_i, \gamma_i\}$, that transform one local coordinate system to the next. In the following sections we will make use of the following sets of Euler angles:

- For $i, i+1 \in I_l$, the angles $\{\alpha_i, \beta_i, \gamma_i\}$ transform from the $\{\mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i\}$ to the $\{\mathbf{a}_{i+1}, \mathbf{b}_{i+1}, \mathbf{c}_{i+1}\}$ coordinate system.

Table 1: Elastic and geometric parameters used in the dinucleosome model.

| Parameter | Description | Value |
|---|---|---|
| $l_o$ | Equilibrium segment length | 3.0 nm |
| $h$ | Stretching constant | $5000\ k_B\mathrm{T}/l_o^2$ |
| $C$ | Twisting rigidity constant | $3.0 \times 10^{-12}$ erg · nm |
| $L_p$ | Elastic bending persistence length of DNA | 50 nm |
| $\theta_o$ | Angular separation between linker segments | 90° |
| $r_o$ | Radius of wound DNA supercoil | 4.8 nm |
| $2w_o$ | Width of wound DNA supercoil | 3.6 nm |
| $\rho_i,\ i \in I_l$ | Hydrodynamic radius of linker bead (set $I_l$) | 1.5 nm |
| $\rho_i,\ i \in I_c$ | Hydrodynamic radius of core bead (set $I_c$) | 5 nm |
| $k_{\mathrm{ex}}$ | Excluded volume parameter | 0.001 |
| $\sigma_1$ | Core/linker excluded volume parameter | 3.0 nm |
| $\sigma_2$ | Core/core excluded volume parameter | 2.0 nm |
| $\Delta t$ | Numerical time step for dynamics simulation | 2.0 ps |

- For $i+1 \in I_c$, the angles $\{\alpha_i, \beta_i, \gamma_i\}$ transform from the $\{\mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i\}$ to the $\{\mathbf{a}_{i+1}^-, \mathbf{b}_{i+1}^-, \mathbf{c}_{i+1}^-\}$ coordinate system.
- For $i \in I_c$, the angles $\{\alpha_i^+, \beta_i^+, \gamma_i^+\}$ transform $\{\mathbf{a}_i^+, \mathbf{b}_i^+, \mathbf{c}_i^+\}$ to $\{\mathbf{a}_i^{\mathrm{DNA}}, \mathbf{b}_i^{\mathrm{DNA}}, \mathbf{c}_i^{\mathrm{DNA}}\}$; and the angles $\{\alpha_i, \beta_i, \gamma_i\}$ transform $\{\mathbf{a}_i^{\mathrm{DNA}}, \mathbf{b}_i^{\mathrm{DNA}}, \mathbf{c}_i^{\mathrm{DNA}}\}$ to $\{\mathbf{a}_{i+1}, \mathbf{b}_{i+1}, \mathbf{c}_{i+1}\}$.

The additional DNA coordinate system associated with each core bead, $\{\mathbf{a}_i^{\mathrm{DNA}}, \mathbf{b}_i^{\mathrm{DNA}}, \mathbf{c}_i^{\mathrm{DNA}}\}$, and the associated Euler angles $\{\alpha_i^+, \beta_i^+, \gamma_i^+\}$, are calculated based on the assumption that the core particle protein/DNA complex remains rigid and twisting of the DNA that is wrapped around the core does not contribute to the mechanics of the model. Therefore $\alpha_i^+ = -\gamma_i^+$. Calculation of the vector $\mathbf{a}_i^{\mathrm{DNA}}$ and the angle $\beta_i^+$ is straightforward:

$$\mathbf{a}_i^{\mathrm{DNA}} = \frac{r_{i+1} - r_i + r_o b_i + w_o c_i}{\|r_{i+1} - r_i + r_o b_i + w_o c_i\|}, \tag{3}$$

$$\beta_i^+ = \cos^{-1}(\mathbf{a}_i^+ \cdot \mathbf{a}_i^{\mathrm{DNA}}). \tag{4}$$

We calculate $\alpha_i^+$ from:

$$\alpha_i^+ = \begin{cases} |\alpha_i| & \text{for } \mathbf{c}_i^+ \cdot \left((\mathbf{a}_i^{\mathrm{DNA}} - \cos\beta_i^+ \mathbf{a}_i^+)/\sin\beta_i^+\right) > 0 \\ -|\alpha_i| & \text{for } \mathbf{c}_i^+ \cdot \left((\mathbf{a}_i^{\mathrm{DNA}} - \cos\beta_i^+ \mathbf{a}_i^+)/\sin\beta_i^+\right) < 0, \end{cases} \tag{5}$$

where

$$|\alpha_i^+| = \cos^{-1}\left[\mathbf{b}_i^+ \cdot \left(\frac{\mathbf{a}_i^{\mathrm{DNA}} - \cos\beta_i^+ \mathbf{a}_i^+}{\sin\beta_i^+}\right)\right]. \tag{6}$$

Then we set $\gamma_i^+ = -\alpha_i^+$ to ensure that no torsion is introduced into the Euler rotation $\{\alpha_i^+, \beta_i^+, \gamma_i^+\}$. Then the Euler rotations are applied to $\{\mathbf{a}_i^+, \mathbf{b}_i^+, \mathbf{c}_i^+\}$ to obtain $\mathbf{b}_i^{\mathrm{DNA}}$ and $\mathbf{c}_i^{\mathrm{DNA}}$.

## Calculation of the Potential

The energy associated with a given polymer structure is estimated from the sum of several elastic energy terms, an electrostatic potential, and an excluded volume term [3]:

$$E = E_S + E_T + E_B + E_C + E_V. \tag{7}$$

The first three terms represent elastic contributions from stretching, twisting, and bending, respectively. The terms $E_C$ and $E_V$ are used to model electrostatic and excluded volume interactions, respectively.

### Stretching

The stretching potential, $E_S$, is a computational device, and its treatment is optimized with respect to the time step of the dynamics simulation [4], so as to balance realized deviations from the target length with the computational time step. $E_S$ is written as:

$$E_S = \frac{h}{2} \sum_{i=1}^{N-1} (l_i - l_o)^2 \tag{8}$$

where $l_i$ is the length of the segment connecting particle $i$ to particle $i+1$, calculated as:

$$l_i = \begin{cases} \|\mathbf{r}_{i+1} - \mathbf{r}_i + r_o \mathbf{b}_i + w_o \mathbf{c}_i\| & \text{for } i \in I_c \\ \|\mathbf{r}_{i+1} - r_o \bar{\mathbf{b}}_{i+1} + w_o \bar{\mathbf{c}}_{i+1} - \mathbf{r}_i\| & \text{for } i+1 \in I_c \\ \|\mathbf{r}_{i+1} - \mathbf{r}_i\| & \text{otherwise.} \end{cases} \tag{9}$$

We use an equilibrium segment length of $l_o = 3$ nm, which corresponds to roughly 9 bp per segment.

It has been shown for the Brownian dynamics simulation of linear and circular DNA [4] that a choice of $h = 100 k_B \mathrm{T}/l_o^2$, where $k_B$ is Boltzmann's constant and T is the absolute temperature, results in standard deviations in segment length of around 10% of $l_o$. The motions of the relatively large nucleosome beads in the present model tend to produce greater stretching and compressive forces on the linker DNA than are typically found in supercoiled DNA alone. This means that a greater value for the stretching rigidity constant is required to achieve comparable accuracy. A value of $h = 5000 k_B \mathrm{T}/l_o^2$ results in segment length deviations of less than 2% of the equilibrium segment length and a mean segment length equal to the equilibrium segment length for time steps of 2 ps.

### Twisting

The torsional rotation about the segment connecting particles $i$ and $(i+1)$ is given by the sum of the Euler angles $\alpha_i + \gamma_i$, and the torsional energy, $E_T$, is calculated from:

$$E_T = \frac{C}{2 l_o} \sum_{i=1}^{N-1} (\alpha_i + \gamma_i)^2, \tag{10}$$

where $C$ is the torsional rigidity constant.

### Bending

The bending energy, $E_B$, is calculated from the set of angles denoting the deformation between the linker DNA segments.

$$E_B = \frac{g}{2}\sum_{i=1}^{N-1}(\beta_i)^2 + \frac{g}{2}\sum_{i\in I_c}(\beta_i^+)^2, \tag{11}$$

The bending constant, $g$, can be calculated from:

$$g = L_p k_B \mathrm{T}/l_o, \tag{12}$$

where $L_p$ is the bending persistence length.

### Electrostatics

Representative charges are assigned to the linker beads as well as on the surface of the core disks. The assignment of charges in the model is based on a discrete $N$-body potential which approximates the solution to the nonlinear Poisson-Boltzmann equation in the solvent surrounding the core particle. This procedure is detailed in Beard & Schlick (2000). A single charge, $q_l$ is assigned to each linker bead; and a set of charges $\{q_c^k\}$ is assigned to each core disk, where the index $k$ refers to the $k^{th}$ charge on the core disk. The position of the $k^{th}$ charge on the $j^{th}$ particle is denoted by $\{\mathbf{x}_c^{jk}\}$ for $j \in I_c$.

The charge on a linker bead is calculated as $q_l = \nu l_o$, where $\nu$ is the effective linear charge density on DNA, calculated by fitting the tail of the Debye-Hückel potential for an infinitely-long cylinder to the Gouy-Chapman potential in the far zone [5]. Values for $\nu$ and $\kappa$, the inverse Debye length for various levels of monovalent salt concentration, are listed in Table 2.

Table 2: Electrostatic parameters for DNA.

| $C_s$ [Molar] | $\nu$ [e/nm] | $\kappa$ [1/nm] |
|---|---|---|
| 0.01 | $-2.43$ | 0.330 |
| 0.02 | $-2.96$ | 0.467 |
| 0.03 | $-3.39$ | 0.572 |
| 0.04 | $-3.91$ | 0.660 |
| 0.05 | $-4.15$ | 0.738 |

The electrostatic contribution to the potential is calculated as the superposition of the fundamental solution to the linearized Poisson-Boltzmann equation:

$$E_C = \sum_{\substack{j>i+1\\ i,j\in I_l}} \frac{q_l^2 e^{-\kappa r_{ij}}}{\epsilon r_{ij}} + \sum_{\substack{j>i+1\\ i\in I_l, j\in I_c}} \left[\sum_{k=1}^{N_c} \frac{q_l q_c^k e^{-\kappa r_{i\{jk\}}}}{\epsilon r_{i\{jk\}}}\right] + \sum_{\substack{j>i+1\\ i,j\in I_c}} \left[\sum_{k=1}^{N_c}\sum_{l=1}^{N_c} \frac{q_c^k q_c^l e^{-\kappa r_{\{ik\}\{jl\}}}}{\epsilon r_{\{ik\}\{jl\}}}\right], \tag{13}$$

where $\kappa$ denotes the inverse Debye length (salt-dependent), $\epsilon$ is the dielectric constant of the medium, and $N_c$ is the number of point charges on each core disk. In equation (13) we have introduced the notation $r_{ij} = \|\mathbf{r}_j - \mathbf{r}_i\|$ to denote the distance between the centers of the $i^{th}$ and $j^{th}$ particles. Similarly, the distance between the center of the $i^{th}$ particle and the $k^{th}$ charge on particle $j \in I_c$ is denoted by $r_{i\{jk\}} = \|\mathbf{x}_c^{jk} - \mathbf{r}_i\|$;

and the distance between the $k^{th}$ charge on particle $i \in I_c$ and the $l^{th}$ charge on particle $j \in I_c$ is denoted by $r_{\{ik\}\{jl\}} = \|\mathbf{x}_c^{ik} - \mathbf{x}_c^{jl}\|$.

The first term in equation (13) is due to linker/linker interactions, and the summation is over all pairs of linker beads. The summation in the second term is over all linker/core pairs and in the last term over all core/core pairs.

### Excluded Volume

It is necessary to include an excluded volume term in the calculation of the potential to avoid the overlap of positive and negative charges. We represent the excluded volume potential, $E_V$, as the sum of Lennard-Jones potentials arising from linker/core pair interactions and from core/core pair interactions as:

$$\begin{aligned} E_V &= k_{\mathrm{ex}} k_B \mathrm{T} \sum_{\substack{j>i \\ i \in I_l, j \in I_c}} \left[ \sum_{k=1}^{N_c} \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^{12} - \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^{6} \right] + \\ & \quad k_{\mathrm{ex}} k_B \mathrm{T} \sum_{\substack{j>i \\ i,j \in I_c}} \left[ \sum_{k=1}^{N_c} \sum_{l=1}^{N_c} \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^{12} - \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^{6} \right]. \end{aligned} \tag{14}$$

The terms in equation (14) have a shallow minimum of value $-k_{\mathrm{ex}} k_B \mathrm{T}/4$ at a separation between charges of $2^{1/6}\sigma$, where $\sigma$ and $k_{\mathrm{ex}}$ are the parameters describing the Lennard-Jones interactions.

The excluded volume parameters (see Table 1) are chosen to ensure that particles do not overlap one another over the course of a simulation. It is not necessary to include a linker/linker excluded volume term because the electrostatic repulsion between DNA segments proves sufficient to prevent overlap.

## Calculation of Forces

The systematic force acting on the $i^{th}$ particle is obtained from the gradient of the potential energy function taken with respect to the position of the particle:

$$\mathbf{f}_i = -\nabla_{\mathbf{r}_i}(E_S + E_T + E_B + E_C + E_V) \tag{15}$$

or

$$\mathbf{f}_i = \mathbf{f}_i^S + \mathbf{f}_i^T + \mathbf{f}_i^B + \mathbf{f}_i^C + \mathbf{f}_i^V. \tag{16}$$

Details of the calculations are given below.

### Stretching

The force due to the stretching potential is expressed as

$$\mathbf{f}_i^{\mathbf{S}} = -h(\mathbf{S}_i - \mathbf{S}_{i-1}), \tag{17}$$

where

$$\mathbf{S}_i = \begin{cases} (l_i - l_o)\mathbf{a}_i & \text{for } i \in I_l \\ (l_i - l_o)\mathbf{a}_i^{\mathrm{DNA}} & \text{for } i \in I_c. \end{cases} \tag{18}$$

### Twisting

A change in the position of the $i^{th}$ particle effects a change in the torsions $(\alpha_{i-2}+\gamma_{i-2})$, $(\alpha_{i-1}+\gamma_{i-1})$ and $(\alpha_i+\gamma_i)$. The torsional force on the $i^{th}$ particle can be expressed as:

$$\mathbf{f}_i^T = \frac{C}{l_o}(\chi_i + \xi_i - \chi_{i-1} - \xi_{i-1}), \tag{19}$$

where the vectors $\chi_i$ and $\xi_i$ are given by

$$\chi_i = \begin{cases} \frac{(\alpha_i+\gamma_i)}{l_i}\tan(\beta_i/2)\left[\cos\alpha_i\mathbf{c}_i - \sin\alpha_i\mathbf{b}_i\right] & \text{for } i \in I_l \\ \frac{(\alpha_i+\gamma_i)}{l_i}\tan(\beta_i/2)\left[\cos\alpha_i\mathbf{c}_i^{\mathrm{DNA}} - \sin\alpha_i\mathbf{b}_i^{\mathrm{DNA}}\right] & \text{for } i \in I_c \end{cases} \tag{20}$$

and

$$\xi_i = \begin{cases} \frac{(\alpha_{i-1}+\gamma_{i-1})}{l_i}\tan(\beta_{i-1}/2)\left[\cos\gamma_{i-1}\mathbf{c}_i + \sin\gamma_{i-1}\mathbf{b}_i\right] & \text{for } i \in I_l \\ \frac{(\alpha_i+\gamma_i)}{l_i}\tan(\beta_i^+/2)\left[\cos\gamma_i^+\mathbf{c}_i^{\mathrm{DNA}} + \sin\gamma_i^+\mathbf{b}_i^{\mathrm{DNA}}\right] & \text{for } i \in I_c. \end{cases} \tag{21}$$

For the end disks, $\chi_0, \xi_0, \chi_N, \xi_N = 0$.

### Bending

The force due to the bending potential is expressed as:

$$\mathbf{f}_i^B = -g(A_i - A_{i-1} + B_i - B_{i-1}) \tag{22}$$

where the $A_i$ and $B_i$ are given as follows:

$$A_i = \begin{cases} \beta_i(\mathbf{a}_{i+1} - \mathbf{a}_i\cos\beta_i)/(l_i\sin\beta_i) & \text{for } i, i+1 \in I_l \\ \beta_i(\mathbf{a}_{i+1}^- - \mathbf{a}_i\cos\beta_i)/(l_i\sin\beta_i) & \text{for } i+1 \in I_c \\ \beta_i(\mathbf{a}_{i+1} - \mathbf{a}_i^{\mathrm{DNA}}\cos\beta_i)/(l_i\sin\beta_i) & \text{for } i \in I_c \end{cases} \tag{23}$$

and

$$B_i = \begin{cases} \beta_{i-1}(\mathbf{a}_{i-1} - \mathbf{a}_i\cos\beta_{i-1})/(l_i\sin\beta_{i-1}) & \text{for } i, i-1 \in I_l \\ \beta_{i-1}(\mathbf{a}_{i-1}^{\mathrm{DNA}} - \mathbf{a}_i\cos\beta_{i-1})/(l_i\sin\beta_{i-1}) & \text{for } i-1 \in I_c \\ \beta_i^+(\mathbf{a}_i^+ - \mathbf{a}_i^{\mathrm{DNA}}\cos\beta_i^+)/(l_i\sin\beta_i^+) & \text{for } i \in I_c. \end{cases} \tag{24}$$

For the end disks, $A_0, B_0, A_N, B_N = 0$.

### Electrostatics

The electrostatic force, $\mathbf{f}_i^C$, acting on bead $i$ is given by a sum of forces due to pairwise interactions of the form:

$$\mathbf{f}_{mn}^C = \frac{q_m q_n e^{-\kappa s_{mn}}}{\epsilon s_{mn}^2}(\kappa s_{mn}+1)\left[\frac{\mathbf{s}_m - \mathbf{s}_n}{s_{mn}}\right] \tag{25}$$

where $\mathbf{f}_{mn}^C$ represents the force on bead $i$ due to interaction of a charge $m$ (located on bead $i$) with charge $n$ (located on another bead). The charges $q_m$ and $q_n$ are the charges at positions $\mathbf{s}_m$ and $\mathbf{s}_n$, respectively. The vector connecting position $m$ to position $n$ is given by $\mathbf{s}_m - \mathbf{s}_n$ and $s_{mn} = \|\mathbf{s}_m - \mathbf{s}_n\|$ is the scalar distance. The total electrostatic force acting on a given bead is:

$$\mathbf{f}_i^C = \sum_{m \in i} \sum_{n \notin i} \mathbf{f}_{mn}^C, \tag{26}$$

where the notation $m \in i$ denotes that summation occurs over all charges that are associated with bead $i$. Similarly, the notation $n \notin i$ denotes the set of all charges not located on bead $i$. Specifically, DNA beads have only one charge, positioned at the center of the bead while core beads have several charges located on the surface of the disk.

### Excluded Volume

The excluded volume force, $\mathbf{f}_i^V$, acting on bead $i$ is given by:

$$\mathbf{f}_i^V = \frac{k_{\text{ex}} k_B \mathrm{T}}{\sigma} \sum_{\substack{j \neq i \\ j \in I_c}} \left\{ \sum_{k=1}^{Nc} \left[ 12 \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^{13} - 6 \left( \frac{\sigma_1}{r_{i\{jk\}}} \right)^{7} \right] \frac{\mathbf{r}_{i\{jk\}}}{r_{i\{jk\}}} \right\} \tag{27}$$

for all $i \in I_l$ and

$$\begin{aligned} \mathbf{f}_i^V \quad &= \quad \frac{k_{\text{ex}} k_B \mathrm{T}}{\sigma_1} \sum_{\substack{j \neq i \\ j \in I_l}} \left\{ \sum_{k=1}^{Nc} \left[ 12 \left( \frac{\sigma_1}{r_{\{ik\}j}} \right)^{13} - 6 \left( \frac{\sigma_1}{r_{\{ik\}j}} \right)^{7} \right] \frac{\mathbf{r}_{\{ik\}j}}{r_{\{ik\}j}} \right\} \\ &+ \quad \frac{k_{\text{ex}} k_B \mathrm{T}}{\sigma_2} \sum_{\substack{j \neq i \\ j \in I_c}} \left\{ \sum_{k=1}^{Nc} \sum_{l=1}^{Nc} \left[ 12 \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^{13} - 6 \left( \frac{\sigma_2}{r_{\{ik\}\{jl\}}} \right)^{7} \right] \frac{\mathbf{r}_{\{ij\}\{jl\}}}{r_{\{ij\}\{jl\}}} \right\} \end{aligned} \tag{28}$$

for all $i \in I_C$. When $i$ is a linker bead (equation (27) the excluded volume force comes from the summation interactions between particle $i$ the charges on the surface of each core disk. When $i$ is a core disk (equation (28)), the force comes from all pairwise interactions with linker beads and with other core particles.

## Calculation of Torques

We express the systematic torque acting on bead $i$ by a vector of torques acting in each of the local coordinate directions, $\tau_i = \{\tau_{a_i}, \tau_{b_i}, \tau_{c_i}\}$.

### Torque on Linker Beads

The torque on the linker DNA beads comes from the elastic twisting potential and acts only in the $\mathbf{a}_i$ direction:

$$\tau_{a_i} = -\frac{C}{l_o}(\phi_i - \phi_{i-1}), \; \tau_{b_i} = 0, \; \tau_{c_i} = 0, \tag{29}$$

where $\phi_i = \alpha_i + \gamma_i$ is the torsional rotation about the segment connecting particle $i$ and $i + 1$.

## Torque on Core Particles

The torque acting on core particles acts not only in the $\mathbf{a}_i$ direction, but also in the directions of the $\mathbf{b}_i$ and $\mathbf{c}_i$ local coordinates. The total torque acting on a core particle can be written as the sum of several terms:

$$\tau_i = \tau_i^F + \tau_i^T + \tau_i^B, \tag{30}$$

where $\tau_i^F$ is the torque associated with contributions to the force $\mathbf{f}_i$ which are not applied at the center of mass of the particle. Additional torques $\tau_i^T$ and $\tau_i^B$ are associated with the torsional and bending potentials.

The $\tau_i^F$ term is expressed in the fixed laboratory reference frame as follows:

$$\{\tau_i^F\}_{\text{lab}} = \sum_j \mathbf{d}_i^j \times \mathbf{f}_i^j, \tag{31}$$

where the summation is over all contributions $\mathbf{f}_i^j$ to the force acting on the particle $i \in I_c$. The vector $\mathbf{d}_i^j$ connects the center of the core particle to the location of the action of the force $\mathbf{f}_i^j$. For electrostatic and excluded volume force terms, $\mathbf{d}_i^j$ is given by the position of the charge on the surface of the core. For elastic forces arising from linker stretching, bending, and twisting, the force is directed at $\mathbf{d}_i^j = \mathbf{r}_i - r_o\mathbf{b}_i - w_o\mathbf{c}_i$ or $\mathbf{d}_i^j = \mathbf{r}_i - r_o\mathbf{b}_i^- + w_o\mathbf{c}_i^-$, depending on whether the force $\mathbf{f}_i^j$ arises from interaction with the proceeding or preceeding segment. The torque can be projected onto the local frame using:

$$\tau_{a_i}^F = \mathbf{a}_i \cdot \{\tau_i^F\}_{\text{lab}}, \quad \tau_{b_i}^F = \mathbf{b}_i \cdot \{\tau_i^F\}_{\text{lab}}, \quad \tau_{c_i}^F = \mathbf{c}_i \cdot \{\tau_i^F\}_{\text{lab}}. \tag{32}$$

The additional torque associated with the torsional potential is expressed in the laboratory frame as:

$$\begin{aligned}\{\tau_i^T\}_{\text{lab}} \quad = \quad & s[\alpha_i + \gamma_i]\mathbf{a}_i^{\text{DNA}} - s[\alpha_{i-1} + \gamma_{i-1}]\mathbf{a}_i^- - \\ & s(\alpha_i + \gamma_i)\tan(\beta_i^+/2)\left[\mathbf{c}_i^{\text{DNA}}\sin\alpha_i^+ + \mathbf{b}_i^{\text{DNA}}\cos\alpha_i^+\right] + \\ & s(\alpha_{i-1} + \gamma_{i-1})\tan(\beta_{i-1}/2)\left[-\mathbf{c}_i^-\sin\gamma_{i-1} + \mathbf{b}_i^-\cos\gamma_{i-1}\right],\end{aligned} \tag{33}$$

which is converted to the local frame using

$$\tau_{a_i}^T = \mathbf{a}_i \cdot \{\tau_i^T\}_{\text{lab}}, \quad \tau_{b_i}^T = \mathbf{b}_i \cdot \{\tau_i^T\}_{\text{lab}}, \quad \tau_{c_i}^T = \mathbf{c}_i \cdot \{\tau_i^T\}_{\text{lab}}. \tag{34}$$

The torque associated with the bending potential, expressed in the local frame, is

$$\begin{aligned}\tau_{a_i}^B &= g\left[\frac{\beta_{i-1}\sin\theta_o}{\sin\beta_{i-1}}(\mathbf{a}_{i-1}\cdot\mathbf{c}_i)\right] \\ \tau_{b_i}^B &= g\left[-\frac{\beta_i^+}{\sin\beta_i^+}(\mathbf{a}_i^{\text{DNA}}\cdot\mathbf{c}_i) - \frac{\beta_{i-1}\cos\theta_o}{\sin\beta_{i-1}}(\mathbf{a}_{i-1}\cdot\mathbf{c}_i)\right] \\ \tau_{c_i}^B &= g\left[\frac{\beta_i^+}{\sin\beta_i^+}(\mathbf{a}_i^{\text{DNA}}\cdot\mathbf{b}_i) + \frac{\beta_{i-1}}{\sin\beta_{i-1}}(\mathbf{a}_{i-1}\cdot\mathbf{b}_i\cos\theta_o - \mathbf{a}_{i-1}\cdot\mathbf{a}_i\sin\theta_o)\right]\end{aligned} \tag{35}$$

# Hydrodynamic Interactions

For hydrodynamic purposes, core particles are treated as spheres, and the rotational frictional coefficients are be expressed as:

$$\xi_{a_i} = \xi_{b_i} = \xi_{c_i} = 8\pi\eta d_{\text{core}}^3, \tag{36}$$

where $d_{\text{core}}$ is the hydrodynamic radius of the core particle. For the linker beads, $\xi_{a_i}$ is the rotational friction coefficient of DNA and can be expressed as:

$$\xi_{a_i} = 4\pi\eta r_h^2 l_o, \tag{37}$$

where $r_h = 1.2$ nm is the hydrodynamic radius of DNA. Since rotation occurs only about the $\mathbf{a}_i$ axis for linker beads, $\xi_{b_i}$ and $\xi_{c_i}$ are effectively infinite.

## Translational hydrodynamics

The movements of the various components of the chromatin system are coupled to one another through the action of the viscous medium. This viscous coupling is approximated by incorporating the configuration-dependent hydrodynamic friction tensor into the the dynamic equations, as outlined below.

Since the beads used to represent the core particles are larger than those used to represent the linker DNA (see below), the hydrodynamic interaction tensor for nonidentical subunits, $\mathbf{H}$, given by Garcia and Bloomfield [6] can be used to calculate the frictional interaction tensor. The diffusion tensor used in the Brownian dynamics algorithm (see below) is proportional to $\mathbf{H}$:

$$\mathbf{D} = k_B \mathrm{T}\, \mathbf{H}. \tag{38}$$

For this $N$-bead system, $\mathbf{H}$ is the $3N \times 3N$ matrix written as:

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} & \cdots & \mathbf{H}_{1N} \\ \mathbf{H}_{21} & \mathbf{H}_{22} & \cdots & \mathbf{H}_{2N} \\ \vdots & \vdots & & \vdots \\ \mathbf{H}_{N1} & \mathbf{H}_{N2} & \cdots & \mathbf{H}_{NN} \end{bmatrix}, \tag{39}$$

where each $\mathbf{H}_{ij}$ is a $3 \times 3$ matrix representing the interaction between the $i^{th}$ and $j^{th}$ beads. Each $\mathbf{H}_{ij}$ can be calculated from [6]:

$$\mathbf{H}_{ij} = \begin{cases} \left(\dfrac{1}{6\pi\eta\rho_i}\right)\mathbf{I} & \text{for } i = j \text{ (same bead)}, \\ \left(\dfrac{1}{8\pi\eta\mathbf{r}_{ij}}\right)\left[\left(\mathbf{I} + \dfrac{\mathbf{r}_{ij}\mathbf{r}_{ij}^T}{r_{ij}^2}\right) + \dfrac{(\rho_i^2+\rho_j^2)}{r_{ij}^2}\left(\dfrac{1}{3}\mathbf{I} - \dfrac{\mathbf{r}_{ij}\mathbf{r}_{ij}^T}{r_{ij}^2}\right)\right] & \text{for } i \neq j \text{ (different beads)}, \end{cases} \tag{40}$$

where $\mathbf{I}$ is the $3 \times 3$ identity matrix, $\rho_i$ is the bead radius, and $\eta$ is the viscosity of the surrounding fluid. We use a touching-bead model for the linker DNA, and thus set the linker bead hydrodynamic radius to $\rho_i = l_o/2 = 1.5$ nm for $i \in I_l$. The core particle is treated as a spherical bead for hydrodynamic purposes. Yao *et al.* (1990) measure the translational diffusion coefficient of a core particle (octamer and wrapped DNA) to be about $3.9 \times 10^{-1}$ cm$^2$ sec$^{-1}$. This allows us to calculate an effective hydrodynamic radius of $\rho_i = 5.0$ nm for $i \in I_c$ particle using the relation:

$$D = k_B\mathrm{T}/6\pi\eta d_i. \tag{41}$$

We remark that the volume of the spherical bead with this radius is nearly equal to the volume of a disk of radius 6 nm and width 5 nm.

The Brownian dynamics (BD) algorithm [7] requires obtaining the Cholesky factorization, $\mathbf{H} = \mathbf{L}\mathbf{L}^T$, where $\mathbf{L}$ is a lower triangular matrix. The entries the matrix $\mathbf{L}$ are given by:

$$l_{ij} = \begin{cases} \left(H_{ii} - \sum_{k=1}^{i-1} l_{ij}^2\right)^{1/2} & \text{if} \quad i = j, \\ \left(H_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{jk}\right)/l_{jj} & \text{if} \quad i > j, \\ 0 & \text{if} \quad i < j. \end{cases} \tag{42}$$

An alternative to the Cholesky factorization of $\mathbf{H}$ is to compute the random force vector as an expansion in terms of Chebyshev polynomials [8]. Our recent application of this alternative showed reduction in computational complexity (roughly from a cubic to quadratic dependence on system size), but the benefits are realized on much larger systems than used here [9].

# Numerical Methods

A given conformation for an $N$-bead system is specified by the set of $N$ local coordinate systems, $\{\mathbf{a}_i^n, \mathbf{b}_i^n, \mathbf{c}_i^n\}$, and the position vector $r^n$, where the superscript $n$ denotes quantities associated with the difference equations at time $n\Delta t$ ($\Delta t =$ time step), and the vector $r^n \in \Re^{3N}$ is the collective position vector listing the three Cartesian components of each vector $r_i^n$ in turn.

## Rotational Transformations

To simulation the dynamics of the system we use a modified BD method [7] (see below) which involves translating and rotating the particles in the system by discrete steps. Rotation of an orthogonal coordinate system at a constant angular velocity over a finite time step involves a transformation governed by the following system of linear differential equations:

$$\begin{aligned} \dot{\mathbf{a}}_i &= \omega_{c_i}\mathbf{b}_i - \omega_{b_i}\mathbf{c}_i \\ \dot{\mathbf{b}}_i &= \omega_{a_i}\mathbf{c}_i - \omega_{c_i}\mathbf{a}_i \\ \dot{\mathbf{c}}_i &= \omega_{b_i}\mathbf{a}_i - \omega_{a_i}\mathbf{b}_i \end{aligned} \tag{43}$$

where $\{\omega_{a_i}, \omega_{b_i}, \omega_{c_i}\}$ are the three components of the angular velocity.

We define $z_i = ({\omega_{a_i}}^2 + {\omega_{b_i}}^2 + {\omega_{c_i}}^2)^{1/2}$ and note that equation (43) has constant coefficients for a constant rate of angular rotation and has the exact solution:

$$\begin{aligned} \mathbf{a}_i(t + \Delta t) &= \mathbf{g}_a\left(\mathbf{a}_i(t), \mathbf{b}_i(t), \mathbf{c}_i(t);\ \omega_{a_i}, \omega_{b_i}, \omega_{c_i};\ \Delta t\right) \\ \mathbf{b}_i(t + \Delta t) &= \mathbf{g}_b\left(\mathbf{a}_i(t), \mathbf{b}_i(t), \mathbf{c}_i(t);\ \omega_{a_i}, \omega_{b_i}, \omega_{c_i};\ \Delta t\right) \\ \mathbf{c}_i(t + \Delta t) &= \mathbf{g}_c\left(\mathbf{a}_i(t), \mathbf{b}_i(t), \mathbf{c}_i(t);\ \omega_{a_i}, \omega_{b_i}, \omega_{c_i};\ \Delta t\right) \end{aligned} \tag{44}$$

where $\Delta t$ is the finite time step and the rotation operators, $\mathbf{g_a}$, $g_\mathbf{b}$, and $g_\mathbf{c}$, are defined as follows:

$$\mathbf{g_a} \quad = \quad \left[\frac{({\omega_{b_i}}^2 + {\omega_{c_i}}^2)\cos z_i \Delta t + {\omega_{a_i}}^2}{z_i^2}\right]\mathbf{a}_i(t) + \left[\frac{\omega_{a_i}\omega_{b_i}}{z_i^2}(1 - \cos z_i\Delta t) + \frac{\omega_{c_i}}{z_i}\sin z_i \Delta t\right]\mathbf{b}_i(t)$$

$$
\begin{aligned}
& + \left[\frac{\omega_{a_i}\omega_{c_i}}{z_i^2}(1-\cos z_i\Delta t) - \frac{\omega_{b_i}}{z_i}\sin z_i\Delta t\right]\mathbf{c}_i(t) \\
\mathbf{g_b} \;=\; & \left[\frac{\omega_{a_i}\omega_{b_i}}{z_i^2}(1-\cos z_i\Delta t) - \frac{\omega_{c_i}}{z_i}\sin z_i\Delta t\right]\mathbf{a}_i(t) + \left[\frac{({\omega_{a_i}}^2+{\omega_{c_i}}^2)\cos z_i\Delta t + {\omega_{b_i}}^2}{z_i^2}\right]\mathbf{b}_i(t) \\
& + \left[\frac{\omega_{b_i}\omega_{c_i}}{z_i^2}(1-\cos z_i\Delta t) + \frac{\omega_{a_i}}{z_i}\sin z_i\Delta t\right]\mathbf{c}_i(t) \\
\mathbf{g_c} \;=\; & \left[\frac{\omega_{a_i}\omega_{c_i}}{z_i^2}(1-\cos z_i\Delta t) + \frac{\omega_{b_i}}{z_i}\sin z_i\Delta t\right]\mathbf{a}_i(t) + \left[\frac{\omega_{b_i}\omega_{c_i}}{z_i^2}(1-\cos z_i\Delta t) - \frac{\omega_{a_i}}{z_i}\sin z_i\Delta t\right]\mathbf{b}_i(t) \\
& + \left[\frac{({\omega_{a_i}}^2+{\omega_{b_i}}^2)\cos z_i\Delta t + {\omega_{c_i}}^2}{z_i^2}\right]\mathbf{c}_i(t). \qquad (45)
\end{aligned}
$$

## Brownian Dynamics Algorithm

We modify the second-order BD algorithm of Iniesta and Garcia de la Torre [10] for translational and rotational motions as follows:

1. A first-order estimate of the rotational and translational configuration update is made. The rotational update is calculated by:

$$
\begin{aligned}
\Delta\Omega_{a_i}^{n,*} &= \frac{\Delta t}{\xi_{a_i}}\left(\tau_{a_i}^n + \tau_{r_{ai}}^n\right) \\
\Delta\Omega_{b_i}^{n,*} &= \frac{\Delta t}{\xi_{b_i}}\left(\tau_{b_i}^n + \tau_{r_{bi}}^n\right) \\
\Delta\Omega_{c_i}^{n,*} &= \frac{\Delta t}{\xi_{c_i}}\left(\tau_{c_i}^n + \tau_{r_{ci}}^n\right), \qquad (46)
\end{aligned}
$$

where $\{\Delta\Omega_{a_i}^{n,*},\, \Delta\Omega_{b_i}^{n,*},\, \Delta\Omega_{c_i}^{n,*}\}$ denote finite rotations of the $i$th particle about its local coordinate system $\{\mathbf{a}_i^n,\, \mathbf{b}_i^n,\, \mathbf{c}_i^n\}$. The random torques are chose from zero-mean Gaussian distributions with variance

$$
\begin{aligned}
\langle \tau_{r_{ai}}^n \tau_{r_{ai}}^m \rangle &= 2k_B\mathrm{T}\;\xi_{a_i}\delta_{nm} \\
\langle \tau_{r_{bi}}^n \tau_{r_{bi}}^m \rangle &= 2k_B\mathrm{T}\;\xi_{b_i}\delta_{nm} \\
\langle \tau_{r_{ci}}^n \tau_{r_{ci}}^m \rangle &= 2k_B\mathrm{T}\;\xi_{c_i}\delta_{nm}, \qquad (47)
\end{aligned}
$$

where $\delta_{nm}$ is the Kroneker delta. Using equations (44) and (45) we rotate the the local coordinate systems according to:

$$
\begin{aligned}
\tilde{\mathbf{a}}_i^{n+1,*} &= \mathbf{g}_a\left(\mathbf{a}_i^n, \mathbf{b}_i^n, \mathbf{c}_i^n;\; \Omega_{a_i}^{n,*}/\Delta t, \Omega_{b_i}^{n,*}/\Delta t, \Omega_{c_i}^{n,*}/\Delta t;\; \Delta t\right) \\
\tilde{\mathbf{b}}_i^{n+1,*} &= \mathbf{g}_b\left(\mathbf{a}_i^n, \mathbf{b}_i^n, \mathbf{c}_i^n;\; \Omega_{a_i}^{n,*}/\Delta t, \Omega_{b_i}^{n,*}/\Delta t, \Omega_{c_i}^{n,*}/\Delta t;\; \Delta t\right) \\
\tilde{\mathbf{c}}_i^{n+1,*} &= \mathbf{g}_c\left(\mathbf{a}_i^n, \mathbf{b}_i^n, \mathbf{c}_i^n;\; \Omega_{a_i}^{n,*}/\Delta t, \Omega_{b_i}^{n,*}/\Delta t, \Omega_{c_i}^{n,*}/\Delta t;\; \Delta t\right). \qquad (48)
\end{aligned}
$$

The asterisk superscript again denotes here the first-order estimate. The tilde notation is used to specify that these estimates of the coordinate axes are made based on the rotation step alone. A further modification (described below) of the local coordinate axes is associated with the translation step due to the constraint that the DNA beads rotate only about the $\mathbf{a}_i$ axes.

2. The first-order translational update is given by:

$$\mathbf{r}^{n+1,*} = \mathbf{r}^n + \frac{\Delta t}{k_B \mathrm{T}} \mathbf{D}^n \mathbf{f}^n + \mathbf{w}^n. \tag{49}$$

where $\mathbf{w}^n$ denotes a random move chosen from a Gaussian distribution with zero mean and covariance structure,

$$\langle (\mathbf{w}^n)(\mathbf{w}^m)^T \rangle = 2\Delta t \ \mathbf{D}^n \delta_{nm}. \tag{50}$$

Here $\mathbf{D}^n$ is the configuration-dependent diffusion matrix calculated for the configuration $\mathbf{r}^n$ and $\delta_{nm}$ is the Kroneker delta. The vector $\mathbf{f}^n$ is the systematic force at the $n$th time step.

3. To enforce the constraint that the linker DNA beads are free to rotate only about the $\mathbf{a}_i$ axes, we recompute the local coordinate systems of the particles after the position vector $\mathbf{r}^{n+1,*}$ has been calculated. Namely, for all linker beads, we calculate $\mathbf{a}_i$ according to its definition in equation (1):

$$\mathbf{a}_i^{n+1,*} = \begin{cases} (\mathbf{r}_{i+1}^{n+1,*} - \mathbf{r}_i^{n+1,*}) / \|\mathbf{r}_{i+1}^{n+1,*} - \mathbf{r}_i^{n+1,*}\| & \text{for } i+1 \in I_l \\ \dfrac{\mathbf{r}_{i+1}^{n+1,*} - r_o(\mathbf{b}_{i+1}^{n+1,*} \cos\theta_o - \mathbf{a}_{i+1}^{n+1,*} \sin\theta_o) + w_o \mathbf{c}_{i+1}^{n+1,*} - \mathbf{r}_i^{n+1,*}}{\|\mathbf{r}_{i+1}^{n+1,*} - r_o(\mathbf{b}_{i+1}^{n+1,*} \cos\theta_o - \mathbf{a}_{i+1}^{n+1,*} \sin\theta_o) + w_o \mathbf{c}_{i+1}^{n+1,*} - \mathbf{r}_i^{n+1,*}\|} & \text{for } i+1 \in I_c \end{cases} \tag{51}$$

We then define $\delta \mathbf{a}_i^* = \mathbf{a}_i^{n+1,*} - \tilde{\mathbf{a}}_i^{n+1,*}$. Since we require all rotations about $\mathbf{a}_i$ to vanish (for the translation step), the new displacements are calculated [4]:

$$\delta \mathbf{b}_i^* = -(\delta \mathbf{a}_i^* \cdot \tilde{\mathbf{b}}_i^{n+1,*}) \tilde{\mathbf{a}}_i^{n+1,*} \tag{52}$$

and then $\mathbf{b'}_i^{n+1,*} = \tilde{\mathbf{b}}_i^{n+1,*} + \delta \mathbf{b}_i^*$. Then $\mathbf{b}_i^{n+1,*}$ is determined as the component of $\mathbf{b'}_i^{n+1,*}$ perpendicular to $\mathbf{a}_i^{n+1,*}$ (see Figure 1):

$$\mathbf{b}_i^{n+1,*} = \frac{\mathbf{b'}_i^{n+1,*} - (\mathbf{b'}_i^{n+1,*} \cdot \mathbf{a}_i^{n+1,*}) \mathbf{a}_i^{n+1,*}}{\|\mathbf{b'}_i^{n+1,*} - (\mathbf{b'}_i^{n+1,*} \cdot \mathbf{a}_i^{n+1,*}) \mathbf{a}_i^{n+1,*}\|}. \tag{53}$$

Finally, $\mathbf{c}_i^{n+1,*}$ can be calculated from the cross product:

$$\mathbf{c}_i^{n+1,*} = \mathbf{a}_i^{n+1,*} \times \mathbf{b}_i^{n+1,*}. \tag{54}$$

4. The first-order estimate of the configuration at time $(n+1)\Delta t$ (given by the position vector $\mathbf{r}^{n+1,*}$ and the local coordinate systems $\{\mathbf{a}_i^{n+1,*}, \mathbf{b}_i^{n+1,*}, \mathbf{c}_i^{n+1,*}\}$) yields an estimate of the forces and torques acting at the end of the $n+1$ time step. These forces and torques, denoted by $\mathbf{f}_s^{n+1,*}$ and $\{\tau_{a_i}^{n+1,*}, \tau_{b_i}^{n+1,*}, \tau_{c_i}^{n+1,*}\}$, are used to construct an explicit second-order coordinate update:

   The finite rotations are given by

$$\begin{aligned} \Delta\Omega_{a_i}^n &= \frac{\Delta t}{\xi_{a_i}} \left( (\tau_{a_i}^n + \tau_{a_i}^{n+1,*})/2 + \tau_{r_{ai}}^n \right) \\ \Delta\Omega_{b_i}^n &= \frac{\Delta t}{\xi_{b_i}} \left( (\tau_{b_i}^n + \tau_{b_i}^{n+1,*})/2 + \tau_{r_{bi}}^n \right) \\ \Delta\Omega_{c_i}^n &= \frac{\Delta t}{\xi_{c_i}} \left( (\tau_{c_i}^n + \tau_{c_i}^{n+1,*})/2 + \tau_{r_{ci}}^n \right), \end{aligned} \tag{55}$$

and the the position update is given by:

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \frac{\Delta t}{2k_B\mathrm{T}}\mathbf{D}^n(\mathbf{f}^n + \mathbf{f}^{n+1,*}) + \mathbf{w}^n. \tag{56}$$

Again, the local coordinate systems of the DNA beads are rotated according to the procedure outlined in equations (51)-(54).

## Setup and Model Parameters

We chose reasonable parameter values from the literature wherever possible. Table 1 lists the elastic and geometric parameters used in the model. The electrostatic parameters discussed above are derived based on a detailed analysis of the solvated core particle [11]. A reasonably accepted value for the twisting energy constant is $C = 3.0 \times 10^{-12}$ erg · nm [12], which corresponds to a twisting persistence length of about 75 nm. The bending rigidity constant is calculated from equation (12) based on the persistence length of DNA which is set here to be 50 nm, which yields $g = 6.9 \times 10^{-13}$ erg. This value is consistent with recent measures of the non-electrostatic contribution to the bending rigidity (e.g., the high-salt limit of the persistence length) [13].

Excluded volume parameters $\sigma_1$, $\sigma_2$, and $k_{\mathrm{ex}}$ are the only free parameters used in the model. We have shown [11] that the Debye-Hückel electrostatic potential is accurate at distances of greater than 1 nm at the salt concentration of $C_s = 0.05$ M. Thus setting the core/core excluded volume distance parameter $\sigma_2 = 2$ nm, ensures that the potential remains fairly accurate and the charges are not allowed to overlap. The linker/core distance parameter is set to $\sigma_1 = 3$ nm, to account for the approximate radius of double helical DNA.

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