Chemotactic Chiral Active Matter

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1 Models

1.1 Definitions

1.1.1 General Model

$$\dot{\mathbf{r}}_i(t) = v\mathbf{p}(\theta_i) + \sum_{j\in A_i^{1,2}} \mathbf{I}(\Delta\mathbf{r}_{ij}) , \tag{1a}$$

$$\dot{\theta}_i(t) = \omega_i + G(\mathbf{r},\theta,c) + \sum_{j\neq i} H(\Delta\theta_{ij},\Delta\mathbf{r}_{ij}) , \tag{1b}$$

$$\dot{c}(\mathbf{r},t) = D\nabla^2 c + F(c)\sum_{j=1}\delta(\mathbf{r}-\mathbf{r}_i) , \tag{1c}$$

for $i = 1, 2, \cdots, N$. Here, $\mathbf{r}_i$ is the position of the i-th particle, θ_i is the orientation of the i-th particle, v is the self-propulsion velocity, $\mathbf{p}(\theta_i) = (\cos\theta_i, \sin\theta_i)$ is the unit vector pointing in the direction of the i-th particle, ω_i is the natural frequency of the i-th particle, $G(\mathbf{r},\theta,c)$ is the coupling function between particles and chemical fields, $H(\Delta\theta_{ij},\Delta\mathbf{r}_{ij})$ is the coupling function between partials, $c(\mathbf{r},t)$ is the chemical concentration, D is the diffusion coefficient, $F(c)$ is the production rate of the chemical field, $A_i^{1,2} = \{j \mid r_c \geqslant |\mathbf{r}_j - \mathbf{r}_i|\}$, $\Delta\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, $\Delta\theta_{ij} = \theta_j - \theta_i$, $\mathbf{I}(\Delta\mathbf{r}_{ij}) = \frac{\Delta\mathbf{r}_{ij}}{|\Delta\mathbf{r}_{ij}|^2}$. The natural frequencies ω_i are distributed with following two cases:

1. **Single-chiral particles:** The natural frequencies ω_i are distributed in $U(\omega_{\min},\omega_{\max})$ for all particles and $\omega_{\min}\omega_{\max} > 0$.

2. **Double-chiral particles:** The frequencies are distributed in two symmetric uniform distributions, representing two types of chirality. Exactly half of the particles have natural frequencies $\omega_i \sim U(\omega_{\min},\omega_{\max})$ and the other half have natural frequencies $\omega_i \sim U(-\omega_{\max},-\omega_{\min})$.

1.1.2 Polar alignment Interaction

- Additive coupling:

$$\dot{\theta}_i = \omega_i + K\sum_{j=1}^{N} f(r_{ij})\sin(\theta_j - \theta_i + \alpha) , \tag{2}$$

- Mean-field coupling by oscillator number:

$$\dot{\theta}_i = \omega_i + \frac{K}{N}\sum_{j=1}^{N} f(r_{ij})\sin(\theta_j - \theta_i + \alpha) , \tag{3}$$

Here, $f(r_{ij})$ is a function of $r = |\mathbf{r}_i - \mathbf{r}_j|$, and K is the coupling strength. The function $f(r)$ can be defined as

1. $f_H(r) = H(d_0 - r),\ r_0 > 0;$
2. $f_E(r) = e^{-\frac{r}{d_0}},\ r_0 > 0.$

1.1.3 Chemotactic Interaction

General Chemotactic Model For Two Species

Type 1:

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \ , \tag{4a}$$

$$\dot{\theta}_i^{1,2} = \omega + |\nabla c_{1,2}| \sin\left(\varphi_{c_{1,2}} - \theta_i^{1,2}\right) + F\left(\theta, \mathbf{r}\right) \ , \tag{4b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + F_1\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \ , \tag{4c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + F_2\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \ , \tag{4d}$$

where $\mathbf{I}_{ij}^{1,2} = \frac{\mathbf{r}_j - \mathbf{r}_i^{1,2}}{|\mathbf{r}_j - \mathbf{r}_i^{1,2}|^2}$, $\varphi_{c_{1,2}} = \arctan\left(\frac{\partial_y c_{1,2}}{\partial_x c_{1,2}}\right)$ and $A_i^{1,2} = \left\{ j \mid r_c \geqslant |\mathbf{r}_j - \mathbf{r}_i^{1,2}| \right\}$.
Type 2:

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) + \alpha_{1,2}\nabla c_{1,2} - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \ , \tag{5a}$$

$$\dot{\theta}_i^{1,2} = \omega + F\left(\theta, \mathbf{r}\right) \ , \tag{5b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + F_1\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \ , \tag{5c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + F_2\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \ , \tag{5d}$$

Chemotactic Model with Lotka-Volterra Functions

Let $F_1\left(c_1, c_2\right) = c_1\left(k_1 - k_2 c_2\right)$ and $F_2\left(c_1, c_2\right) = c_2\left(k_3 c_1 - k_4\right)$, where k_1, k_2, k_3, k_4 are constants.

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \ , \tag{6a}$$

$$\dot{\theta}_i^{1,2} = \omega + |\nabla c_{1,2}| \sin\left(\varphi_{c_{1,2}} - \theta_i^{1,2}\right) + F\left(\theta, \mathbf{r}\right) \ , \tag{6b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + c_1\left(k_1 - k_2 c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \ , \tag{6c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + c_2\left(k_3 c_1 - k_4\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \ , \tag{6d}$$

2 Continuum model

We start with the model as given by Eqs. (6) in the main text but replace the finite range alignment interaction by a pseudopotential (δ-interaction), which is justified if the interaction is short ranged enough, such that the shape of the associated interaction potential is irrelevant to the many particle dynamics:

In the thermodynamic limit $N \to \infty$, the Eqs. (6a) and (6b) give rise to the following continuum model:

$$\frac{\partial}{\partial t} f^{1,2}\left(\mathbf{r}, \theta, t\right) = -\frac{\partial}{\partial \theta}\left(f^{1,2} v_\theta^{1,2}\right) - \nabla \cdot \left(f^{1,2} \mathbf{v}_\mathbf{r}^{1,2}\right) \ , \tag{7}$$

where $f^{1,2}\left(\mathbf{r}, \theta, t\right)$ is the probability density of particles of species 1 or 2 at position $\mathbf{r}$ and orientation θ at time t, and $\mathbf{v}_\mathbf{r}^{1,2}$ and $v_\theta^{1,2}$ are the velocity fields in the position and orientation space, respectively.

The velocity fields are given by

$$v_\theta^{1,2}(\mathbf{r},\theta,t) = \omega + |\nabla c_{1,2}| \sin\left(\varphi_{c_{1,2}} - \theta\right) + F(\theta,\mathbf{r}) \ , \tag{8a}$$

$$\mathbf{v}_\mathbf{r}^{1,2}(\mathbf{r},\theta,t) = v\mathbf{p}(\theta) - \int \mathrm{d}\theta' \mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\, \mathbf{I}(\mathbf{r}'-\mathbf{r}) \ , \tag{8b}$$

where $\mathbf{I}(\mathbf{r}) = |\mathbf{r}|^{-2}\mathbf{r}$. By substituting Eqs. (8) into Eq. (7), we obtain

$$\begin{aligned}\frac{\partial}{\partial t} f^{1,2}(\mathbf{r},\theta,t) = &- v\mathbf{p}(\theta)\cdot\nabla f^{1,2} - \nabla\cdot\mathbf{F}^{1,2}(\mathbf{r},\theta,t) \\ &- \omega\partial_\theta f^{1,2} - |\nabla c_{1,2}|\, \partial_\theta \left[f^{1,2}\sin\left(\varphi_{c_{1,2}} - \theta\right)\right] \ ,\end{aligned} \tag{9}$$

where

$$\mathbf{F}^{1,2}(\mathbf{r},\theta,t) = \nabla\cdot\int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\, f^{1,2}(\mathbf{r},\theta,t)\, \frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^2} \ , \tag{10}$$

and

$$\begin{aligned}\nabla\cdot\mathbf{F}^{1,2}(\mathbf{r},\theta,t) &= \nabla\cdot\int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\, f^{1,2}(\mathbf{r},\theta,t)\, \frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^2} \\ &= \int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\, \nabla\cdot\left[f^{1,2}(\mathbf{r},\theta,t)\, \frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^2}\right] \\ &= \int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\left[-2\pi\delta(\mathbf{r}'-\mathbf{r})\, f^{1,2}(\mathbf{r},\theta,t) + \nabla f^{1,2}(\mathbf{r},\theta,t)\cdot\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^2}\right] \\ &= -2\pi\left[f^{1,2}(\mathbf{r},\theta,t)\right]^2 + \int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\, \nabla f^{1,2}(\mathbf{r},\theta,t)\cdot\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^2}\end{aligned} \tag{11}$$

The equation accounts for self-propulsion, and short-range repulsion between particles, rotational diffusion and chemotactic alignment. From here, we expand $f^{1,2}(\mathbf{r},\theta,t)$ in a Fourier series

$$f^{1,2}(\mathbf{r},\theta,t) = \sum_{k=-\infty}^{\infty} f_k^{1,2}(\mathbf{r},t)\, \mathrm{e}^{\mathrm{i}k\theta} \ , \tag{12}$$

with the projection

$$f_k^{1,2}(\mathbf{r},t) = \frac{1}{2\pi}\int \mathrm{d}\theta f^{1,2}(\mathbf{r},\theta,t)\, \mathrm{e}^{-\mathrm{i}k\theta} \ , \tag{13}$$

and define the coefficients as the particle density $\rho(\mathbf{r},t)$ and the density-weighted polar order $\boldsymbol{p}(\mathbf{r},t)$ by relating them to the harmonics via the Fourier expansion:

$$\rho^{1,2}(\mathbf{r},t) \equiv \int_0^{2\pi} \mathrm{d}\theta f^{1,2}(\mathbf{r},\theta,t) = 2\pi f_0^{1,2}(\mathbf{r},t) \tag{14a}$$

$$\begin{aligned}\boldsymbol{p}^{1,2}(\mathbf{r},t) &\equiv \int_0^{2\pi} \mathrm{d}\theta\mathbf{p}(\theta)\, f^{1,2}(\mathbf{r},\theta,t) \\ &= \int_0^{2\pi}\mathrm{d}\theta \begin{bmatrix}\cos\theta \\ \sin\theta\end{bmatrix} f^{1,2}(\mathbf{r},\theta,t) = \int_0^{2\pi}\mathrm{d}\theta\frac{1}{2}\begin{bmatrix}\mathrm{e}^{\mathrm{i}\theta}+\mathrm{e}^{-\mathrm{i}\theta} \\ \mathrm{i}\left(\mathrm{e}^{-\mathrm{i}\theta}-\mathrm{e}^{\mathrm{i}\theta}\right)\end{bmatrix} f^{1,2}(\mathbf{r},\theta,t) \\ &= \pi\begin{bmatrix}\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta\left(\mathrm{e}^{\mathrm{i}\theta}+\mathrm{e}^{-\mathrm{i}\theta}\right) f^{1,2}(\mathbf{r},\theta,t) \\ \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta\mathrm{i}\left(\mathrm{e}^{-\mathrm{i}\theta}-\mathrm{e}^{\mathrm{i}\theta}\right) f^{1,2}(\mathbf{r},\theta,t)\end{bmatrix} = \pi\begin{bmatrix}f_1^{1,2}(\mathbf{r},t)+f_{-1}^{1,2}(\mathbf{r},t) \\ \mathrm{i}\left(f_1^{1,2}(\mathbf{r},t)-f_{-1}^{1,2}(\mathbf{r},t)\right)\end{bmatrix}\end{aligned} \tag{14b}$$

In the following, the different contributions to the continuum model, Eq. (7), are analyzed separately. First, in order to derive expressions for the self-propulsion, $-v\mathbf{p}(\theta)\cdot\nabla f^{1,2}$, we apply the projection operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

$$
\begin{aligned}
\frac{\partial}{\partial t} f_{k,\mathrm{prop}}^{1,2} =& \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \mathrm{e}^{-\mathrm{i}k\theta}\left[-v\mathbf{p}(\theta)\cdot\nabla f^{1,2}\right] \\
=& -\frac{v}{4\pi}\int_0^{2\pi} \mathrm{d}\theta \mathrm{e}^{-\mathrm{i}k\theta}\left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left(\mathrm{e}^{\mathrm{i}(m+1)\theta}+\mathrm{e}^{\mathrm{i}(m-1)\theta}\right)+\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left(\mathrm{e}^{\mathrm{i}(m-1)\theta}-\mathrm{e}^{\mathrm{i}(m+1)\theta}\right)\right] \\
=& -\frac{v}{4\pi}\int_0^{2\pi} \mathrm{d}\theta \left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left(\mathrm{e}^{\mathrm{i}(m-k+1)\theta}+\mathrm{e}^{\mathrm{i}(m-k-1)\theta}\right)+\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left(\mathrm{e}^{\mathrm{i}(m-k-1)\theta}-\mathrm{e}^{\mathrm{i}(m-k+1)\theta}\right)\right] \\
=& -\frac{v}{2}\left\{\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left[\delta(m-k+1)+\delta(m-k-1)\right]+\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left[\delta(m-k-1)-\delta(m-k+1)\right]\right\} .
\end{aligned}
\tag{15}
$$

With the definitions, Eqs. (14a) and (14b), we obtain for the field variables

$$
\begin{aligned}
\frac{\partial}{\partial t}\rho_{\mathrm{prop}}^{1,2} =& 2\pi\frac{\partial}{\partial t} f_{0,\mathrm{prop}}^{1,2} \\
=& -v\pi\left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left[\delta(m+1)+\delta(m-1)\right] +\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left[\delta(m-1)-\delta(m+1)\right]\right] \\
=& -v\pi\left[\partial_x\left(f_{-1}^{1,2}+f_1^{1,2}\right)+\mathrm{i}\partial_y\left(f_1^{1,2}-f_{-1}^{1,2}\right)\right] \\
=& -v\nabla\cdot\boldsymbol{p}_{\mathrm{prop}}^{1,2} ,
\end{aligned}
\tag{16}
$$

and because of

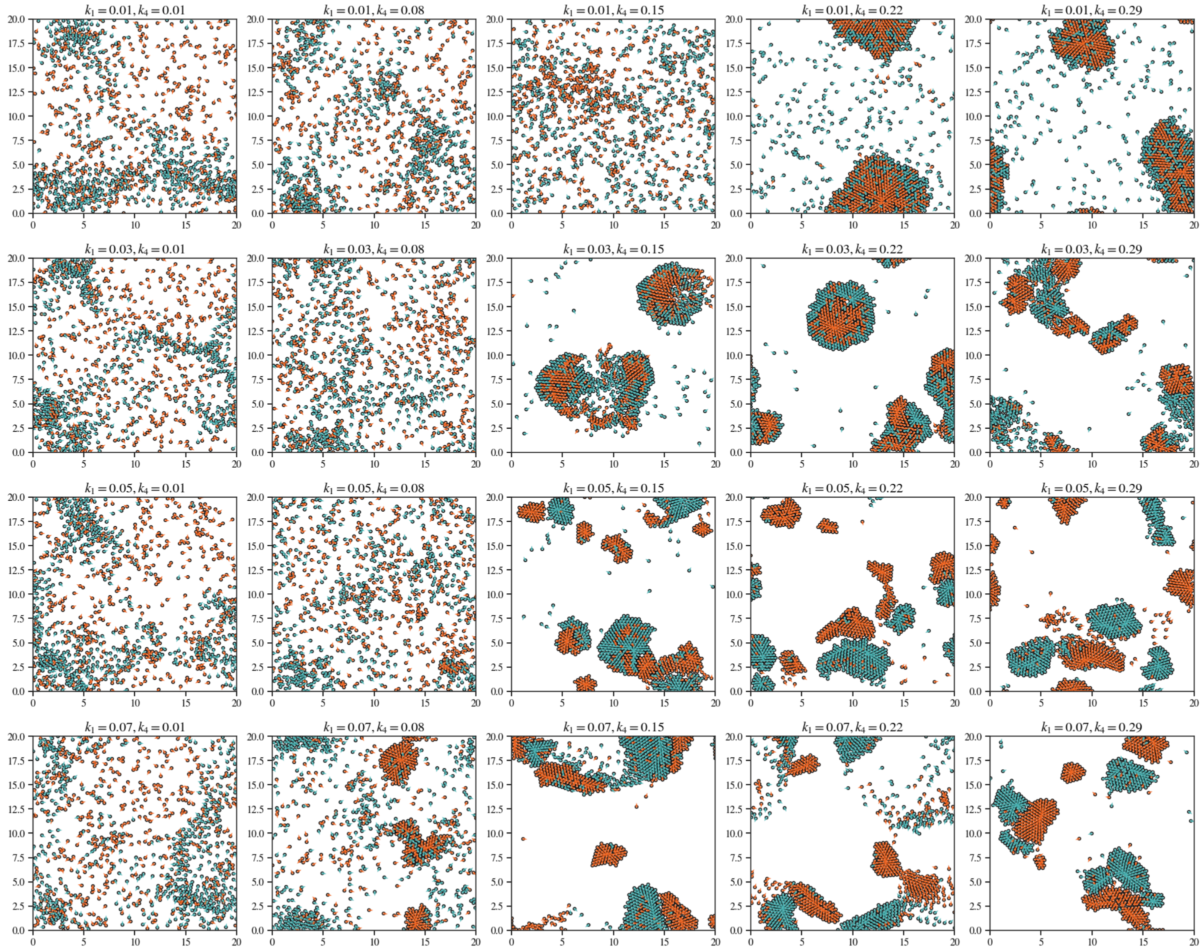
$$
\begin{aligned}
\partial_t f_1^{1,2} &= -\frac{v}{2}\left\{\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left[\delta(m)+\delta(m-2)\right]+\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left[\delta(m-2)-\delta(m)\right]\right\} \\
&= -\frac{v}{2}\left[\partial_x\left(f_0^{1,2}+f_2^{1,2}\right)+\mathrm{i}\partial_y\left(f_2^{1,2}-f_0^{1,2}\right)\right] && (17\mathrm{a}) \\
\partial_t f_{-1}^{1,2} &= -\frac{v}{2}\left\{\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2}\left[\delta(m-2)+\delta(m)\right]+\mathrm{i}\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2}\left[\delta(m)-\delta(m-2)\right]\right\} \\
&= -\frac{v}{2}\left[\partial_x\left(f_0^{1,2}+f_2^{1,2}\right)+\mathrm{i}\partial_y\left(f_0^{1,2}-f_2^{1,2}\right)\right] , && (17\mathrm{b})
\end{aligned}
$$

we have

$$
\frac{\partial}{\partial t}\boldsymbol{p}_{\mathrm{prop}}^{1,2} = \pi\begin{bmatrix} \partial_t\left(f_1^{1,2}+f_{-1}^{1,2}\right) \\ \mathrm{i}\partial_t\left(f_1^{1,2}-f_{-1}^{1,2}\right)\end{bmatrix} = \pi\begin{bmatrix} -v\partial_x\left(f_0^{1,2}+f_2^{1,2}\right) \\ v\partial_y\left(f_2^{1,2}-f_0^{1,2}\right)\end{bmatrix} \approx -\frac{v}{2}\begin{bmatrix}\partial_x f_0^{1,2} \\ \partial_y f_0^{1,2}\end{bmatrix} = -\frac{v}{2}\nabla\rho_{\mathrm{prop}}^{1,2} . \tag{18}
$$

Next, we turn to the short-range repulsion, $-\nabla\cdot\int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f^{1,2}(\mathbf{r}',\theta',t)\,\mathbf{I}(\mathbf{r}-\mathbf{r}')$. We apply the projection operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

3 Behaviors



$k_1 = 0.01, k_4 = 0.01$
$k_1 = 0.01, k_4 = 0.08$
$k_1 = 0.01, k_4 = 0.15$
$k_1 = 0.01, k_4 = 0.22$
$k_1 = 0.01, k_4 = 0.29$
$k_1 = 0.03, k_4 = 0.01$
$k_1 = 0.03, k_4 = 0.08$
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