

Supplemental Materials: DNA Barcode by Flossing through a Cylindrical Nanopore

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I. SECTION 1: THE MODEL

Our BD scheme is implemented on a bead-spring model of a polymer with the monomers interacting via an excluded volume (EV), a Finite Extension Nonlinear Elastic (FENE) spring potential, and a bond-bending potential enabling variation of the chain persistence length ℓ_p (Fig.S1). The model, originally introduced for a fully flexible chain by Grest and Kremer [S1], has been studied quite extensively by many groups using both Monte Carlo (MC) and various molecular dynamics (MD) methods [S2]. Recently we have generalized the model for a semi-flexible chain and studied both equilibrium and dynamic properties [S3–S5] and studied compression dynamics of a model dsDNA inside a nanochannel [S6, S7]. The mutual EV interaction among any two monomers are given by the truncated Lennard-Jones (LJ) potential with a cut-off radius $2^{1/6}\sigma$

$$U_{LJ}(r_{ij}) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] + \epsilon, & \text{for } r < 2^{1/6}\sigma \\ 0, & \text{otherwise} \end{cases} \quad (\text{S1})$$

where σ is the effective diameter of a monomer and ϵ is the interaction strength. To mimic the connectivity between two adjacent monomers, finite-extensible-non-linear elastic (FENE) potential

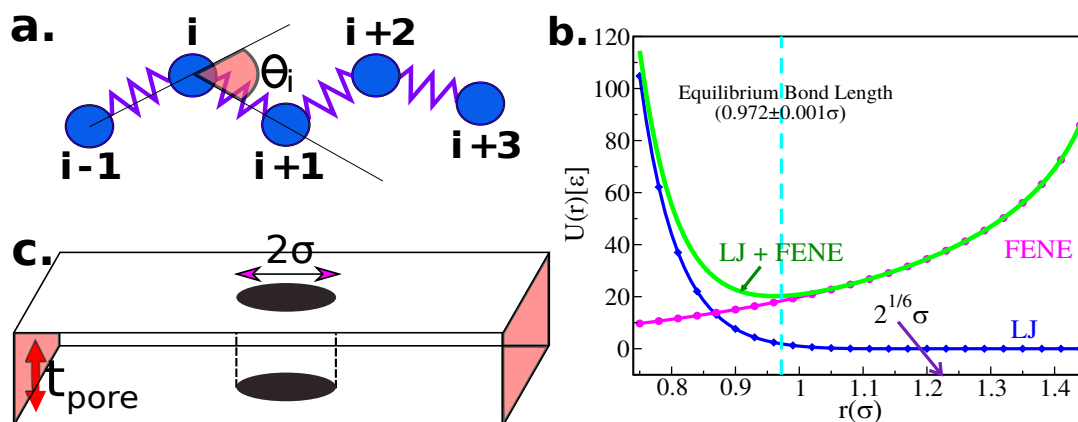


FIG. S1. (a) Illustration depicts the monomers are interacting via LJ and FENE potential. The three body bending potential is calculated using the angle θ_i between two adjacent bond vectors \vec{b}_i and \vec{b}_{i+1} respectively. (b) Interaction potential between two consecutive monomers is given by the green line for a separation distance r in unit of σ . The blue diamonds denote the LJ potential with a cutoff radius $2^{1/6}\sigma$ and the magenta circles correspond to the FENE potential with a spring constant $\kappa_F = 30.0\epsilon/\sigma^2$. (c) A cylindrical nanopore of diameter 2σ is drilled into a material of thickness t_{pore} . The walls consist of purely repulsive LJ particles.

$$U_{FENE}(r_{ij}) = -\frac{1}{2}\kappa_F R_0^2 \ln \left[1 - \left(\frac{r_{ij}}{R_0} \right)^2 \right] \quad (\text{S2})$$

is used with the maximum bond-stretching length $R_0 = 1.5\sigma$ and spring constant $\kappa_F = 30\epsilon/\sigma^2$. Here, $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the separation distance between two adjacent monomers i and $j = i \pm 1$ located at \vec{r}_i and \vec{r}_j respectively. Along with these two potentials, we introduce a bending potential

$$U_{bend}(\theta_i) = \kappa (1 - \cos(\theta_i)) \quad (\text{S3})$$

with bending rigidity κ . In three dimensions, for $\kappa \neq 0$, the persistence length ℓ_p of the chain is related to κ via [S8]

$$\ell_p = \frac{\kappa}{k_B T}, \quad (\text{S4})$$

where k_B is the Boltzmann constant and T is the temperature. Here θ_i is the bond angle between two subsequent bond vectors $\vec{b}_i = \vec{r}_{i+1} - \vec{r}_i$ and $\vec{b}_{i-1} = \vec{r}_i - \vec{r}_{i-1}$. A cylindrical nanopore of diameter 2σ is drilled through a solid material of thickness t_{pore} consists of immobile and purely repulsive LJ particles. Our model of DNA polymer consists 1016 monomer beads along with 8 heavier tags ($T_1 - T_8$) located at positions 154, 369, 379, 399, 614, 625, 696, and 901 respectively (please refer to Fig. 2 and Table-I in the main article). A recent study by Zhang et al. on 48512 bp long dsDNA uses 75 bp long protein tags as barcodes [S9]. In simulation, we purposely choose the mass of a tag (m_{tag}) three times heavier of a normal monomer to replicate the tags used in the experiments. We proportionally increase the solvent friction of the tags $\Gamma_{tag} = 3\Gamma_i$. We use the Brownian dynamics to solve the equation of motion of a monomer i having a mass m_i and solvent friction Γ_i as

$$m_i \ddot{\vec{r}}_i = \vec{\nabla}_i [U_{LJ} + U_{FENE} + U_{bend} + U_{wall}] - \Gamma_i \vec{v}_i + \eta_i \quad (S5)$$

where $\Gamma_i = 0.7\sqrt{m_i\epsilon^2/\sigma^2}$ is the frictional coefficient arising from solvent-monomer interaction. For the case of a tag, $m_{tag} = 3m_i$ and $\Gamma_{tag} = 2.1\sqrt{m_i\epsilon^2/\sigma^2}$. The Gaussian white noise η_i arising from thermal fluctuation is delta correlated and expressed as $\langle \eta_i(t) \cdot \eta_j(t') \rangle = 2dk_B T \Gamma_i \delta_{ij} \delta(t - t')$ with $d = 3$ in three dimension. We express length and energy in units of σ and ϵ respectively such that $k_B T / \epsilon = 1.0$. The parameters for FENE potential in Eq. (S2) are κ_F and R_0 , and set to be $\kappa_F = 30\epsilon/\sigma^2$ and $R_0 = 1.5\sigma$. The numerical integration of Eq. (S5) is implemented using the algorithm introduced by Gunsteren and Berendsen [S10]. Our previous experiences with BD simulation suggests that for a time step $\Delta t = 0.01$ these parameters values produce stable trajectories over a very long period of time and do not lead to unphysical crossing of a bond by a monomer [S4, S5]. The average bond length stabilizes to $\langle b_l \rangle = 0.971 \pm 0.001\sigma$ with negligible fluctuation regardless of the chain size and rigidity [S4]. Hence we relate the polymer's contour length L and the number of monomers N as $L = (N - 1)\langle b_l \rangle$.

II. SECTION 2: THE TENSION PROPAGATION THEORY AND THE MOVIE

The non-monotonic velocity profile can be explained using tension propagation theory. Fig. S2 shows an example on how the segment connecting T_7 and T_8 has non-monotonic velocity under the influence of the tension front. The accompanying movie (Fig. S3) shows the uncoiling of the chain and the corresponding velocities of the monomers and the tags.

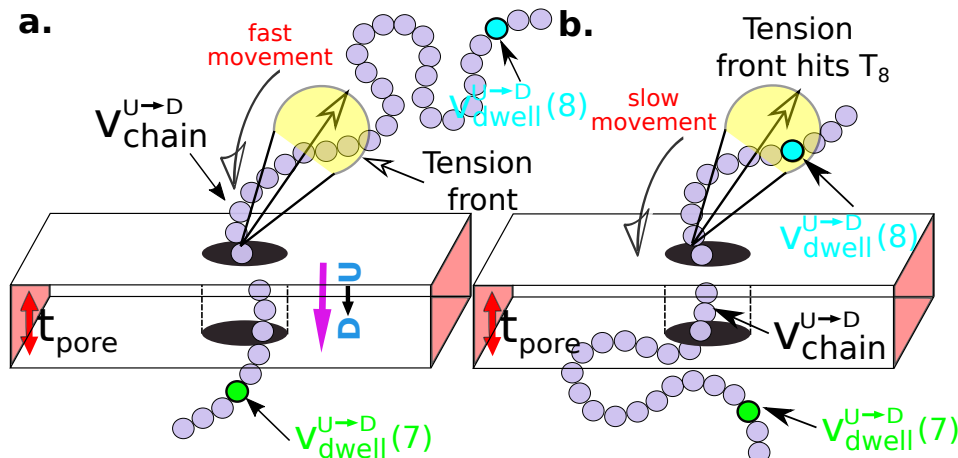


FIG. S2. Tension propagation (TP) through the chain backbone connecting T_7 and T_8 . (a) Figure shows a sudden fast movement of monomers right after T_7 's passage through the pore. Due to the TP front's influence (yellow blob region), subsequent monomers are sucked into the pore quickly. (b) TP front finally reaches T_8 , leading to a slower translocation speed due to the tag's large inertia and higher viscous drag.

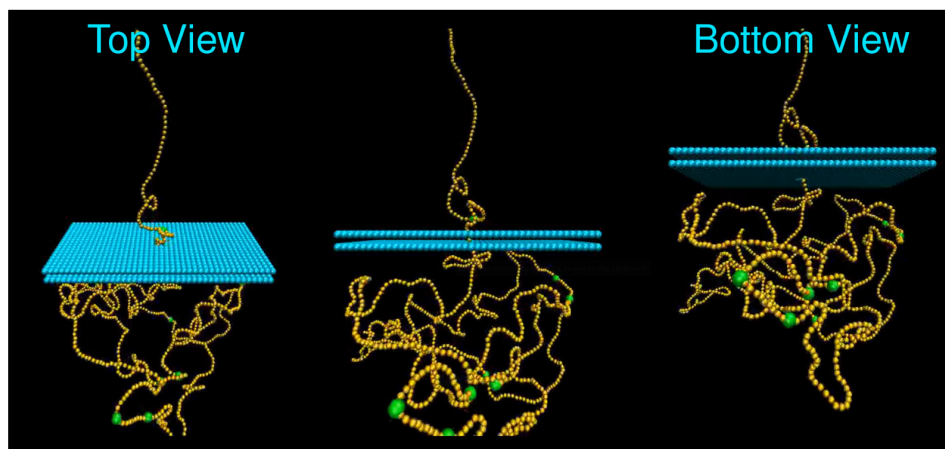


FIG. S3. A single movie frame (screen-shot) depicting the translocation process of a dsDNA through the cylindrical nanopore. The movie captures three different angle views (from Top, Middle and Bottom side) in synchronization and presented in three columns. Monomers are depicted using yellow ● beads and tags are colored in green ●.

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