Electronic Supplementary Material (ESI) for Soft Matter

Dynamics of self-organized rotating spiral-coils in bacterial swarms Supplementary Information

Szu-Ning Lin, Wei-Chang Lo and Chien-Jung Lo

1 Videos

1.1 Video One: Rotating Spiral Coil

This video shows a self-organized spiral coil rotating at $\sim$ 12 rad/s. The size of view is 44×44 μm^2, and the video is displayed at real time 50 frames per second (fps) for two seconds.

1.2 Video Two: Spiral Coil Folding

This video shows a folding process of a single spiral coil. The size of view is 26×26 μm^2, and the video is displayed at real time 50 fps for 2.2 seconds. The long cells turned into itself and then folded in 2D.

1.3 Video Three: Spiral Coil Unfolding

This video shows an unfolding process of a double spiral coil. The size of view is 46×52 μm^2, and the video is displayed at real time 50 fps for 6.4 seconds. One end of the cell changed the moving direction that unfolded the whole coil.

1.4 Video Four: Simulating Rotating Spiral Coil

This video shows a simulated self-organized spiral coil rotating at $\sim$ 6 rad/s. The size of view is 60×60 μm^2, and the video is displayed at real time 50 fps for 2 seconds.

2 Brownian Dynamics Simulations

As outlined in the main text, the dynamics of the long and short bacteria is simulated through the quasi-two-dimensional Brownian dynamics simulation. Both types of bacteria are composed of identical beads (diameter $\sigma = 1$ μm). The short bacterium has N_r beads, and the long one has N_s. Each bead obeys the overdamped Langevin equation as follows:

$$\xi \frac{\mathrm{d}\vec{R}_n(t)}{\mathrm{d}t} = -\nabla U(\{\vec{R}_n\}) + \vec{f}_p^{(n)}(t) + \vec{f}^{(n)}(t), \quad n = 1, \cdots, N, \tag{1}$$

where ξ is the friction constant, $\vec{R}_n$ the position of the n-th bead, $U(\{\vec{R}_n\}) = U_W(r) + U_F(r) + U_b(\theta)$ the interaction potential between beads, $\vec{f}_p^{(n)}$ the propulsion force, $\vec{f}^{(n)}$ the random force acting on the n-th bead, and N the total number of beads. The random force $\vec{f}^{(n)}$ is characterized by a Gaussian probability distribution, as usual, with the correlation function $\langle f_i^{(m)}(t) f_j^{(n)}(t') \rangle = 2\xi k_B T \delta_{mn} \delta_{ij} \delta(t - t')$.

As shown above, there are three kinds of interactions between beads in the simulation. The first type is the excluded volume interaction that is modeled by using the Weeks-Chandler-Andersen potential (WCA),

$$U_W(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon & r < 2^{1/6}\sigma \\ 0 & r \geq 2^{1/6}\sigma, \end{cases} \tag{2}$$

where r is the separation between the centers of mass of two beads. Since this is a short ranged interaction, in practice we can ignore any beads farther than the cut-off distance $2^{1/6}\sigma$. In the simulation, the well depth ε is set as the thermal energy k_BT, and the program ignores any beads outside of a $3\sigma \times 3\sigma$ area while calculating the excluded volume interaction to save the computation time.

The second kind of interactions is the bonding between beads within either long or short bacteria. Here we apply the finitely extensible nonlinear elastic potential (FENE) to confine the distance between connected beads. With careful choices of k and R_0 and the WCA potential, the chains cannot move through one another. In the simulation the FENE potential is given as follows:

$$U_F(r) = \begin{cases} -\frac{1}{2}kR_0^2 \log[1 - (r/R_0)^2] & r < R_0 \\ \infty & r \geq R_0, \end{cases} \tag{3}$$

where $k = 60k_BT/\sigma^2$ and $R_0 = 1.25\sigma$. The choice of these values are simply based on matching the separation between consecutive beads to the set diameter $\sigma = 1$ μm and the stability of the bonding under the circumstances of frequent collisions from other cells.

The last kind of interactions is the elastic bending between bonds. We calculate the position vectors of consecutive beads $\vec{R}_a = \vec{R}_i - \vec{R}_{i-1}$ and $\vec{R}_b = \vec{R}_{i+1} - \vec{R}_i$, for $1 < i < N_r$ or $1 < i < N_s$, and the angle between $\vec{R}_a$ and $\vec{R}_b$ via $\theta_b = \cos^{-1}(\vec{R}_a \cdot \vec{R}_b/|\vec{R}_a||\vec{R}_b|)$. The elastic bending energy is simply given by

$$U_b = \frac{1}{2}k_l\theta_b^2, \tag{4}$$

where $k_l = 60\sigma k_BT$ in the simulation. The choice of this value is based on matching the curvature of the long bacterium in the simulation compared to that observed in experiments. Without interactions with other short bacteria, the long bacterium maintains a straight conformation for most of times due to the long persistence length.

In order to model the change of propelling direction of flagella on the bacteria, we propose a simple way to model the propulsion generated by the flagella. First we assume that each bead is propelled by a constant propulsion force $|\vec{f}_p^{(n)}| = 0.2$ pN. Despite the magnitude is fixed, the direction of the propulsion can be changed according to the current speed of the bead. We first compute the tangential direction by simply using the position vectors between consecutive beads. Then we add an angle deviation $\Delta\theta_p$,

$$\Delta\theta_p = \frac{2\pi}{1 + C_o|\vec{v}|}X, \quad \forall\, X \in \mathbb{R} : -\frac{1}{2} < X < \frac{1}{2}, \tag{5}$$

where X is a uniformly distributed random variable, to the tangential direction. Here the coefficient C_o controls how large the deviation can be according to the current speed $|\vec{v}|$. In this way, even when a bacterium is blocked by other bacteria, it still has ways to turn and escape from the obstacles. On the other hand, when it is relatively free to move, the propulsion tends to align along the long axis of the bacterium. In this work, C_o is set to be 10^3 to imitate the average speed of the bacteria observed in experiments.

A typical simulation comprised $N = 2208$ beads, including $N_s = 48$ for the long bacterium and others for the short ones ($N_r = 4$). There were 540 short bacteria and a long one in the 60×60 μm^2 area, in which periodic boundary conditions were implemented at the edges of the square area. In order to investigate the effects of the contour length of the long cell, we also reduced N_s to smaller values ($N_s = 4, 8, 12, 16, 20, 24$, and 36) in some simulation runs and made the reduced part become short cells; namely, the total number of beads were retained throughout the whole study. The simulation was typically run with the temperature at 25°C, the viscosity of water $\eta = 8.9 \times 10^{-4}$ Pa·s and the friction constant $\xi = 3\pi\eta\sigma$. Each time step of the simulation was 50 μs, and the infinitesimal length interval for spatial derivatives was set to $10^{-4}\sigma$.

3 The Elastic Restoring Force of a Spiral Coil

In what follows we explain the calculation of elastic restoring force of a spiral coil. Here we only take the Single Clockwise (SCW) spiral as the example. The calculation of other three types of spiral coils shall be similar to this case, although it may be tricky for the cases of "S-centered" double spirals. The SCW spiral coil can be mathematically represented as an Archimedes' spiral in the polar coordinates,

$$r = \frac{b}{2\pi}\theta, \tag{6}$$

where b is the width of the bacterium and $\theta \in (2\pi, 2(n+1)\pi]$, n being the number of rounds. Note that the curve does not begin at the origin. This is because the bacterium has finite volume and stiffness, and it is difficult to accommodate itself in that region, $\theta \in [0, 2\pi]$, due to either the high cost of bending energy or the excluded volume interaction. In the experimental observation, we always can see an empty hole or space at the center of spiral coils. Therefore, around the center of the Archimedes' spiral it does not represent the geometry of the spiral coils in our experiments.

Because of the stiffness of the bacterial cell wall, there is energy cost to bend the bacterium. Here the bending energy per unit arc length is thought of as proportional to the quadratic of the curvature

$$\delta U_b = \frac{1}{2}E\kappa^2, \tag{7}$$

where κ is the curvature of the Archimedes' spiral,

$$\kappa = \frac{2\pi(\theta^2+2)}{b(\theta^2+1)^{3/2}}. \tag{8}$$

The constant E is related to the persistence length of the cell l_p and the thermal energy k_BT, according to the worm-like chain model,

$$l_p^{-1} = \frac{k_BT}{E}. \tag{9}$$

In order to compute the elastic restoring force along the spiral coil, one needs to know how to calculate the arc length first. The unit arc length of the Archimedes' spiral can be written as

$$\mathrm{d}s = \frac{b}{2\pi}\sqrt{\theta^2+1}\mathrm{d}\theta. \tag{10}$$

The elastic restoring force per unit arc length now can be obtained by differentiating the bending energy density δU_b with respect to the arc length s,

$$\begin{aligned}
\delta f_b &= -\frac{1}{2}E\frac{\partial \kappa^2}{\partial s} \\
&= -\frac{1}{2}E\frac{\partial}{\partial \theta}\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\right)\left[\frac{2\pi(\theta^2+2)}{b(\theta^2+1)^{3/2}}\right]^2 \\
&= \frac{4\pi^3 l_p k_B T}{b^3}\left[\frac{\theta(\theta^2+2)(3\theta^2+10)}{(\theta^2+1)^{9/2}}\right]. \qquad (11)
\end{aligned}$$

When one puts the values used in the simulation, $b = 1$ μm, $l_p = 60$ μm, and $k_B T \approx 4.12 \times 10^{-3}$ pN-μm, into the result above, the restoring force per unit arc length is monotonically decreasing with the increasing θ in the range $\theta \in (2\pi, 2(n+1)\pi]$, and its maximum at $\theta = 2\pi$ is of the order 10^{-2} pN/μm. For comparison, the propulsion force in the simulation is 0.2 pN per bead. The result of decreasing restoring force per unit arc length is consistent with the direct observation. When one follows the contour of the spiral coil from the center moving toward the outer rim, the degree of bending (i.e. the curvature) is decreasing, thus the elastic restoring force is reducing.