1 Definition of classes

2 Field-theoretic treatment of interactions

Our treatment of interactions uses a field-theoretic treatment of the densities to determine the interactions between polymer segments. Following work by de Pick, *et al.* [1], we define

The simulation has a fixed volume with sides lengths L_x, L_y, and L_z. These lengths are discretize into M_x, M_y, and M_z bins of length $\Delta_x = L_x/M_x$, $\Delta_y = L_y/M_y$, and $\Delta_z = L_z/M_z$. The bins are defined by the three indices i_x, i_y, and i_z that run from zero to $M_x - 1$, $M_y - 1$, and $M_z - 1$, respectively.

We consider the nth bead located at position $\vec{r}^{(n)}$. We define a weight function $w_I(\vec{r}^{(n)})$ within the Ith bin. The Ith index is defined to be a superindex that combines i_x, i_y, and i_z into a single unique index $I = i_x + M_x i_y + M_x M_z i_z$ that runs from zero to $M_x M_y M_z - 1$ (total of $M_x M_y M_z$ unique indices) The total weight on the Ith bin is given by the contributions from the three cartesian directions, *i.e.* $w_I(\vec{r}^{(n)}) = w_{i_x}^{(x)}(x^{(n)}) w_{i_y}^{(y)}(y^{(n)}) w_{i_z}^{(z)}(z^{(n)})$. Figure 1 shows a schematic of the x-direction weight function (same method for y and z). This shows a linear interpolation weighting method, consistent with Ref. [1].

The number of epigenetic proteins (*e.g.* HP1) to the nth site is given by $N_I^{(\alpha)}$, where α determines the type of epigenetic mark. The α-protein density within the Ith bin is given by

$$\rho_I^{(\alpha)} = \frac{1}{v_{\text{bin}}} \sum_{n=0}^{n_b-1} w_I(\vec{r}^{(n)}) N_I^{(\alpha)} \tag{1}$$

where $v_{\text{bin}} = \Delta_x \Delta_y \Delta_z$ is the volume of a bin. The maximum number of epigenetic proteins bound $N_{\text{max}}^{(\alpha)}$ gives an upper bound on the number of proteins that can bind to a bead, accounting for coarse graining of a bead to represent multiple nucleosomes. For discretization of one nucleosome per bead, the maximum $N_{\text{max}}^{(\alpha)} = 2$ implies binding of a protein to the two histone tail proteins for the α epigenetic mark. We define the number of α marks on the Ith bead as $M_I^{(\alpha)}$, which can take values from zero to $N_{\text{max}}^{(\alpha)}$.

Protein binding to a marked tail results in energy $-\beta\varepsilon_m$ [non-dimensionalized by $\beta = 1/(k_B T)$], and protein binding to an unmarked tail is associated with energy $-\beta\varepsilon_u$. The chemical potential of the α protein is defined as $\beta\mu^{(\alpha)}$. The binding of $N_I^{(\alpha)}$ proteins to a bead with $M_I^{(\alpha)}$ marks results in a free energy that accounts for all of the combinatoric ways of binding.

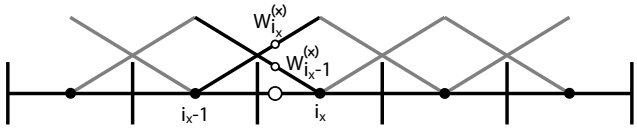

Figure 1: Schematic of the weight function $w_{i_x}^{(x)}$ that gives the weighting of the particle in the i_x site in the x-direction based on a linear interpolation method [1].

3 Energetic contributions to the Monte Carlo simulation

3.1 Polymer chain model: shearable, stretchable wormlike chain

We consider a polymer with n_b number of beads. We consider the shearable, stretchable wormlike chain potential, given by

$$\beta E_{\text{elas}} = \sum_{n=0}^{n_b-2} \left[\frac{\varepsilon_b}{2\Delta} \left| \vec{t}_3^{(n+1)} - \vec{t}_3^{(n)} - \eta \Delta \vec{r}_\perp^{(n)} \right|^2 + \frac{\varepsilon_\parallel}{2\Delta} \left(\Delta \vec{r}^{(n)} \cdot \vec{t}_3^{(n)} - \Delta\gamma \right)^2 + \frac{\varepsilon_\perp}{2\Delta} \left| \Delta \vec{r}_\perp^{(n)} \right|^2 \right], \qquad (2)$$

where $\Delta\vec{r}^{(n)} = \vec{r}^{(n+1)} - \vec{r}^{(n)}$ is the bond vector, $\Delta\vec{r}_\perp^{(n)} = \Delta\vec{r}^{(n)} - (\Delta\vec{r}^{(n)} \cdot \vec{t}_3^{(n)})\vec{t}_3^{(n)}$ is the perpendicular component of the bond vector to the tangent vector.

References

[1] Darin Q. Pike, François A. Detcheverry, Marcus Müller, and Juan J. de Pablo. Theoretically informed coarse grain simulations of polymeric systems. *The Journal of Chemical Physics*, 131(8):084903, August 2009.