

Biophysical Journal, Volume 122

Supplemental information

Epigenetic switching with asymmetric bridging interactions

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1 Simulation details

1.1 Nucleosome dynamics

The nucleosome dynamics is evolved using the Euler–Maruyama method,

$$\mathbf{X}_i(t + \Delta t) = \mathbf{X}_i(t) - \nabla_{\mathbf{X}_i} U(\mathbf{X}(t)) \Delta t + \sigma \mathbf{N}_i(t) \sqrt{\Delta t}, \quad (\text{S1})$$

where U is the potential described in the main text, σ is the noise scale (stemming from diffusion), and $\mathbf{N}_i(t)$ is a vector of standard Gaussian distributed random numbers.

Our model polymer is completely inelastic, which we implement by only permitting monomer motion that consists of rotations in the plane perpendicular to the distance vector between adjacent monomers (except at the end-points). To achieve this, each time step is subdivided into a three-step process:

- For *endpoint* monomers we use Eq. (S1) directly, and subsequently the position of the monomers are moved along the distance vector to their respective neighbors, such that the distance between the monomers is restored to ℓ_0 .
- For *even-indexed, non-endpoint* monomers, we update the position indirectly via the angle updates:

$$\theta_i(t + \Delta t) - \theta_i(t) = -\nabla_{\theta_i} U(\mathbf{X}(t)) \Delta t + \sigma/r_i \mathbf{N}_i(t) \sqrt{\Delta t}, \quad (\text{S2})$$

where θ_i is the angle of rotation (with respect to a fixed starting-point) for the i 'th monomer, and r_i is the radius of rotation of the i 'th monomer at time step t .

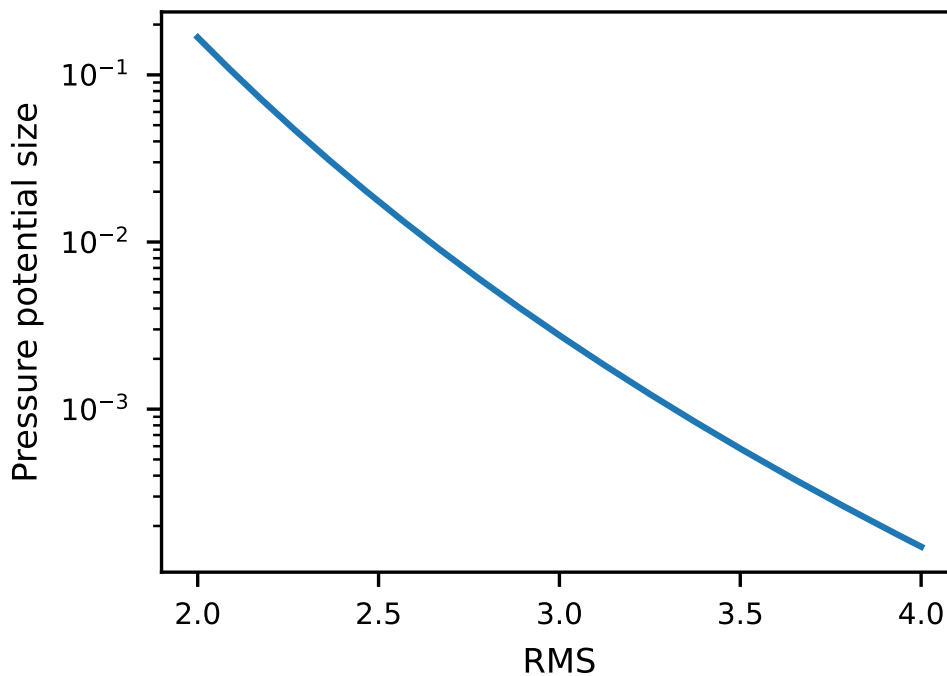


Figure S1: The relationship between the pressure potential size and the average RMS.

- For *odd-indexed, non-endpoint* monomers the same procedure is performed as for even-indexed monomers.

The potential gradients are calculated using automatic differentiation via the `torch.autograd` functionality from the PYTORCH library [1].

1.2 Parameters

- The distance within which S-S bonds are allowed to be formed is set equal to ℓ_0 .
- The noise scale is fixed to $\sigma = \frac{1}{\sqrt{2}}$.

- The proportionality constant of Eq. (2), corresponding to the scaling parameter for the interaction potential, is equal to 50.
- The proportionality constant of Eq. (3), i.e., the pressure potential size, is calculated as a function of the desired average RMS of the polymer, determined empirically from simulations (Fig. S1).

2 Bistability

Fig. S2 shows the bistability of the system, i.e. that active polymers remain active and silent polymers remain silent in the absence of *cenH*.

References

- [1] Paszke, Adam *et. al.* *PyTorch: An Imperative Style, High-Performance Deep Learning Library* Advances in Neural Information Processing Systems 32 (2019).

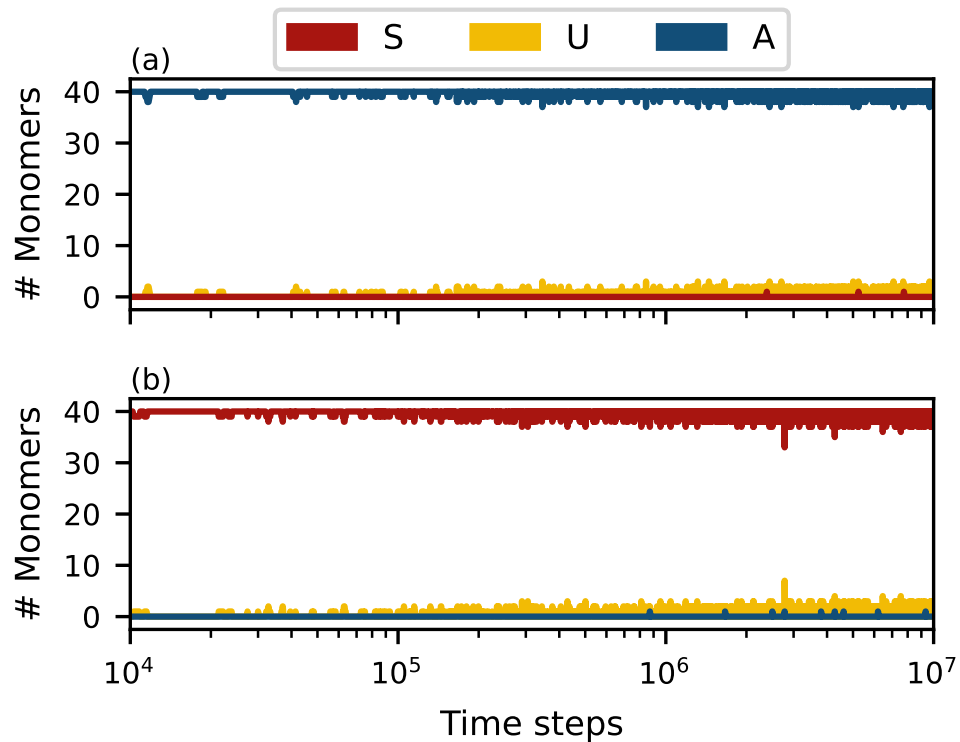


Figure S2: Time-space plots showing the development of polymers without a *cenH* region. All monomers were initialized in the (a) ‘A’ and (b) ‘S’ states, respectively. Each polymer retains its overall active and silent states, which indicates that the system is bistable. Parameters: As in Figure 2, except: $\text{RMS} \approx 2.0$. Note that the x-axis is log-scaled — the density of random events is *not* increasing as a function of time.