Effects of inertia on conformation and dynamics of tangentially-driven active filaments
Supplementary Material

I. TANGENTIALLY DRIVEN ACTIVE POLYMER SIMULATIONS

A. Model definition

We use a tangentially-driven active polymer model identical to the model put forward by Isele-Holder et al. [1] to examine the effect of inertia on the conformational dynamics of active flexible filaments. The active filament is modelled as a flexible linear polymer composed of a sequence of \( N \) bead-like units connected via harmonic springs. The chains are under the influence of an active force which is tangential to the polymer backbone. Hence, the active force is directly coupled to the polymer conformation. The dynamics of each bead of an active polymer with mass \( m \) is described by the Langevin equation of motion:

\[
m \ddot{r}_i = -\gamma \dot{r}_i - \sum_j \nabla_{r_i} U(r_{ij}) + f^a_i + f^r_i, \tag{1}
\]

in which \( r_i \) is the coordinate of the bead \( i \) with the dots denoting derivatives with respect to time and \( \gamma \) is the effective friction coefficient of the bead. \( r_{ij} = |r_j - r_i| \) denotes the distance between bead \( i \) and \( j \) and \( U(r_{ij}) \) is the potential energy of inter-particle interactions. \( f^a_i \) and \( f^r_i \) are the active and random thermal forces acting on the bead \( i \), respectively.

The total potential energy of a bead \( U = U_{\text{Bond}} + U_{\text{excl}} \) includes contributions from springs connecting the monomer to its adjacent monomers along the chain backbone \( U_{\text{Bond}} \) and excluded volume potential \( U_{\text{excl}} \) between any two monomers which guarantees the self avoidance of the polymers. The bond potential used throughout our simulations is a harmonic oscillator potential:

\[
U_{\text{Harmonic}}(r) = \frac{1}{2}k_s(r - \ell)^2, \tag{2}
\]

in which \( \ell \) is the length of the spring at rest and \( k_s \) is its stiffness. The excluded volume interactions between any two beads, bonded or non-bonded, at a distance \( r \) are modelled by the truncated and shifted Lennard-Jones potential, i.e., Weeks-Chandler-Andersen (WCA) potential,

\[
U_{\text{excl}}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} + \frac{1}{4} \right], \quad r < r_{\text{cut}} \tag{3}
\]

where \( \epsilon \) sets the strength of pairwise interaction energy, and \( r_{\text{cut}} = 2^{1/6}\sigma \) is the cutoff distance such that \( U_{\text{excl}}(r > r_{\text{cut}}) = 0 \).

By defining the bond vector \( r_{i,i+1} = r_{i+1} - r_i \), the active force on each bead \( i \) is modeled as:

\[
f^a_i = \frac{f^a}{\ell} (r_{i,i+1} + r_{i-1,i}), \tag{4}
\]

which mimics a homogeneous active force driving along the backbone of the chain. Here, \( f^a \) is the strength of active force, \( \ell \) is the mean bond length and the orientation of force on end beads is parallel to end bonds. The thermal noise \( f^r_i \) in Eq. (1) is a delta correlated random force acting on particle \( i \) with zero mean and strength \( 2D_0\gamma^2 \)

\[
\langle f^r_i(t)f^r_j(t') \rangle = 2D_0\gamma^2\delta_{ij}\delta(t-t'), \tag{5}
\]

where \( D_0 \) is the diffusion coefficient of a single passive monomer particle, the \( \delta_{ij} \) is the Kronecker delta and \( \delta(t-t') \) is the Dirac delta.

In the overdamped limit, where we can neglect inertial effects, the Langevin equations of motion Eq.(1) result in Brownian Dynamics equations of motion:

\[
\gamma \dot{r}_i = -\sum_j \nabla_{r_i} U(r_{ij}) + f^a_i + f^r_i \tag{6}
\]
FIG. S1. a) PDF of bond length for underdamped chains of $N = 500$ and different activities. b) Same graph for overdamped polymers.

TABLE I. Summary of simulation for $N = 500$ for underdamped (left) and overdamped (right) cases. The tables contains the information about the number of thermalizing steps $N_{\text{run}}$ before the actual simulation and then the total production steps of $N_{\text{pro}}$, the corresponding step size $dt$ and the bond spring constants for each activity.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$f^a$</th>
<th>$N_{\text{run}}$</th>
<th>$N_{\text{pro}}$</th>
<th>$dt$</th>
<th>$k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>0.01</td>
<td>5.0e+08</td>
<td>9.0e+08</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>0.025</td>
<td>3.6e+08</td>
<td>3.6e+08</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>0.05</td>
<td>1.8e+08</td>
<td>1.8e+08</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>0.1</td>
<td>9.0e+07</td>
<td>9.0e+07</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>0.25</td>
<td>3.6e+07</td>
<td>3.6e+07</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>0.5</td>
<td>1.8e+07</td>
<td>1.8e+07</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>1</td>
<td>9.0e+06</td>
<td>9.0e+06</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>2.5</td>
<td>9.0e+06</td>
<td>9.0e+06</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>5</td>
<td>9.0e+06</td>
<td>9.0e+06</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>10</td>
<td>9.0e+06</td>
<td>9.0e+06</td>
<td>1.0e-03</td>
<td>1.0e+06</td>
</tr>
<tr>
<td>500</td>
<td>25</td>
<td>1.8e+07</td>
<td>1.8e+07</td>
<td>2.0e-04</td>
<td>1.0e+07</td>
</tr>
<tr>
<td>500</td>
<td>50</td>
<td>1.8e+07</td>
<td>1.8e+07</td>
<td>1.0e-04</td>
<td>1.0e+07</td>
</tr>
<tr>
<td>500</td>
<td>100</td>
<td>4.0e+07</td>
<td>4.0e+07</td>
<td>5.0e-05</td>
<td>1.0e+07</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N$</th>
<th>$f^a$</th>
<th>$N_{\text{run}}$</th>
<th>$N_{\text{pro}}$</th>
<th>$dt$</th>
<th>$k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>0.01</td>
<td>6.8e+08</td>
<td>6.8e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>0.025</td>
<td>9.0e+08</td>
<td>9.0e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>0.05</td>
<td>9.0e+08</td>
<td>9.0e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>0.1</td>
<td>9.0e+08</td>
<td>9.0e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>0.25</td>
<td>3.6e+08</td>
<td>3.6e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>0.5</td>
<td>1.8e+08</td>
<td>1.8e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>1</td>
<td>1.8e+08</td>
<td>1.8e+08</td>
<td>1.0e-04</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>2.5</td>
<td>9.0e+07</td>
<td>9.0e+07</td>
<td>5.0e-05</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>5</td>
<td>1.8e+08</td>
<td>1.8e+08</td>
<td>5.0e-05</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>10</td>
<td>9.0e+07</td>
<td>9.0e+07</td>
<td>1.0e-05</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>25</td>
<td>9.0e+07</td>
<td>9.0e+07</td>
<td>1.0e-05</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>50</td>
<td>9.0e+07</td>
<td>9.0e+07</td>
<td>1.0e-05</td>
<td>5.0e+03</td>
</tr>
<tr>
<td>500</td>
<td>100</td>
<td>4.5e+07</td>
<td>1.5e+07</td>
<td>1.0e-05</td>
<td>1.0e+05</td>
</tr>
</tbody>
</table>

B. Dimensionless groups and simulation details

The simulations are carried out in HOOMD-BLUE [2] package with home-made modification to include the active force using a GPU implementation. The equations of motion are solved using a velocity-Verlet scheme.

We choose $\ell_u = \sigma$, $E_u = \epsilon$ and $\tau_u = \gamma \sigma^2/\epsilon$, with $\gamma = 1$, as the units of length, energy and time, respectively and reduced quantities are denoted by * superscript. We fix $\ell/\sigma = 1$ and dimensionless diffusion coefficient $D_0^* = 0.1$, whereas we vary dimensionless active force strength $f^a_\ast = f^a_\ast \sigma \epsilon$ in the range $0.01 \leq f^a_\ast \leq 100$ for chain lengths $50 \leq N \leq 1000$. The reduced mass $m^* = m \epsilon / (\gamma \sigma)^2 = 1$ is varied in the range $0 \leq m^* \leq 5$. However, the majority of simulations focus on the overdamped limit $m^*_\ast = 0$ and the underdamped case of $m^*_\ast = 1$. The spring constant of bond potential $k_s^* = k_s \sigma^2/\epsilon$ is chosen according to active force strength, such that the maximum bond length fluctuation is less than %5 of average bond length which is $\sigma$, see Table I for the chosen values of $k_s^*$. Fig. S1 shows the distribution of bond length in simulations, which is defined as $\ell_b = |r_{i+1}(t) - r_i(t)|$ for ith monomer, at several $f^a_\ast$.

To produce the desired statistics, for each set of parameters i.e. $(N, f^a_\ast)$ we have simulated 120 independent chain configurations. For this purpose, we first equilibrated passive polymers of different chain lengths and then we used them as starting configurations for active polymers. The simulations consist of $N_{\text{run}}$ timesteps until the polymers reach a dynamical steady state, to ensure that no vestige of the initial conditions are remained. Subsequently they are followed by a production run of $N_{\text{pro}}$ timesteps to compute the structural and dynamical observable quantities.
We verified that the total time in the production run \( t_{\text{pro}} = n_{\text{pro}} \ast dt \) is at least four times larger than the relaxation time of the end-to-end vector \( \tau^*_e \). A summary of simulation parameters, including timestep \( dt \) can be found in Table I.

C. Exponential decay of \( C^*_e \)

In Fig. S2, \( \tilde{C}_e = \lim_{t' \to \infty} \langle R_e(t + t') \cdot R_e(t') \rangle / \langle R^2_e(t') \rangle \) is fitted by exponential functions with the form \( \exp(-t^*/\tau^*_e) \) and the \( \tau^*_e \) for each \( N \) correspond to the times that their normalized end-to-end vector time correlation function \( \tilde{C}_e \) reaches the value of \( 1/e \).

![Figure S2](image)

**FIG. S2.** Normalized end-to-end vector TACF for chains of \( N = 500 \) and different activities (symbols) and their corresponding exponential fits (lines) \( \tilde{C}_e = \exp(-t^*/\tau^*_e) \). The bold symbols and solid lines correspond to inertial active chains, whereas empty symbols and dashed lines represent the overdamped active chains.

II. VIDEOS

Videos of the time evolution of an active polymer configuration starting from a passive state have been provided. These include one video for an overdamped active chain and two videos for an inertial active polymer. In all of them, the chain length is \( N = 500 \) and \( f^{a*} = 100 \). To show the polarity of polymer, the six starting monomers are colored in blue and the rest of monomers are red. The specification of the videos are as follows:

The video file "LD-N500-f100.mp4" is for inertial polymer including the period that it reaches a steady state. The video file "LD-N500-f100-zoomed.mp4" also shows the same active inertial chain, however with a zoomed-in view for a more detailed visualisation of the transition from coil-like to elongated configuration in the steady-state due to impacts from inertial collisions. The snapshots are recorded each 2000 timesteps with \( dt = 5 \times 10^{-5} \).

Finally, the video file "BD-N500-f100.mp4" is for overdamped polymer and shows how the chain tends to swirl around itself like a yarn ball. The snapshots are recorded each 20000 timesteps with \( dt = 10^{-6} \).

III. THE ACTIVE BROWNIAN POLYMER

The very basic model for active chains is a sequence of active Brownian particles connected with springs, forming an Active Brownian Polymer (ABPO) [3]. A flexible ABPO is composed of \( N \) active Brownian particles \((i = 1, ..., N)\).
which their translational and rotational dynamics are described by the following equations of motion:

$$m\ddot{\mathbf{r}}_i(t) = -\gamma_T \dot{\mathbf{r}}_i(t) + \gamma_T v_0 \mathbf{e}_i(t) - \sum_j \nabla_{\mathbf{r}_j} U(r_{ij}) + \mathbf{f}_i^a(t)$$

(7)

$$\dot{\mathbf{e}}_i(t) = \eta_i(t) \times \mathbf{e}_i(t),$$

(8)

where $\mathbf{r}_i$ is the position of particle $i$, and $\gamma_T v_0 \mathbf{e}_i(t)$ is the active self-propulsion with the speed of $v_0$ and direction of $\mathbf{e}_i(t)$ which diffuses according to Eq. 8. $\gamma_T$ is the translational friction and the interparticle forces between particles $j$ and $i$ are given by the the same two potentials $U(r_{ij}) = U_{\text{Harmonic}} + U_{\text{excl}}$, as in Sec. I. The noise terms $\mathbf{f}_i^a$ and $\eta_i$ are Gaussian and Markovian stochastic processes with mean value of zero and second moments of:

$$\langle \mathbf{f}_i^a(t) \cdot \mathbf{f}_j^a(t') \rangle = 6D_0 \gamma^2 \delta_{ij}\delta(t-t')$$

(9)

$$\langle \eta_i(t)\eta_j(t') \rangle = 2D_\tau \delta_{ij}\delta(t-t'),$$

(10)

in which, $D_0$ is the single passive particle diffusion coefficient and $D_\tau$ is the rotational diffusion coefficient. The correlation of the orientation vector $\mathbf{e}_i$ is given by [4]

$$\langle \mathbf{e}_i(t) \cdot \mathbf{e}_i(t') \rangle = e^{-2D_\tau|t-t'|},$$

(11)

where $\tau_\tau = 1/(2D_\tau)$ denotes the rotational relaxation time.

Noting that the total active force on an ABPO of chain length $N$ is $\mathbf{F}_a = \gamma_T v_0 \sum_{i=1}^N \mathbf{e}_i$, its time autocorrelation function using Eq. (11) becomes

$$C_f = \langle \mathbf{F}_a(0) \cdot \mathbf{F}_a(t) \rangle = N(\gamma_T v_0)^2 e^{-|t|/\tau_\tau},$$

(12)

For inertial ABPOs, velocity auto-correlation can be obtained from Eq. (6) of the main manuscript using the explicit form of active force auto-correlation given by Eq. (12).

$$C_{v,\text{ABPO}}^A(s) = \frac{3D_0\gamma_T}{Nm} e^{-\frac{s}{\tau_m}} + \frac{v_0^2}{N} \frac{\tau_\tau}{\tau_\tau^2 - \tau_m^2} \left[ \tau_\tau e^{-s/\tau_\tau} - \tau_m e^{-s/\tau_m} \right].$$

(13)

We can also find the long time diffusion coefficient as follows,

$$D_L = \frac{1}{3} \int_0^\infty dt \langle \mathbf{V}_\text{cm}(t) \cdot \mathbf{V}_\text{cm}(0) \rangle = \frac{D_0}{N} + \frac{v_0^2 \tau_\tau}{6N},$$

(14)

which turns out to be independent of $\tau_m$, similar to the case of inertial ABPs without orientational inertia [4]. For non-inertial ABPOs we have,

$$\lim_{m \to 0} C_r(s > 0) = \frac{v_0^2}{N} e^{-|t|/\tau_\tau},$$

(15)

$$\lim_{m \to 0} D_L = \frac{D_0}{N} + \frac{v_0^2 \tau_\tau}{3N}.$$  

(16)

In panel (a) of Fig.S3, we see the predictions of Eq. (13) and eq. (15) show very good agreement with the results of simulations for the velocity auto-correlation of ABPOs and the differences between inertial and overdamped cases. We normalised all the values with respect to the squared center of mass velocities that are predicted by theory, which gives $\langle \mathbf{V}_\text{cm}^2 \rangle = 0.71$ for the ABPO with inertia and $\langle \mathbf{V}_\text{cm}^2 \rangle = 5$ for the overdamped one for this particular chain length and active force strength. Furthermore, using eq. 14 and eq. 16 for long time diffusion coefficients of ABPOs, we have $D_L/D_0 = 2.77$ for both inertial and overdamped cases (N.B, the two formulas are identical and mass-independent). From the simulations, we have found that for inertial case $D_L/D_0 = 2.62$ and for overdamped one $D_L/D_0 = 2.59$.

Finally, we report the end-to-end distance of each case. For inertial ABPO it is $R^*_e = 57.4$ and for polymers with overdamped dynamics, we have $R^*_e = 53.4$, which are quite the similar within error bar. This shows the impact of inertia on the size of active polymers are much more significant when the active driving force is tangential leading to a self-amplifying feedback loop between active force direction and polymer conformation.
FIG. S3. a) Comparison of the normalised velocity auto-correlation functions of underdamped (inertial) and overdamped ABPOs with their corresponding analytical predictions, namely eq. (13) and eq. (15) which are plotted in solid blue and purple lines respectively. The chains are both active with $v_0^* = 50$ (in the same dimension-less system as tangentially driven ones) and chain length of $N = 500$. b) Comparison of the MSDs of the overdamped and underdamped ABPOs.