

# Supplementary material: Effect of local active fluctuations in structure and dynamics of flexible biopolymers

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## 1 Temporal correlation for normal modes of a flexible polymer subject to active fluctuations

In this section, we will sketch a derivation of the temporal correlation of the normal modes  $p$  and  $q$  (i.e.  $C_{pq}$ ) in time  $t$  for a flexible polymer subject to active fluctuations. We start our analysis by writing down the equation of motion of normal mode  $p$  (for  $p > 0$ ) as stated in Eq. (5) of the main text.

$$N\xi \frac{d\vec{X}_p}{dt} = -\frac{3p^2\pi^2 k_B T}{Nb^2} \vec{X}_p + \vec{f}_p^B(t) + \vec{f}_p^A(t), \quad (1)$$

Next we introduce the time-scale of internal relaxation of the polymer  $\tau_R = \xi N^2 b^2 / (3\pi^2 k_B T)$ , popularly known as Rouse time, and a non-dimensional time  $\tau = t/\tau_R$ , which allows us to rewrite Eq. 1 as,

$$\frac{d\vec{X}_p}{d\tau} + p^2 \vec{X}_p = \frac{\tau_R}{N\xi} [\vec{f}_p^B(t) + \vec{f}_p^A(t)], \quad (2)$$

Solution of Eq. 2 leads to:

$$\vec{X}_p(\tau) = \frac{\tau_R}{N\xi} \exp(-p^2\tau) \int_{-\infty}^{\tau} \exp(p^2\tau_1) [\vec{f}_p^B(\tau_1) + \vec{f}_p^A(\tau_1)] d\tau_1. \quad (3)$$

Similarly, we can find the solution for mode  $q$  at time 0 as.

$$\vec{X}_q(0) = \frac{\tau_R}{N\xi} \int_{-\infty}^0 \exp(q^2\tau_2) [\vec{f}_q^B(\tau_2) + \vec{f}_q^A(\tau_2)] d\tau_2. \quad (4)$$

From the definition of  $C_{pq}$ , we can write,

$$C_{pq}(\tau) = \langle \vec{X}_p(\tau) \cdot \vec{X}_q(0) \rangle = \left[ \frac{\tau_R}{N\xi} \right]^2 \exp(-p^2\tau) \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \left\langle [\vec{f}_p^B(\tau_1) + \vec{f}_p^A(\tau_1)] \cdot [\vec{f}_q^B(\tau_2) + \vec{f}_q^A(\tau_2)] \right\rangle d\tau_2 d\tau_1. \quad (5)$$

As the Brownian and active fluctuations are decorrelated to each other we can further decompose and simplify this expression for three dimensions as,

$$\begin{aligned} C_{pq}(\tau) &= \left[ \frac{\tau_R}{N\xi} \right]^2 \exp(-p^2\tau) \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \left[ \langle \vec{f}_p^B(\tau_1) \cdot \vec{f}_q^B(\tau_2) \rangle + \langle \vec{f}_p^A(\tau_1) \cdot \vec{f}_q^A(\tau_2) \rangle \right] d\tau_2 d\tau_1 \\ &= \left[ \frac{\tau_R}{N\xi} \right]^2 \exp(-p^2\tau) \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \frac{3k_B T N \xi}{\tau_R} [2\delta_{pq}\delta(\tau_1 - \tau_2) + L_{pq}\tau_R\kappa(|\tau_1 - \tau_2|)] d\tau_2 d\tau_1 \\ &= \frac{3k_B T \tau_R}{N\xi} \exp(-p^2\tau) \left[ 2\delta_{pq} \int_{-\infty}^0 \exp(2p^2\tau_1) d\tau_1 + L_{pq}\tau_R \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \kappa(|\tau_1 - \tau_2|) d\tau_2 d\tau_1 \right] \\ &= \frac{Nb^2}{\pi^2} \exp(-p^2\tau) \left[ \frac{\delta_{pq}}{p^2} + L_{pq}\tau_R \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \kappa(|\tau_1 - \tau_2|) d\tau_2 d\tau_1 \right] \end{aligned} \quad (6)$$

For the specific definition of a point active force at a bead with exponential decay of correlation defined in Eq. (7-8) of the main text leads to:

$$L_{pq} = N^{-1} \int_0^N \int_0^N Z(n, n') \phi_p(n) \phi_q(n') dn' dn = N^{-1} \int_0^N \int_0^N N \Gamma \delta(n - n_0) \delta(n' - n_0) \phi_p(n) \phi_q(n') dn' dn = \Gamma \phi_p(n_0) \phi_q(n_0). \quad (7)$$

Using this expression, we find the  $C_{pq}$  for this case using the relation derived in Eq. 6 as,

$$\begin{aligned} C_{pq}(\tau) &= \frac{Nb^2}{\pi^2} \exp(-p^2\tau) \left[ \frac{\delta_{pq}}{p^2} + L_{pq} \tau_R \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \kappa(|\tau_1 - \tau_2|) d\tau_2 d\tau_1 \right] \\ &= \frac{Nb^2}{\pi^2} \exp(-p^2\tau) \left[ \frac{\delta_{pq}}{p^2} + \Gamma \phi_p(n_0) \phi_q(n_0) \frac{\tau_R}{t_A} \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2] \exp[-\tau_R|\tau_1 - \tau_2|/t_A] d\tau_2 d\tau_1 \right] \\ &= \frac{Nb^2}{\pi^2} \exp(-p^2\tau) \left[ \frac{\delta_{pq}}{p^2} + \Gamma k_A \phi_p(n_0) \phi_q(n_0) \int_{-\infty}^{\tau} \int_{-\infty}^0 \exp[p^2\tau_1 + q^2\tau_2 - k_A|\tau_1 - \tau_2|] d\tau_2 d\tau_1 \right] \\ &= \frac{Nb^2}{\pi^2} \exp(-p^2\tau) \left[ \frac{\delta_{pq}}{p^2} + \Gamma k_A \phi_p(n_0) \phi_q(n_0) \left[ \int_{-\infty}^0 d\tau_2 \int_{\tau_2}^0 d\tau_1 \exp[(p^2 - k_A)\tau_1] \exp[(q^2 + k_A)\tau_2] \right. \right. \\ &\quad \left. \left. + \int_{-\infty}^0 d\tau_1 \int_{\tau_1}^0 d\tau_2 \exp[(q^2 - k_A)\tau_2] \exp[(p^2 + k_A)\tau_1] \right. \right. \\ &\quad \left. \left. + \int_{-\infty}^0 d\tau_2 \int_0^{\tau} d\tau_1 \exp[(q^2 + k_A)\tau_2] \exp[(p^2 - k_A)\tau_1] \right] \right] \\ &= \frac{Nb^2}{\pi^2} \left[ \frac{\delta_{pq} \exp(-p^2\tau)}{p^2} + \Gamma k_A \phi_p(n_0) \phi_q(n_0) \left[ \frac{\exp(-p^2\tau)}{(q^2 + k_A)(p^2 + q^2)} + \frac{\exp(-p^2\tau)}{(p^2 + k_A)(p^2 + q^2)} + \frac{\exp(-k_A\tau) - \exp(-p^2\tau)}{(p^2 - k_A)(q^2 + k_A)} \right] \right] \\ &= \frac{Nb^2}{\pi^2} \left[ \frac{\delta_{pq} \exp(-p^2\tau)}{p^2} + \Gamma k_A \phi_p(n_0) \phi_q(n_0) \left[ \frac{2k_A \exp(-p^2\tau)}{(k_A^2 - p^4)(p^2 + q^2)} - \frac{\exp(-k_A\tau)}{(k_A - p^2)(k_A + q^2)} \right] \right]. \quad (8) \end{aligned}$$

## 2 Mean squared displacement of tracer on a flexible polymer subject to active fluctuations

We define the mean squared displacement (MSD) of a tracer situated at segment  $n$  and decompose the contributions of center of mass motion and different orthogonal modes.

$$\begin{aligned} \text{MSD}(n, t) &= \langle [|\vec{r}(n, t) - \vec{r}(n, 0)|^2] \rangle = \left\langle \left[ \vec{r}_{\text{com}}(t) + \sum_{p=1}^{\infty} \vec{X}_p(t) \phi_p(n) - \vec{r}_{\text{com}}(0) - \sum_{p=1}^{\infty} \vec{X}_p(0) \phi_p(n) \right]^2 \right\rangle \\ &= \left\langle \left[ \vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0) \right]^2 \right\rangle + 2 \sum_{p=1}^{\infty} \phi_p(n) \left\langle \left[ \vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0) \right] \cdot \left[ \vec{X}_p(t) - \vec{X}_p(0) \right] \right\rangle \\ &\quad + \left\langle \left[ \sum_{p=1}^{\infty} \left[ \vec{X}_p(t) \phi_p(n) - \vec{X}_p(0) \phi_p(n) \right]^2 \right] \right\rangle. \quad (9) \end{aligned}$$

First, we express the contribution of the purely non-zero modes in terms of the correlation of modal amplitudes  $C_{pq}$ :

$$\begin{aligned}
\left\langle \sum_{p=1}^{\infty} [\vec{X}_p(t)\phi_p(n) - \vec{X}_p(0)\phi_p(n)]^2 \right\rangle &= \left\langle \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} [\vec{X}_p(t)\phi_p(n) - \vec{X}_p(0)\phi_p(n)] \cdot [\vec{X}_q(t)\phi_q(n) - \vec{X}_q(0)\phi_q(n)] \right\rangle \\
&= \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \phi_p(n)\phi_q(n) \left[ \langle \vec{X}_p(t) \cdot \vec{X}_q(t) \rangle - \langle \vec{X}_p(t) \cdot \vec{X}_q(0) \rangle - \langle \vec{X}_q(t) \cdot \vec{X}_p(0) \rangle + \langle \vec{X}_p(0) \cdot \vec{X}_q(0) \rangle \right] \\
&= \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \phi_p(n)\phi_q(n) \left[ 2C_{pq}(0) - C_{pq}(t) - C_{qp}(t) \right].
\end{aligned} \tag{10}$$

Next, for the specific definition of a point active force at a bead with exponential decay of correlation defined in Eq. (7-8) of the main text, we derive the other two components of the right hand side. To analyze the contributions of center of mass, we begin from the equation of motion of the chain stated in Eq (1).

$$\xi \frac{\partial \vec{r}(n, t)}{\partial t} = \frac{3k_B T}{b^2} \frac{\partial^2 \vec{r}(n, t)}{\partial n^2} + \vec{f}^B(n, t) + \vec{f}^A(n, t) \tag{11}$$

Integrating both side of the equation with respect to  $n$  and dividing by  $N$ , we obtain:

$$\begin{aligned}
\xi \frac{d\vec{r}_{\text{com}}(t)}{dt} &= \frac{3k_B T}{Nb^2} \left[ \frac{\partial \vec{r}(n)}{\partial n} (n=N) - \frac{\partial \vec{r}(n)}{\partial n} (n=0) \right] + \frac{1}{N} \int_0^N [\vec{f}^B(n, t) + \vec{f}^A(n, t)] dn \\
\Rightarrow [\vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0)] &= \frac{1}{N\xi} \int_0^t \int_0^N [\vec{f}^B(n, t) + \vec{f}^A(n, t)] dn dt \\
\Rightarrow [\vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0)]^2 &= \frac{1}{N^2 \xi^2} \int_0^t \int_0^N \int_0^t \int_0^N \langle [\vec{f}^B(n_1, t_1) + \vec{f}^A(n_1, t_1)] \cdot [\vec{f}^B(n_2, t_2) + \vec{f}^A(n_2, t_2)] \rangle dn_1 dt_1 dn_2 dt_2 \\
&= \frac{1}{N^2 \xi^2} \int_0^t \int_0^N \int_0^t \int_0^N \left[ \langle \vec{f}^B(n_1, t_1) \cdot \vec{f}^B(n_2, t_2) \rangle + \langle \vec{f}^A(n_1, t_1) \cdot \vec{f}^A(n_2, t_2) \rangle \right] dn_1 dt_1 dn_2 dt_2 \\
&= \frac{3k_B T}{N^2 \xi^2} \int_0^t \int_0^N \int_0^t \int_0^N \left[ 2\delta(t_1 - t_2)\delta(n_1 - n_2) + \right. \\
&\quad \left. N\Gamma\delta(n - n_0)\delta(n' - n_0) \frac{\exp(-|t_1 - t_2|/t_A)}{t_A} \right] dn_1 dt_1 dn_2 dt_2 \\
&= \frac{3k_B T}{N^2 \xi^2} \left[ 2Nt + N\Gamma \int_0^t \int_0^t \frac{\exp(-|t_1 - t_2|/t_A)}{t_A} dt_1 dt_2 \right] \\
&= \frac{3k_B T \tau_R}{N \xi^2} \left[ 2\tau + \frac{\Gamma \tau_R}{t_A} \int_0^\tau \int_0^\tau \exp(-k_A |\tau_1 - \tau_2|) d\tau_1 d\tau_2 \right] \\
&= \frac{Nb^2}{\pi^2} \left[ 2\tau + \Gamma k_A \left[ \int_0^\tau \int_0^{\tau_1} \exp[-k_A(\tau_1 - \tau_2)] d\tau_2 d\tau_1 + \int_0^\tau \int_{\tau_1}^\tau \exp[-k_A(\tau_2 - \tau_1)] d\tau_2 d\tau_1 \right] \right] \\
&= \frac{Nb^2}{\pi^2} \left[ 2\tau + \Gamma k_A \left[ \frac{2k_A \tau + 2 \exp(-k_A \tau) - 2}{k_A^2} \right] \right] \\
&= \frac{2Nb^2}{\pi^2} \left[ (1 + \Gamma)t + \Gamma \left[ \frac{\exp(-k_A \tau) - 1}{k_A} \right] \right].
\end{aligned} \tag{12}$$

Similarly, from the solution of equation of motion of modal amplitudes demonstrated in Eq. 3 we obtain,

$$\begin{aligned}
\vec{X}_p(t) - \vec{X}_p(0) &= \frac{\tau_R}{N\xi} \left[ \exp(-p^2 \tau) \int_{-\infty}^\tau \int_0^N \exp(p^2 \tau') [\vec{f}^B(n, \tau') + \vec{f}^A(n, \tau')] \phi_p(n) dn d\tau' - \right. \\
&\quad \left. \int_{-\infty}^0 \int_0^N \exp(p^2 \tau') [\vec{f}^B(n, \tau) + \vec{f}^A(n, \tau')] \phi_p(n) dn d\tau' \right]
\end{aligned} \tag{13}$$

Utilizing this expression and the fact that the Brownian contribution for the modal amplitudes and the center

of mass motion is decorrelated, we write:

$$\begin{aligned}
& \left\langle \left[ \vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0) \right] \cdot \left[ \vec{X}_p(t) - \vec{X}_p(0) \right] \right\rangle \\
&= \frac{\tau_R^2}{N^2 \xi^2} \left[ \exp(-p^2 \tau) \int_0^t \int_0^N \int_0^\tau \int_0^N \exp(p^2 \tau_2) \langle \vec{f}^A(n, \tau_1) \vec{f}^A(n', \tau_2) \rangle \phi_p(n') dn d\tau_1 dn' d\tau_2 \right. \\
&\quad \left. + \left[ \exp(-p^2 \tau) - 1 \right] \times \int_{-\infty}^0 \int_0^N \int_0^\tau \int_0^N \exp(p^2 \tau_2) \langle \vec{f}^A(n, \tau_1) \vec{f}^A(n', \tau_2) \rangle \phi_p(n') dn d\tau_1 dn' d\tau_2 \right] \\
&= \left[ \frac{3\tau_R k_B T \Gamma k_A}{N \xi} \int_0^N \int_0^N \delta(n - n_0) \delta(n' - n_0) \phi_p(n') dn dn' \right] \times \left[ \exp(-p^2 \tau) \int_0^\tau \int_0^\tau \exp[p^2 \tau_2 - k_A(|\tau_1 - \tau_2|)] d\tau_1 d\tau_2 + \right. \\
&\quad \left. \left[ \exp(-p^2 \tau) - 1 \right] \times \int_{-\infty}^0 \int_0^\tau \exp[p^2 \tau_2 - k_A(|\tau_1 - \tau_2|)] d\tau_1 d\tau_2 \right] \\
&= \frac{N b^2}{\pi^2} \Gamma k_A \phi_p(n_0) \left[ I_1 + I_2 \right], \tag{14}
\end{aligned}$$

where

$$\begin{aligned}
I_1 &= \exp(-p^2 \tau) \int_0^\tau \int_0^\tau \exp[p^2 \tau_2 - k_A(|\tau_1 - \tau_2|)] d\tau_1 d\tau_2 \\
&= \exp(-p^2 \tau) \left[ \int_0^\tau \int_0^{\tau_1} \exp[(p^2 + k_A)\tau_2 - k_A \tau_1] d\tau_2 d\tau_1 + \int_0^\tau \int_{\tau_1}^\tau \exp[(p^2 - k_A)\tau_2 + k_A \tau_1] d\tau_2 d\tau_1 \right] \\
&= \exp(-p^2 \tau) \left[ \frac{\exp(p^2 \tau) - 1}{p^2(k_A + p^2)} - \frac{1 - \exp(-k_A \tau)}{k_A(k_A + p^2)} + \frac{\exp(p^2 \tau) - 1}{p^2(k_A - p^2)} - \frac{\exp(p^2 \tau)[1 - \exp(-k_A \tau)]}{k_A(k_A - p^2)} \right], \tag{15}
\end{aligned}$$

and

$$\begin{aligned}
I_2 &= \left[ \exp(-p^2 \tau) - 1 \right] \times \int_{-\infty}^0 \int_0^\tau \exp[p^2 \tau_2 - k_A(|\tau_1 - \tau_2|)] d\tau_1 d\tau_2 \tag{16} \\
&= \left[ \exp(-p^2 \tau) - 1 \right] \times \int_{-\infty}^0 \int_0^\tau \exp[(p^2 + k_A)\tau_2 - k_A \tau_1] d\tau_1 d\tau_2 \\
&= \frac{[\exp(-p^2 \tau) - 1][1 - \exp(-k_A \tau)]}{k_A(k_A + p^2)}. \tag{17}
\end{aligned}$$

The addition of these terms and further algebraic simplification leads to

$$\begin{aligned}
\left\langle \left[ \vec{r}_{\text{com}}(t) - \vec{r}_{\text{com}}(0) \right] \cdot \left[ \vec{X}_p(t) - \vec{X}_p(0) \right] \right\rangle &= \frac{N b^2}{\pi^2} \Gamma k_A \phi_p(n_0) \left[ I_1 + I_2 \right] \\
&= N b^2 \Gamma k_A \phi_p(n_0) \frac{2k_A[1 - \exp(-p^2 \tau)] - 2p^2[1 - \exp(-k_A \tau)]}{p^2 \pi^2 (k_A^2 - p^4)} \tag{18}
\end{aligned}$$

### 3 Numerical simulations of dynamics of a flexible polymer subject to active fluctuations

To simulate a flexible polymer subject to active fluctuations, we perform a numerical integration of a discrete form of the Langevin equation introduced in Eq. (1) of the main text. We non-dimensionalize this equation by scaling the positions with respect to the root mean squared end-to-end distance of a Rouse chain with same number of segments ( $\vec{\rho} = \vec{r}/\sqrt{N b^2}$ ), time with respect to Rouse time ( $\tau = t/\tau_R$ ), and segment position with respect to total number of Kuhn segments ( $\eta = n/N$ ).

This results in the expression

$$\frac{\partial \vec{\rho}(\eta, \tau)}{\partial \tau} = \frac{\partial^2 \vec{\rho}(\eta, \tau)}{\partial \eta^2} + \vec{\Phi}^B(\eta, \tau) + \vec{\Phi}^A(\eta, \tau), \tag{19}$$

where, the dimensionless Brownian and active forces  $\vec{\Phi}^B(\eta, \tau)$ , and  $\vec{\Phi}^A(\eta, \tau)$  has the property  $\langle \vec{\Phi}^B(\eta, \tau) \vec{\Phi}^B(\eta', \tau') \rangle = (2/3\pi^2) \delta(\eta - \eta') \delta(\tau - \tau') \mathbf{I}$ , and  $\langle \vec{\Phi}^A(\eta, \tau) \vec{\Phi}^A(\eta', \tau') \rangle = (\Gamma k_A / 3\pi^2) \delta(\eta - \eta_0) \delta(\eta' - \eta_0) \exp(-k_A |\tau - \tau'|) \mathbf{I}$ .

For numerical integration, we discretize the polymer into  $N$  segments represented by  $(N + 1)$  beads. We simulate the time evolution of the coordinates of the  $i$ th bead in dimension  $\alpha$  as,

$$\rho_{i,\alpha}(\tau + \delta\tau) = \rho_{i,\alpha}(\tau) + \frac{\rho_{i-1,\alpha}(\tau) - 2\rho_{i,\alpha}(\tau) + \rho_{i+1,\alpha}(\tau)}{\pi^2 \delta \hat{n}^2} \delta\tau + \sqrt{\frac{2\delta\tau}{3\pi^2 \delta \eta}} \mathbb{N}(0, 1) + \frac{\delta(i - n_0)}{\delta N} \Phi_\alpha^A(\tau) \delta\tau. \tag{20}$$

The normalized active fluctuation  $\vec{\Phi}_A$  evolves as,

$$\Phi_\alpha^A(\tau + \delta\tau) = \Phi_\alpha^A(\tau) - (k_A \delta\tau) \Phi_\alpha^A(\tau) + \sqrt{\frac{2\Gamma k_A^2 \delta\tau}{3\pi^2}} \mathbb{N}(0, 1), \tag{21}$$

where,  $\delta\eta = 1/N$  is the normalized spacing between the beads,  $\delta\tau$  is the normalized timestep for integration, and  $\mathbb{N}(0,1)$  is taken from a Gaussian distribution of numbers with 0 mean and unit variance. We generate the initial configurations of the simulation from an equilibrium distribution of the Rouse polymer by setting  $\rho_{i+1,\alpha}(0) = \rho_{i,\alpha}(0) + \sqrt{\frac{\delta\eta}{3}}\mathbb{N}(0,1)$ . For the simulations presented in this manuscript, we choose  $N = 100$  and  $\delta\tau = 10^{-5}$ .

## Supplementary Figure

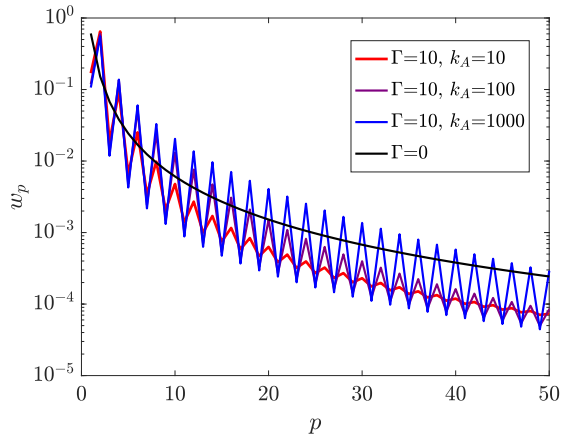


Figure 1: Relative contributions of modal amplitudes  $w_p$ , defined as  $\frac{\langle \vec{X}_p \cdot \vec{X}_p \rangle}{\sum_{p=1}^{\infty} \langle \vec{X}_p \cdot \vec{X}_p \rangle}$ , as a function of mode number  $p$  in absence of active force (i.e.  $\Gamma = 0$ ) and in presence of strong active force (i.e.  $\Gamma = 10$ ) with different persistence time (i.e.,  $k_A = 10, 100, 1000$ ).