

Appendix A: Details of the SAW simulation with the pivot algorithm

The simulation details using the pivot algorithm in each space are listed below [Fig. 1].

- *In 3-D space.* A bead is randomly selected as a “pivot”, with the beads on both sides defined as left and right arms. The shorter arm is then randomly rotated about the pivot bead through the following steps: 1) Translate the entire chain so that the pivot bead is located at the origin of the xyz-coordinate system (the position of the pivot bead refers to its center and this applies consistently). 2) Rotate the shorter arm around the z -axis by an angle ϕ , randomly sampled from the uniform distribution $U(0, 2\pi)$. 3) Rotate the shorter arm around y -axis by an angle θ , where $\cos \theta$ is randomly sampled from $U(-1, 1)$. 4) Optionally, translate the chain back to restore the pivot bead to its original position. Denote the coordinate of bead i ($\in \{1, 2, \dots, N\}$) as $B_i = (x_i, y_i, z_i)$ and assume the p -th (e.g., $p > N/2$) bead as the pivot. Then the coordinates of rotated beads can be mathematically represented by $B_p + (B_i - B_p)R_z(\phi)R_y(\theta)$ (e.g., $i \in \{p+1, \dots, N\}$) and the rotation matrices $R_z(\phi) = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$ and $R_y(\theta) = \begin{pmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{pmatrix}$. If the rotated arm overlaps with the other arm, the rotation is rejected, and the previous conformation’s count increases by ‘1’. Rotation operations are executed at least 2×10^5 times. Other operations, e.g. reflection, may also be preformed but have minimal impact on the results. Gyration radius and EED are calculated for each step. The simulation runs until both variables show no upward/downward trend over a given period or reach a set time limit.
- *In 2-D space (i.e., plane).* The procedure mirrors the 3-D method. For the shorter arm, the rotation axis (z axis) is perpendicular to the walking plane (xy -plane) and passes through the pivot bead; the rotation angle (ϕ) is randomly sampled from the uniform distribution $U(0, 2\pi)$ with the modified rotation formula $B_p + (B_i - B_p)R_z(\phi)$.
- *On a spherical surface.* The procedure follows the same steps in 3-D space. For the rotated shorter arm: the rotation axis passes through the pivot bead and the sphere’s center; the rotation angle ϕ is randomly sampled from $U(0, 2\pi)$; the rotation formula is $B_i R_z(-\phi_1) R_y(-\theta_1) R_z(\phi) R_y(\theta_1) R_z(\phi_1)$, where the origin is the spherical center, and (θ_1, ϕ_1) represents the orientation of the rotation axis.
- *Inside a sphere.* Same as 3-D space, but reject rotation if any bead exits the sphere.
- *Partially confined to a spherical surface.* The confined beads (preset in number) are assumed to be evenly spaced along the chain. The left and right arms are defined as in 3-D space. The segment between two adjacent confined beads is termed a subchain. A random bead is selected as the pivot, and the subchain containing it is the pivot subchain. The portion of the pivot subchain to the left (or right) of the pivot is defined as the left (or right) subarm. If the pivot bead is restricted to the spherical surface, rotate the shorter arm by a random angle ($\phi \sim U(0, 2\pi)$) around the axis passing through the pivot bead and the sphere’s center, similar to the rotation when the entire chain is confined to the sphere. If the pivot bead is not confined, 1) rotate the right (or left) subarm around an axis through the pivot bead, perpendicular to the plane defined by the pivot bead, the spherical center, and the right (or left) end bead; 2) to return the right (or left) end bead of the pivot subchain to the surface, rotate the entire pivot subchain around an axis through the left (or right) end bead, perpendicular to the plane formed by the pivot bead and both end beads of the pivot subchain; 3) rotate the subchains on the right (or left) side of the pivot subchain to reconnect with its moved end, using an axis through the spherical center, perpendicular to the plane containing the spherical center and the right (or left) end bead of the pivot subchain before and after the previous movements.
- *Partially confined inside a sphere.* Same as 3-D space, reject rotation if one confined bead leaves the sphere.