Supplementary Materials: Loop extrusion drives very different dynamics for Rouse chains in bulk solutions and at interfaces

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S1 Rouse model

We use the Rouse model to treat the dynamics of a chromatin fiber that is extruded by cohesin. With this model, the chromatin fiber is treated as beads that are connected by springs of the spring constant k $(= 3k_{\rm B}T/b^2)$, where $k_{\rm B}$ is the Boltzmann constant, T is the absolute temperature, and b is the Kuhn length. For simplicity, we here treat the dynamics of the z-component of the positions of the beads. The position $z_n(t)$ of the n-th bead is derived as a function of time t by the Langevin equation

$$\zeta \frac{\partial}{\partial t} z_n(t) = k \frac{\partial^2}{\partial n^2} z_n(t) + f_n(t) + F_m(t)\delta_{mn}, \quad \text{(S1)}$$

where $n = 1, 2, \cdots$. Eq. (S1) represents the fact that the friction force applied to the bead (the left side) is balanced by the elastic force generated by the springs (the first term in the right side), the random force $f_n(t)$ due to the random collision of solvent molecules (the second term in the right side), and the force $F_m(t)$ generated by the loop extrusion process (the third term in the right side). ζ is the friction constant of a bead. The random force $f_n(t)$ is the Wiener process with $\langle f_n(t)\rangle = 0$ and $\langle f_n(t) f_{n'}(t')\rangle = 2\zeta k_{\rm B}T\delta_{nn'}\delta(t-t')$. δ_{mn} is 1 for $m = n$ and 0 otherwise; eq. (S1) implies that the force $F_m(t)$ is applied only to the m-th bead at which the cohesin is located. The boundary condition of eq. (S1) is $\frac{\partial z_n}{\partial n} = 0$ at the ends of the chain.

Taking the average to the both sides of eq. (S1) leads to the form

$$\zeta \frac{\partial}{\partial t} \langle z_n(t)\rangle = k \frac{\partial^2}{\partial n^2} \langle z_n(t)\rangle + F_m(t)\delta_{mn}. \quad \text{(S2)}$$

The Green function $G(t)$ of eq. (S2) is thus defined by the solution of the equation

$$\frac{\partial}{\partial t} G(n,m,t) = \frac{k}{\zeta} \frac{\partial^2}{\partial n^2} G(n,m,t) + \delta(t)\delta_{mn}. \quad \text{(S3)}$$

Comparing eqs. (S2) and (S3) leads to the form

$$\langle z_n(t)\rangle - \langle z_n(0)\rangle = \frac{1}{\zeta}\int_0^t dt'\, G(n,m,t-t')F(t'). \tag{S4}$$

When the chain is infinitly long, the solution of eq. (S3) has the form

$$G(n,m,t) = \left(\frac{\zeta}{4\pi k t}\right)^{1/2} \mathrm{e}^{-\zeta(n-m)^2/(4kt)}, \tag{S5}$$

where this solution satisfies the boundary condition $\frac{\partial}{\partial n}G(n,m,t) = 0$ for $n \to \infty$ and $-\infty$. Eqs. (S4) and (S5) imply that distant beads are not influenced by the force $F_m(t)$ until the tension generated by the force diffuses to these beads. Restoring the contribution of the random force to eq. (S4) leads to the form

$$z_n(t) - z_n(0) = \frac{1}{\zeta}\int_0^t dt'\, G(n,m,t-t')F(t') + r_n(t), \tag{S6}$$

where $r_n(t)$ is the Wiener process with $\langle r_n(t)\rangle = 0$ and

$$\langle r_n(t) r_m(t)\rangle = \frac{2k_{\mathrm{B}}T}{\zeta}\int_0^t dt'\, G(n,m,t-t'). \tag{S7}$$

Eq. (S7) is derived by using the fluctuation-dissipation theorem. For simplicity, we neglect the contribution $r_n(t)$ of the random force in the main article and the rest of this Supplementary Material.

S2 Loop extrusion at an interface

The Laplace transformation of the both sides of eq. (S6) has the form

$$\Delta z_n^{\mathrm{L}}(s) = \frac{1}{\zeta} G^{\mathrm{L}}(n,m,s) F^{\mathrm{L}}(s), \tag{S8}$$

where $\Delta z_n^{\mathrm{L}}(s)$ is the Laplace transform of the displacement $\Delta z_n(t)$ $(= z_n(t) - z_n(0))$, $G^{\mathrm{L}}(n,m,s)$ is the Laplace transform of the Green function $G(n,m,t)$, and $F^{\mathrm{L}}(s)$ is the Laplace transform of the force $F_m(t)$ generated by the loop extrusion process (the superscript L indicates the Laplace transform). The Green function $G^{\mathrm{L}}(n,m,s)$ has the form

$$G^{\mathrm{L}}(n,m,s) \quad = \quad \frac{\pi}{2}\tau_1 \frac{\mathrm{e}^{-\pi|n-m|\sqrt{s\tau_1}}}{\sqrt{s\tau_1}}, \tag{S9}$$

where τ_1 $(= \zeta/(\pi^2 k))$ is the relaxation time of a monomer.

We here treat the case in which the cohesin is entrapped at the interface $(z = 0)$. The force that is necessary to displace the m-th bead (which is bound by the cohesin) by u_m and to fix the bead at the position has the form

$$\begin{aligned} F^{\mathrm{L}}(s) &= \frac{\zeta u_m}{sG^{\mathrm{L}}(m,m,s)} \\ &= \frac{2}{\pi}\frac{\zeta u_m}{\sqrt{s\tau_1}}, \end{aligned} \tag{S10}$$

where we used the fact that the Laplace transform of the displacement is u_m/s. The inverse Laplace transform of eq. (S10) leads to eq. (7) in the main article. Substituting eq. (S10) into eq. (S8) leads to the displacement $\Delta z_n^{\mathrm{L}}(s)$ of the n-th bead

$$\Delta z_n^{\mathrm{L}}(s) = \frac{u_m}{s}\mathrm{e}^{-\pi|n-m|\sqrt{s\tau_1}}. \tag{S11}$$

The inverse Laplace transform of eq. (S11) leads to the form

$$z_n(t) - z_n(0) = u_m \mathrm{erfc}\left(\frac{\pi}{2}|n-m|\sqrt{\frac{\tau_1}{t}}\right), \tag{S12}$$

where $\mathrm{erfc}(x)$ is the complementary error function that is defined by

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty du\, \mathrm{e}^{-u^2}. \tag{S13}$$

The cohesin drives the loop extrusion process with a constant rate τ_{c}^{-1} in a finite region, starting from $n=1$ and ending at $n=N$. This region is bound by the CTCF molecules that suppress the cohesin to diffuse outside of this region. The m-th bead (from the starting site) is extruded at time $m\tau_{\mathrm{c}}$. The displacement of the n-th bead at time t due to the extrusion of the m-th bead has the form

$$z_n(t) - z_n(m\tau_{\mathrm{c}}) = -z_m(m\tau_{\mathrm{c}})\mathrm{erfc}\left(\frac{\pi}{2}|n-m|\sqrt{\frac{\tau_1}{t-m\tau_{\mathrm{c}}}}\right), \tag{S14}$$

where we used the fact that the $m-1$-th bead is localized at the interface ($z=0$) and the displacement u_m thus has the form $u_m = -z_m(m\tau_{\mathrm{c}})$, see eq. (S12). The beads 1, 2, $\cdots$, $m-1$ have been extruded by the time that the cohesin extrudes the m-th bead. Summing up the contributions of the extrusion steps leads to the form

$$z_n(t) - z_n(0) = -\sum_{l=2}^{m-1} z_l(l\tau_{\mathrm{c}})\mathrm{erfc}\left(\frac{\pi}{2}|n-l|\sqrt{\frac{\tau_1}{t-l\tau_{\mathrm{c}}}}\right), \tag{S15}$$

see eq. (8) in the main article.

The position $z_m(m\tau_{\mathrm{c}})$ of the m-th bead at the moment of the extrusion process is derived by using the form

$$z_m(m\tau_{\mathrm{c}}) - z_m(0) = -\sum_{l=2}^{m-1} z_l(l\tau_{\mathrm{c}})\mathrm{erfc}\left(\frac{\pi}{2}\sqrt{m-l}\sqrt{\frac{\tau_1}{\tau_{\mathrm{c}}}}\right), \tag{S16}$$

where this equation is derived by replacing t and n in eq. (S15) to $m\tau_\mathrm{c}$ and m. We solve eq. (S16) in the form

$$z_m(m\tau_\mathrm{c}) = \sum_{l=0}^{m} \Gamma_{ml} z_l(0), \tag{S17}$$

where Γ_{ml} is derived by the form

$$\Gamma_{mm'} = \delta_{mm'} - \sum_{l=m'}^{m-1} \Gamma_{lm'} \mathrm{erfc}\left(\frac{\pi}{2}\sqrt{\alpha}\sqrt{\frac{m-l}{N}}\right). \tag{S18}$$

We used the parameter

$$\alpha = \frac{\tau_N}{\tau_\mathrm{ex}}. \tag{S19}$$

to represent the ratio of the Rouse time τ_N $(= N^2\tau_1)$ to the time scale τ_ex $(= N\tau_\mathrm{c})$ of the loop extrusion process. Eq. (S18) is derived by substituting eq. (S17) into eq. (S16).

Substituting eq. (S17) into eq. (S15) leads to the form

$$z_n(t) - z_n(0) = -\sum_{l=2}^{m} \Xi_{nl}(t) z_l(0), \tag{S20}$$

where $\Xi_{nl}(t)$ has the form

$$\Xi_{nm}(t) = \sum_{l=m}^{t/\tau_\mathrm{c}} \Gamma_{lm} \mathrm{erfc}\left(\frac{\pi}{2}|n-l|\sqrt{\frac{\tau_1}{t-l\tau_\mathrm{c}}}\right). \tag{S21}$$

Because the starting site is bound by the cohesin, the mean square of the end-to-end distance has the form

$$\begin{aligned}
\frac{3\langle z_N^2(t)\rangle}{Nb^2} &= \frac{3\langle z_N^2(0)\rangle}{Nb^2} - \frac{6}{Nb^2}\sum_{l=2}^{t/\tau_\mathrm{c}} \Xi_{Nl}(t)\langle z_N(0) z_l(0)\rangle \\
&\quad + \frac{3}{Nb^2}\sum_{p=2}^{t/\tau_\mathrm{c}}\sum_{q=2}^{t/\tau_\mathrm{c}} \Xi_{Np}(t)\Xi_{Nq}(t)\langle z_p(0) z_q(0)\rangle \\
&= 1 - \frac{2}{N}\sum_{l=2}^{t/\tau_\mathrm{c}} l\Xi_{Nl}(t) + \frac{2}{N}\sum_{p=2}^{t/\tau_\mathrm{c}}\sum_{q=2}^{p-1} q\Xi_{Np}(t)\Xi_{Nq}(t) \\
&\quad + \frac{1}{N}\sum_{l=2}^{t/\tau_\mathrm{c}} l\Xi_{Nl}^2(t),
\end{aligned} \tag{S22}$$

where we used $\langle z_n(0) z_m(0)\rangle = \frac{b^2}{6}(m+n-|m-n|)$ to derive the last equation.

For $\alpha \to \infty$, the solution of eq. (S18) has an asymptotic form

$$\Gamma_{mm'} = \delta_{mm'}. \tag{S23}$$

Substituting eq. (S23) into eq. (S21) leads to the form

$$\begin{aligned}\Xi_{nm} &= \operatorname{erfc}\left(\frac{\pi}{2}(n-m)\sqrt{\frac{\tau_1}{t-m\tau_{\rm c}}}\right) \\ &\simeq \frac{2N}{\pi^{3/2}}\frac{1}{\sqrt{\alpha}}\frac{1}{1-u}\sqrt{\frac{t}{\tau_{\rm ex}}-u}\,\mathrm{e}^{-\frac{\pi^2}{4}\alpha(1-u)^2/(t/\tau_{\rm ex}-u)},\end{aligned} \tag{S24}$$

where we used $u = m/N$ and the steepest descent to derive the last equation. The mean square of the end-to-end distance thus has an asymptotic form

$$\begin{aligned}\frac{3\langle z_N^2(t)\rangle}{Nb^2} &= 1-\frac{4}{\pi^{3/2}}\frac{N}{\sqrt{\alpha}}\int_0^{t/\tau_{\rm c}} du\,\frac{u}{1-u}\sqrt{\frac{t}{\tau_{\rm ex}}-u}\,\mathrm{e}^{-\frac{\pi^2}{4}\alpha(1-u)^2/(t/\tau_{\rm ex}-u)} \\ &\simeq 1-\frac{4}{\pi^2}\frac{N}{\alpha}\left(2\frac{t}{\tau_{\rm ex}}-1\right)\mathrm{e}^{-\pi^2\alpha(1-t/\tau_{\rm ex})},\end{aligned} \tag{S25}$$

where we used the steepest descent to derive the last equation.

S3 Loop extrusion in a bulk solution

The bead that is bound by the cohesin diffuses freely in the bulk solution. The force $F_m(t)$ is thus applied to the bead only during the extrusion process. For the case in which the applied force is a constant F_0 during the extrusion process, the displacement $\Delta z_m(t)$ of the m-th bead (at which the cohesin is located) due to the extrusion process has the form

$$\begin{aligned}\Delta z_m &= \frac{F_0}{\zeta}\int_0^{r\tau_{\rm c}} dt'\, G(m,m,r\tau_{\rm c}-t') \\ &= \sqrt{\pi}\frac{F_0}{\zeta}\sqrt{r\tau_1\tau_{\rm c}},\end{aligned} \tag{S26}$$

which is derived by using eq. (S6), neglecting the contribution $r_n(t)$ of the random force. r is the duty ratio of the cohesin. The force F_0 that is necessary to displace the m-th bead by u_m thus has the form

$$F_0 = \frac{1}{\sqrt{\pi}}\frac{\zeta u_m}{\sqrt{r\tau_{\rm c}\tau_1}}. \tag{S27}$$

In a long time scale, $t > r\tau_{\rm c}$, the force $F_m(t)$ that is applied to the bead has an asymptotic form

$$\begin{aligned}F_m(t) &= F_0 r\tau_{\rm c}\delta(t) \\ &= \frac{\zeta u_m}{\sqrt{\pi}}\sqrt{\frac{r\tau_{\rm c}}{\tau_1}}\delta(t).\end{aligned} \tag{S28}$$

Substituting eq. (S28) into eq. (S6) leads to the displacement $z_n(t)$ of the n-th bead due to the extrusion of the m-th bead. The displacement $z_n(t)$ has the form

$$z_n(t) - z_n(m\tau_c) = -(z_m(m\tau_c) - z_{m-1}(m\tau_c))K(n, m, t - m\tau_c), \tag{S29}$$

where we used the fact that the extrusion of the m-th bead starts at $t = m\tau_c$ and the displacement u_m of the m-th bead has the form $u_m = z_{m-1}(m\tau_c) - z_m(m\tau_c)$. The function $K(n, m, t)$ is defined by the form

$$K(n, m, t) = \frac{1}{\sqrt{\pi}} \sqrt{\frac{r\tau_c}{\tau_1}} G(n, m, t). \tag{S30}$$

The beads 1, 2, $\cdots$, $m - 1$ have been extruded by the time that the cohesin extrudes the m-th bead. Summing up the contributions of the extrusion steps leads to the form

$$z_n(t) - z_n(0) = -\sum_{l=2}^{m} (z_l(l\tau_c) - z_{l-1}(l\tau_c))K(n, l, t - l\tau_c). \tag{S31}$$

Eq. (S31) implies that the position of the m-th bead right before the extrusion of this bead has the form

$$z_m(m\tau_c) - z_m(0) = -\sum_{l=2}^{m-1} (z_l(l\tau_c) - z_{l-1}(l\tau_c))K(m, l, (m - l)\tau_c). \tag{S32}$$

The position of the $m - 1$-th bead at the time has the form

$$z_{m-1}(m\tau_c) - z_{m-1}(0) = -\sum_{l=2}^{m-1} (z_l(l\tau_c) - z_{l-1}(l\tau_c))K(m - 1, l, (m - l)\tau_c). \tag{S33}$$

By using eqs. (S32) and (S33), we derive the relationship

$$\begin{aligned} z_m(m\tau_c) - z_{m-1}(m\tau_c) &= z_m(0) - z_{m-1}(0) - \sum_{l=2}^{m-1} (z_l(l\tau_c) - z_{l-1}(l\tau_c)) \\ &\quad \times [K(m, l, (m - l)\tau_c) - K(m - 1, l, (m - l)\tau_c)]. \end{aligned} \tag{S34}$$

We derive the solution of eq. (S34) in the form of

$$z_m(m\tau_c) - z_{m-1}(m\tau_c) = \sum_{l=1}^{m} \Gamma_{ml}(z_l(0) - z_{l-1}(0)), \tag{S35}$$

where Γ_{ml} follows from the form

$$\Gamma_{mn} = \delta_{mn} - \sum_{l=n}^{m-1} \Gamma_{ln} \left[K(m, l, (m - l)\tau_c) - K(m - 1, l, (m - l)\tau_c)\right]. \tag{S36}$$

Eq. (S36) is derived by substituting eq. (S35) into eq. (S34).

Substituting eq. (S35) into eq. (S31) leads to the form

$$z_n(t) - z_n(0) = -\sum_{l=2}^{t/\tau_c - 1} \Xi_{nl}(t)(z_l(0) - z_{l-1}(0)), \tag{S37}$$

where the function $\Xi_{nl}(t)$ has the form

$$\Xi_{nl}(t) = \sum_{m=l}^{t/\tau_c - 1} \Gamma_{ml} K(n, m, t - m\tau_c). \tag{S38}$$

The mean square of the end-to-end distance thus has the form

$$\begin{aligned}
\langle (z_N(t) - z_{t/\tau_c}(t))^2 \rangle &= \langle (z_N(0) - z_{t/\tau_c}(0))^2 \rangle \\
&\quad -2 \sum_{l=2}^{t/\tau_c - 1} (\Xi_{Nl}(t) - \Xi_{t/\tau_c - 1, l}(t)) \langle (z_l(0) - z_{l-1}(0))(z_N(0) - z_{t/\tau_c}(0) \rangle \\
&\quad + \sum_{p=1}^{t/\tau_c - 1} \sum_{q=1}^{t/\tau_c - 1} (\Xi_{Np}(t) - \Xi_{t/\tau_c - 1, p}(t)) \\
&\quad \times (\Xi_{Nq}(t) - \Xi_{t/\tau_c - 1, q}(t)) \langle (z_p(0) - z_{p-1}(0))(z_q(0) - z_{q-1}(0) \rangle \\
&= \frac{b^2}{3}\left(N - \frac{t}{\tau_c}\right) + \frac{b^2}{3} \sum_{l=2}^{t/\tau_c} (\Xi_{Nl}(t) - \Xi_{t/\tau_c - 1, l}(t))^2,
\end{aligned} \tag{S39}$$

where we used $\langle (z_p(0) - z_{p-1}(0))(z_q(0) - z_{q-1}(0) \rangle = \delta_{pq}$ and $\langle (z_l(0) - z_{l-1}(0))(z_n(0) - z_{t/\tau_c}(0) \rangle = 0$ for $l < t/\tau_c$ to derive the last equation.

For large values of α (defined by eq. (S19)), the square bracket in eq. (S36) has an approximate form

$$\begin{aligned}
& K(m, l, (m-l)\tau_c) - K(m-1, l, (m-l)\tau_c) \\
= \ & \frac{1}{\pi}\sqrt{\frac{r\tau_c}{\tau_N}} \left(\frac{\pi^2}{4}\alpha \frac{N}{m-l}\right)^{1/2} \left(\mathrm{e}^{-\frac{\pi^2}{4}\alpha \frac{m-l}{N}} - \mathrm{e}^{-\frac{\pi^2}{4}\alpha \frac{1}{N} \frac{(m-l-1)^2}{m-l}}\right) \\
\simeq \ & -\frac{\sqrt{r}}{2}\delta_{l,m-1},
\end{aligned} \tag{S40}$$

where we used the fact that the right hand side is very small except at $m - l \simeq 1$. Substituting eq. (S40) into eq. (S36) leads to the form

$$\Gamma_{mn} = \delta_{mn} + \frac{\sqrt{r}}{2}(1 - \delta_{mn})\Gamma_{m-1,n}. \tag{S41}$$

The solution of the recursion relationship has the form

$$\Gamma_{mn} = \left(\frac{\sqrt{r}}{2}\right)^{m-n}. \tag{S42}$$

Substituting eq. (S42) into eq. (S38) leads to the form

$$\begin{aligned}
\Xi_{Nl}(t) - \Xi_{t/\tau_c-1,l}(t) &= \sum_{m=l}^{t/\tau_c-1} \Gamma_{ml}(K(N,m,t-m\tau_c) - K(t/\tau_c-1,m,t-m\tau_c)) \\
&= \sqrt{N}\int_{l/N}^{t/\tau_{ex}} du \, \frac{1}{\sqrt{t/\tau_{ex}-u}} \left(\frac{\sqrt{r}}{2}\right)^{Nu-l+1} \left(\mathrm{e}^{-\frac{\pi^2}{4}\alpha\frac{(1-u)^2}{\frac{t}{\tau_{ex}}-u}} - \mathrm{e}^{-\frac{\pi^2}{4}\alpha(\frac{t}{\tau_{ex}}-u)}\right) \\
&\simeq -\frac{2\sqrt{N}}{\sqrt{\pi\alpha}} \left(\frac{\sqrt{r}}{2}\right)^{N(t/\tau_{ex}-l/N)+1} \left[1 - \mathrm{e}^{-\pi^2\alpha(1-t/\tau_{ex})}\left(\frac{\sqrt{r}}{2}\right)^{N(t/\tau_{ex}-1)}\right],
\end{aligned} \tag{S43}$$

where we used the steepest descent to derive the last equation. The second term of the last form of eq. (S39) is rewritten in the form

$$\begin{aligned}
\sum_{l=2}^{t/\tau_c} (\Xi_{Nl}(t) - \Xi_{t/\tau_c-1,l}(t))^2 &= \frac{N^2 r}{\pi\alpha}\int_{1/N}^{t/\tau_{ex}} du \left(\frac{\sqrt{r}}{2}\right)^{2N(t/\tau_{ex}-u)} \\
&\quad \times \left[1 - \mathrm{e}^{-\pi^2\alpha(1-t/\tau_{ex})}\left(\frac{\sqrt{r}}{2}\right)^{N(t/\tau_{ex}-1)}\right]^2 \\
&= -\frac{Nr}{2\pi\alpha\log(\sqrt{r}/2)}\left[1 - \left(\frac{\sqrt{r}}{2}\right)^{2Nt/\tau_{ex}}\right] \\
&\quad \times \left[1 - \left(\frac{\sqrt{r}}{2}\right)^{-N(1-t/\tau_{ex})} \mathrm{e}^{-\pi^2\alpha(1-t/\tau_{ex})}\right]^2.
\end{aligned} \tag{S44}$$

The mean square of the end-to-end distance thus has the form

$$\begin{aligned}
\frac{3\langle(z_N(t) - z_{t/\tau_c}(t))^2}{Nb^2} &= 1 - \frac{t}{\tau_{ex}} - \frac{Nr}{2\pi\alpha\log(\sqrt{r}/2)}\left[1 - \left(\frac{\sqrt{r}}{2}\right)^{2Nt/\tau_{ex}}\right] \\
&\quad \times \left[1 - \left(\frac{\sqrt{r}}{2}\right)^{-N(1-t/\tau_{ex})} \mathrm{e}^{-\pi^2\alpha(1-t/\tau_{ex})}\right]^2.
\end{aligned} \tag{S45}$$