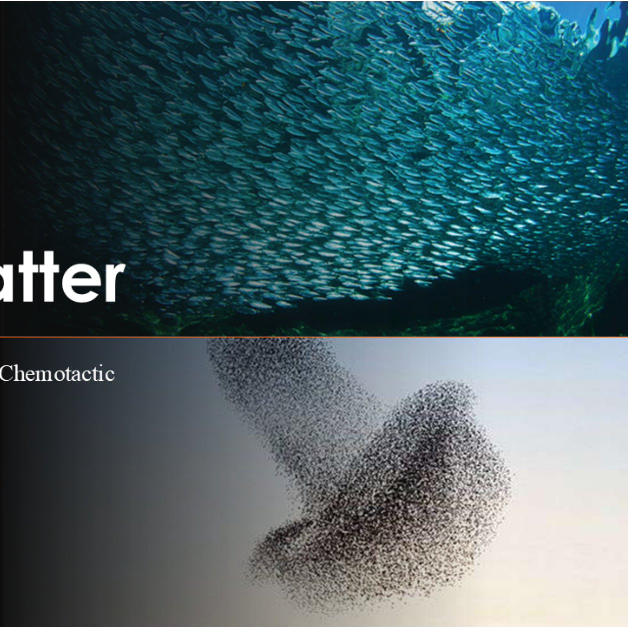
Active Matter



Flocking, Self-propelled, Chiral & Chemotactic

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$$\dot{\mathbf{r}}_i(t) = v\mathbf{p}(\theta_i) + \sum_{j \neq i} \mathbf{I}\left(\Delta \mathbf{r}_{ij}\right), \tag{1a}$$

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

for $i = 1, 2, \cdots, N$. Here, $\mathbf{r}_i$ and θ_i is the position and orientation of the i-th particle, respectively, v is the self-propulsion velocity, $\mathbf{p}(\theta_i) = (\cos\theta_i, \sin\theta_i)$ is the instantaneous unit orientation, ω_i is the natural frequency, $H\left(\Delta\theta_{ij}, \Delta\mathbf{r}_{ij}\right)$ is the coupling function between partials, $\Delta\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\Delta\theta_{ij} = \theta_i - \theta_j$.

$$\mathbf{I}(\Delta\mathbf{r}) = \frac{\Delta\mathbf{r}}{|\Delta\mathbf{r}|} k\left(R_r - |\Delta\mathbf{r}|\right) \Theta\left(R_r - |\Delta\mathbf{r}|\right) \tag{2}$$

$$H(\Delta\theta, \Delta\mathbf{r}) = K \sin(\Delta\theta)\, \Theta\left(R_\theta - |\Delta\mathbf{r}|\right) \tag{3}$$

In the thermodynamic limit $N \to \infty$, the agent-based model gives rise to the following continuum form:

$$\frac{\partial}{\partial t} f\left(\mathbf{r}, \theta, t\right) = -\frac{\partial}{\partial \theta}\left(f v_\theta\right) - \nabla \cdot \left(f \mathbf{v_r}\right) \ , \tag{4}$$

where $f\left(\mathbf{r}, \theta, t\right)$ is the probability density of particles at position $\mathbf{r}$ and orientation θ at time t, and $\mathbf{v_r}$ and v_θ are the velocity fields in the position and orientation space, respectively. The velocity fields are given by

$$v_\theta\left(\mathbf{r}, \theta, t\right) = \omega + K \int \mathrm{d}\theta' f\left(\mathbf{r}, \theta', t\right) \sin\left(\theta' - \theta\right) \ , \tag{5a}$$

$$\mathbf{v_r}\left(\mathbf{r}, \theta, t\right) = v\mathbf{p}\left(\theta\right) + \int \mathrm{d}\theta' \mathrm{d}\mathbf{r}' f\left(\mathbf{r}', \theta', t\right) \mathbf{I}\left(\mathbf{r} - \mathbf{r}'\right) \ . \tag{5b}$$

By substituting Eqs. (5) into Eq. (4), we obtain

$$\begin{aligned}\frac{\partial}{\partial t} f\left(\mathbf{r}, \theta, t\right) = & - v\mathbf{p}\left(\theta\right) \cdot \nabla f - \nabla \cdot \left[f\left(\mathbf{r}, \theta, t\right) \int \mathrm{d}\theta' \mathrm{d}\mathbf{r}' f\left(\mathbf{r}', \theta', t\right) \mathbf{I}\left(\mathbf{r} - \mathbf{r}'\right)\right] \\ & - \omega \partial_\theta f - K \partial_\theta \left[f\left(\mathbf{r}, \theta, t\right) \int \mathrm{d}\theta' f\left(\mathbf{r}, \theta', t\right) \sin\left(\theta' - \theta\right)\right] \ ,\end{aligned} \tag{6}$$

$$\frac{\partial}{\partial t} f(\mathbf{r},\theta,t) = -v\mathbf{p}(\theta)\cdot\nabla f - \nabla\cdot\left[f(\mathbf{r},\theta,t)\int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f(\mathbf{r}',\theta',t)\,\mathbf{I}(\mathbf{r}-\mathbf{r}')\right]$$
$$-\omega\partial_\theta f - K\partial_\theta \int \mathrm{d}\theta'\mathrm{d}\mathbf{r}' f(\mathbf{r},\theta',t)\sin(\theta'-\theta)\ , \tag{7}$$

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

$$f(\mathbf{r},\theta,t) = \sum_{k=-\infty}^{\infty} f_k(\mathbf{r},t)\,\mathrm{e}^{\mathrm{i}k\theta}\ , \tag{8}$$

with the projection

$$f_k(\mathbf{r},t) = \frac{1}{2\pi}\int \mathrm{d}\theta f(\mathbf{r},\theta,t)\,\mathrm{e}^{-\mathrm{i}k\theta}\ , \tag{9}$$

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

$$\rho\left(\mathbf{r},t\right) \equiv \int_0^{2\pi} \mathrm{d}\theta f\left(\mathbf{r},\theta,t\right) = 2\pi f_0\left(\mathbf{r},t\right) \tag{10a}$$

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

In the following, the different contributions to the continuum model, are analyzed separately.
Firstly, in order to derive expressions for the self-propulsion, $-v\mathbf{p}(\theta)\cdot\nabla f$, we apply the projection operator, $f_k(\mathbf{r},t)=\frac{1}{2\pi}\int \mathrm{d}\theta f(\mathbf{r},\theta,t)\,\mathrm{e}^{-\mathrm{i}k\theta}$, onto the corresponding term and obtain

$$\begin{aligned}\frac{\partial}{\partial t}f_{k,\mathrm{prop}} =& \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta \mathrm{e}^{-\mathrm{i}k\theta}\left[-v\mathbf{p}(\theta)\cdot\nabla f\right] \\ =& -\frac{v}{4\pi}\int_0^{2\pi}\mathrm{d}\theta\left\{\mathrm{e}^{-\mathrm{i}k\theta}\left[\partial_x\sum_{m=-\infty}^{\infty}f_m\left(\mathrm{e}^{\mathrm{i}(m+1)\theta}+\mathrm{e}^{\mathrm{i}(m-1)\theta}\right)\right.\right. \\ & \left.\left. +\mathrm{i}\partial_y\sum_{k=-\infty}^{\infty}f_m\left(\mathrm{e}^{\mathrm{i}(m-1)\theta}-\mathrm{e}^{\mathrm{i}(m+1)\theta}\right)\right]\right\} \\ =& -\frac{v}{2}\left\{\partial_x\sum_{m=-\infty}^{\infty}f_m\left[\delta(m-k+1)+\delta(m-k-1)\right]\right. \\ & \left. +\mathrm{i}\partial_y\sum_{k=-\infty}^{\infty}f_m\left[\delta(m-k-1)-\delta(m-k+1)\right]\right\}.\end{aligned} \tag{11}$$

With the definitions of $\rho\left(\mathbf{r},t\right)$ and $p\left(\mathbf{r},t\right)$, we obtain for the field variables

$$\begin{aligned}\frac{\partial}{\partial t}\rho_{\text{prop}} =&2\pi\frac{\partial}{\partial t}f_{0,\text{prop}}\\ =&-v\pi\left[\partial_x\sum_{m=-\infty}^{\infty}f_m\left(\delta_{m+1}+\delta_{m-1}\right)+\mathrm{i}\partial_y\sum_{k=-\infty}^{\infty}f_m\left(\delta_{m-1}-\delta_{m+1}\right)\right]\\ =&-v\pi\left[\partial_x\left(f_{-1}+f_1\right)+\mathrm{i}\partial_y\left(f_1-f_{-1}\right)\right]\\ =&-v\nabla\cdot p_{\text{prop}}\ ,\end{aligned}\tag{12}$$

and because of

$$\partial_t f_1=-\frac{v}{2}\left[\partial_x\left(f_0+f_2\right)+\mathrm{i}\partial_y\left(f_2-f_0\right)\right]\ ,\tag{13a}$$

$$\partial_t f_{-1}=-\frac{v}{2}\left[\partial_x\left(f_0+f_2\right)+\mathrm{i}\partial_y\left(f_0-f_2\right)\right]\ ,\tag{13b}$$

we have

$$\frac{\partial}{\partial t}p_{\text{prop}}=\pi\begin{bmatrix}-v\partial_x\left(f_0+f_2\right)\\ v\partial_y\left(f_2-f_0\right)\end{bmatrix}\approx-\frac{v}{2}\begin{bmatrix}\partial_x f_0\\ \partial_y f_0\end{bmatrix}=-\frac{v}{2}\nabla\rho_{\text{prop}}\tag{14}$$

Next, we turn to the rotational diffusion, $-\omega\partial_\theta f$.

$$\begin{aligned}\frac{\partial}{\partial t} f_{k,\mathrm{rota}}(\mathbf{r},t) &= -\frac{\omega}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \mathrm{e}^{-\mathrm{i}k\theta}\partial_\theta f(\mathbf{r},\theta,t) \\ &= -\frac{\omega}{2\pi}\sum_{m=-\infty}^{\infty} \mathrm{i}m f_{m,\mathrm{rota}}(\mathbf{r},t)\int_0^{2\pi} \mathrm{d}\theta \mathrm{e}^{\mathrm{i}(m-k)\theta} \\ &= -\omega\sum_{m=-\infty}^{\infty} \mathrm{i}m f_{m,\mathrm{rota}}(\mathbf{r},t)\,\delta(m-k) \\ &= -\mathrm{i}k\omega f_{k,\mathrm{rota}}(\mathbf{r},t)\end{aligned} \tag{15}$$

With the definitions of $\rho(\mathbf{r},t)$ and $p(\mathbf{r},t)$, we obtain for the field variables

$$\begin{aligned}\frac{\partial}{\partial t}\rho_{\mathrm{rota}} &= 0\ , \\ \frac{\partial}{\partial t}p_{\mathrm{rota}} &= \omega\pi\begin{bmatrix} \mathrm{i}\left(f_{-1,\mathrm{rota}} - f_{1,\mathrm{rota}}\right) \\ f_{-1,\mathrm{rota}} + f_{1,\mathrm{rota}}\end{bmatrix} = \omega p_{\mathrm{rota},\perp}\ ,\end{aligned} \tag{16}$$

where $p_{\mathrm{rota},\perp} = \left(-p_{\mathrm{rota},y}, p_{\mathrm{rota},x}\right)$.

Next, we turn to the alignment interactions,

$$
\begin{aligned}
\frac{\partial}{\partial t} f_{\text{alig}}(\mathbf{r},\theta,t) =& -K\partial_\theta\left[f(\mathbf{r},\theta,t)\int \mathrm{d}\theta' f(\mathbf{r},\theta',t)\sin(\theta'-\theta)\right] \\
=& K\mathrm{i}\pi\left(\mathrm{e}^{-\mathrm{i}\theta} f_{-1,\text{alig}} - \mathrm{e}^{\mathrm{i}\theta} f_{1,\text{alig}}\right)\sum_{-\infty}^{+\infty} m f_{k,\text{alig}} \mathrm{e}^{\mathrm{i}m\theta} + \\
& K\pi\left(\mathrm{e}^{-\mathrm{i}\theta} f_{-1,\text{alig}} + \mathrm{e}^{\mathrm{i}\theta} f_{1,\text{alig}}\right) f_{\text{alig}}
\end{aligned}
\tag{17}
$$

and

$$
\begin{aligned}
\frac{\partial}{\partial t} f_{k,\text{alig}}(\mathbf{r},t) =& \frac{1}{2\pi}\int \mathrm{d}\theta f_{\text{alig}}(\mathbf{r},\theta,t)\,\mathrm{e}^{-\mathrm{i}k\theta} \\
=& -K\pi\left(f_{-1,\text{alig}}\sum_{-\infty}^{+\infty} m f_{k,\text{alig}}\delta_{k-m+1} - f_{1,\text{alig}}\sum_{-\infty}^{+\infty} m f_{k,\text{alig}}\delta_{k-m-1}\right) \\
& + K\pi\left(f_{k+1,\text{alig}} f_{-1,\text{alig}} + f_{k-1,\text{alig}} f_{1,\text{alig}}\right) \\
=& -K\pi\left[(k+1) f_{-1,\text{alig}} f_{k,\text{alig}} - (k-1) f_{1,\text{alig}} f_{k,\text{alig}}\right] \\
& + K\pi\left(f_{k+1,\text{alig}} f_{-1,\text{alig}} + f_{k-1,\text{alig}} f_{1,\text{alig}}\right)
\end{aligned}
\tag{18}
$$

With the definitions of $\rho(\mathbf{r},t)$ and $p(\mathbf{r},t)$, we obtain for the field variables

$$\begin{aligned} &\frac{\partial}{\partial t}\rho_{\text{alig}} = 0 \, , \\ &\frac{\partial}{\partial t}p_{\text{alig}} = \pi \begin{bmatrix} \partial_t \left[f_1(\mathbf{r},t) + f_{-1}(\mathbf{r},t)\right] \\ \mathrm{i}\partial_t \left[f_1(\mathbf{r},t) - f_{-1}(\mathbf{r},t)\right] \end{bmatrix} = K\rho_{\text{alig}}p_{\text{alig}} \end{aligned} \tag{19}$$

because of

$$\begin{aligned} \frac{\partial}{\partial t}f_1 &= K\pi\left(f_2 f_{-1} + f_0 f_1 - 2f_{-1}f_1\right) = K\pi f_1\left(f_0 - 2f_{-1}\right) \\ \frac{\partial}{\partial t}f_{-1} &= K\pi\left(f_0 f_{-1} + f_{-2} f_1 - 2f_{-1}f_1\right) = K\pi f_{-1}\left(f_0 - 2f_1\right) \end{aligned} \tag{20}$$

Next, we turn to the short-range repulsion

$$\begin{aligned}\int F_{\mathrm{sr}} f\left(\mathbf{r}', \theta', t\right) \mathrm{d}\mathbf{r}' \mathrm{d}\theta' &= 2\pi \int \frac{\mathbf{r}-\mathbf{r}'}{\left|\mathbf{r}-\mathbf{r}'\right|} k\left(R_r - \left|\mathbf{r}-\mathbf{r}'\right|\right) \Theta\left(R_r - \left|\mathbf{r}-\mathbf{r}'\right|\right) f\left(\mathbf{r}', t\right) \mathrm{d}\mathbf{r}' \\ &= 2\pi \int_0^{R_r} \int_0^{2\pi} \mathbf{p}(\phi) k\left(R_r - d\right)\left[f(0, t) + d\nabla f\left(\mathbf{r}', t\right)\right] \mathrm{d}d\mathrm{d}\phi \\ &= \frac{4\pi^2}{3} R_r^4 \nabla f\left(\mathbf{r}', t\right)\end{aligned} \tag{21}$$

To summarize, the continuum model can be written as

$$\dot{\rho}^{1,2}(\mathbf{r},t) = -v\nabla\cdot p^{1,2} + D\nabla^2\rho^{1,2}\ , \tag{22a}$$

$$\dot{p}^{1,2}(\mathbf{r},t) = -\frac{v}{2}\nabla\rho^{1,2} + D\nabla^2 p^{1,2} + \omega p_{\perp}^{1,2} - K\rho p\ , \tag{22b}$$