

# Chemotactic Chiral Active Matter

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# 1 Models

## 1.1 Definitions

### 1.1.1 General Model

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

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

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

for  $i = 1, 2, \dots, N$ . Here,  $\mathbf{r}_i$  is the position of the  $i$ -th particle,  $\theta_i$  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,  $\omega_i$  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 particles,  $c(\mathbf{r}, t)$  is the chemical concentration,  $D$  is the diffusion coefficient,  $F(c)$  is the production rate of the chemical field,  $A_i^{1,2} = \{j \mid r_c \geq |\mathbf{r}_j - \mathbf{r}_i|\}$ ,  $\Delta\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ ,  $\Delta\theta_{ij} = \theta_j - \theta_i$ ,  $\mathbf{I}(\Delta\mathbf{r}_{ij}) = \frac{\Delta\mathbf{r}_{ij}}{|\Delta\mathbf{r}_{ij}|^2}$ . The natural frequencies  $\omega_i$  are distributed with following two cases:

1. **Single-chiral particles:** The natural frequencies  $\omega_i$  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:

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

- Mean-field coupling by oscillator number:

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

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:

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

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

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

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

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  $A_i^{1,2} = \left\{j \mid r_c \geq |\mathbf{r}_j - \mathbf{r}_i^{1,2}|\right\}$ .  
Type 2:

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

$$\dot{\theta}_i^{1,2} = \omega_i + F(\theta, \mathbf{r}), \quad (5b)$$

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

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

### Chemotactic Model with Lotka-Volterra Functions

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

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

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

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

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

## 2 Continuum model

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

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

where  $f^{1,2}(\mathbf{r}, \theta, t)$  is the probability density of particles of species 1 or 2 at position  $\mathbf{r}$  and orientation  $\theta$  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

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

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

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

$$\begin{aligned} \frac{\partial}{\partial t} f^{1,2}(\mathbf{r}, \theta, t) = & -\omega \partial_\theta f^{1,2} - |\nabla c_{1,2}| \partial_\theta [f^{1,2} \sin(\varphi_{c_{1,2}} - \theta)] \\ & - v \mathbf{p}(\theta) \cdot \nabla f^{1,2} - \nabla \cdot \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) \mathbf{I}(\mathbf{r} - \mathbf{r}') . \end{aligned} \quad (9)$$

From here, we expand  $f^{1,2}(\mathbf{r}, \theta, t)$  in a Fourier series  $f^{1,2}(\mathbf{r}, \theta, t) = \sum_{k=-\infty}^{\infty} f_k^{1,2}(\mathbf{r}, t) e^{-ik\theta}$  with  $f_k^{1,2}(\mathbf{r}, t) = \frac{1}{2\pi} \int d\theta f^{1,2}(\mathbf{r}, \theta, t) e^{ik\theta}$  and define the coefficients as the particle density  $\rho(\mathbf{r}, t)$  and the density-weighted polar order  $\mathbf{p}(\mathbf{r}, t)$  by relating them to the harmonics via the Fourier expansion:

$$\rho(\mathbf{r}, t) \equiv \int_0^{2\pi} d\theta f^{1,2}(\mathbf{r}, \theta, t) = 2\pi f_0^{1,2}(\mathbf{r}, t) \quad (10a)$$

$$\begin{aligned} \mathbf{p}(\mathbf{r}, t) & \equiv \int_0^{2\pi} d\theta \mathbf{p}(\theta) f^{1,2}(\mathbf{r}, \theta, t) \\ & = \int_0^{2\pi} d\theta \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} f^{1,2}(\mathbf{r}, \theta, t) = \int_0^{2\pi} d\theta \frac{1}{2} \begin{bmatrix} e^{i\theta} + e^{-i\theta} \\ i(e^{-i\theta} - e^{i\theta}) \end{bmatrix} f^{1,2}(\mathbf{r}, \theta, t) \\ & = \pi \begin{bmatrix} \frac{1}{2\pi} \int_0^{2\pi} d\theta (e^{i\theta} + e^{-i\theta}) f^{1,2}(\mathbf{r}, \theta, t) \\ \frac{1}{2\pi} \int_0^{2\pi} d\theta i(e^{-i\theta} - e^{i\theta}) f^{1,2}(\mathbf{r}, \theta, t) \end{bmatrix} = \pi \begin{bmatrix} f_1^{1,2}(\mathbf{r}, t) + f_{-1}^{1,2}(\mathbf{r}, t) \\ i(f_1^{1,2}(\mathbf{r}, t) - f_{-1}^{1,2}(\mathbf{r}, t)) \end{bmatrix} \end{aligned} \quad (10b)$$

### 3 Behaviors

