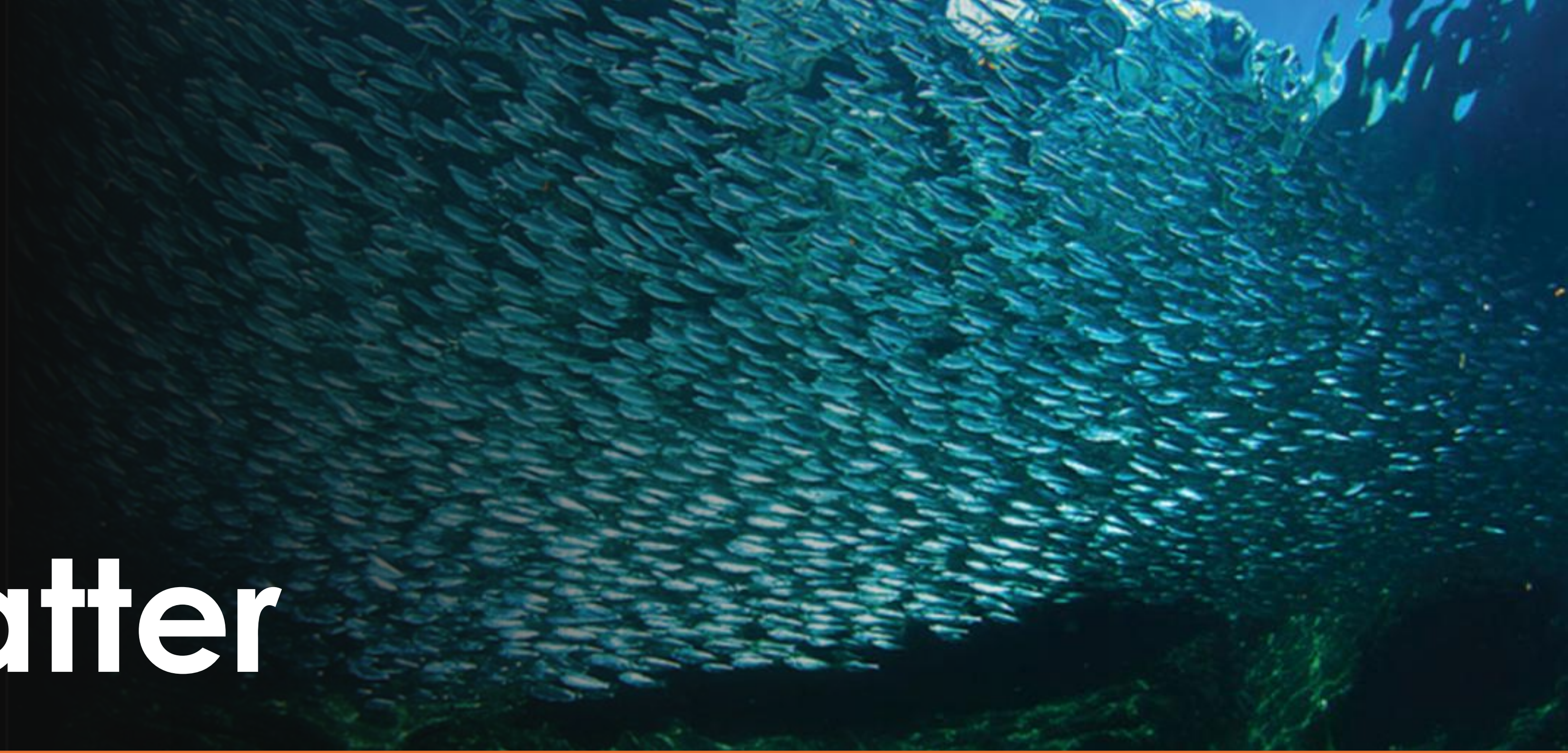
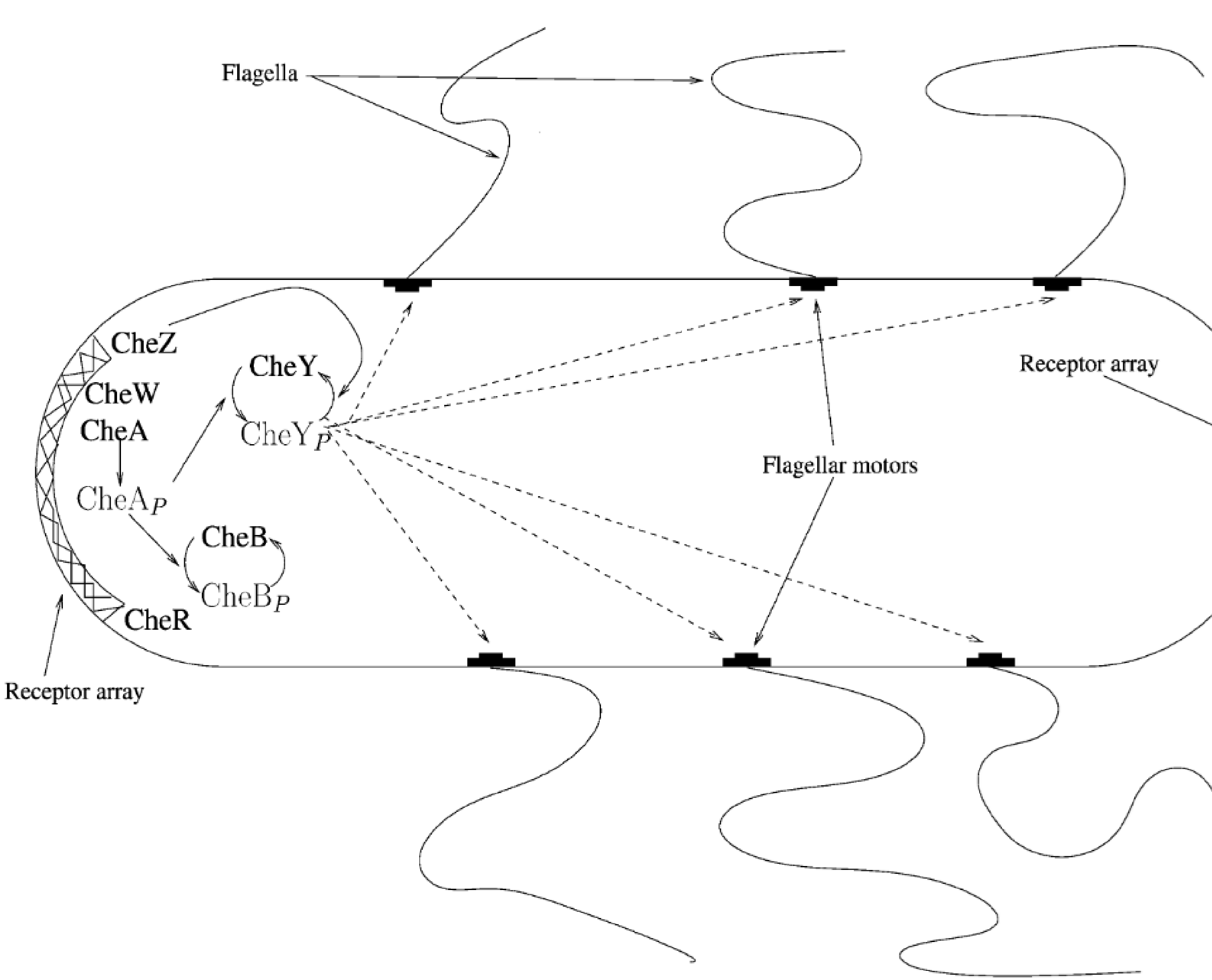
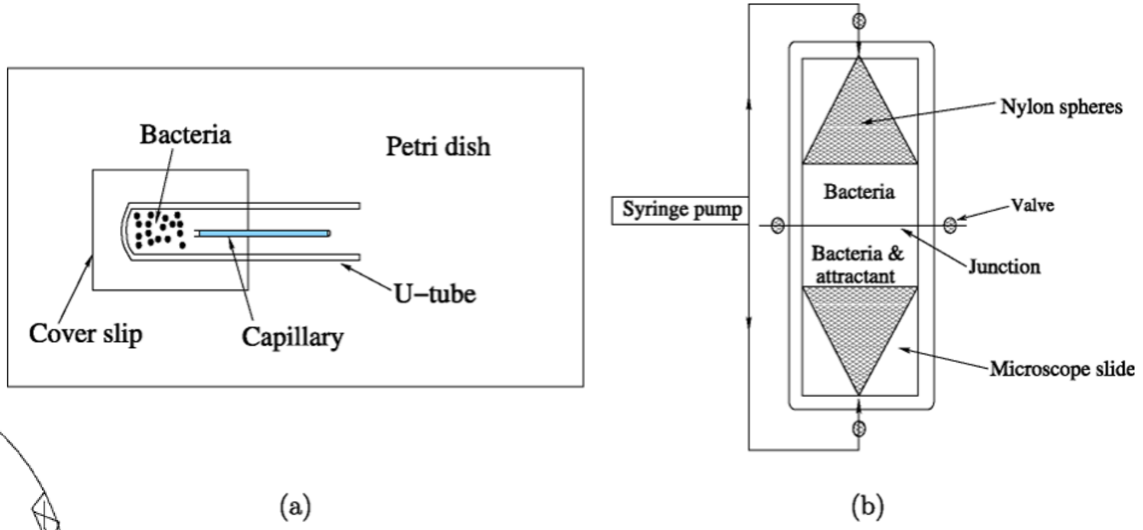
Active Matter

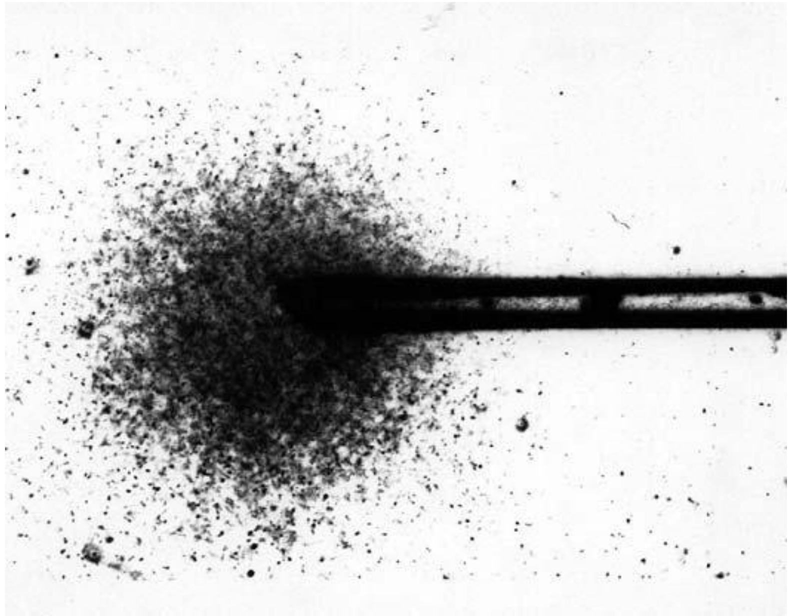


Flocking, Self-propelled, Chiral & Chemotactic

Chemotaxis Bacteria







[1] M. J. Tindall, P. K. Maini, S. L. Porter, and J. P. Armitage, Overview of Mathematical Approaches Used to Model Bacterial Chemotaxis II: Bacterial Populations, Bull. Math. Biol. 70, 1570 (2008).

Agent-based Chemotaxis Model to Smoluchowski Equation

Single Agent

$$\dot{\mathbf{r}}_1(t) = \beta_D \nabla_c(\mathbf{r}_1(t), t) + \sqrt{2D}\,\boldsymbol{\xi}(t)$$

$$\dot{c}(\mathbf{r}, t) = D_c \nabla^2 c(\mathbf{r}, t) + k_0 \delta(\mathbf{r} - \mathbf{r}_1) - k_d c(\mathbf{r}, t)$$

Multi Agents

$$\dot{\mathbf{r}}_i(t) = \beta_D \nabla_c(\mathbf{r}_i(t), t) + \sqrt{2D}\,\boldsymbol{\xi}(t)$$

$$\dot{c}(\mathbf{r}, t) = D_c \nabla^2 c(\mathbf{r}, t) + k_0 \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) - k_d c(\mathbf{r}, t)$$

Smoluchowski Equation

$$\rho(\mathbf{r}, t) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))$$

$$\dot{\rho} = -\nabla \cdot (\beta_D \rho \nabla c) + D \nabla^2 \rho$$

$$\dot{c} = D_c \nabla^2 c + k_0 \rho - k_d c$$

Generalized Keller–Segel (K–S) model

$$\frac{\partial b}{\partial t} = \nabla \cdot (\mu(s) \nabla b) - \nabla \cdot (\chi(s) b \nabla s) + g(b, s) - h(b, s),$$

$$\frac{\partial s}{\partial t} = D \nabla^2 s - f(b, s),$$

[1] Keller, E., Segel, L., 1970. Initiation of slime mold aggregation viewed as an instability. J. Theor. Biol. 26, 399–415.

[2] Keller, E., Segel, L., 1971a. Model for chemotaxis. J. Theor. Biol. 30(2), 225–234.

A trivial solution:

Uniform disordered phase / Equilibrium state

$$\rho(\mathbf{r}, t) \equiv \rho_0$$

$$c(\mathbf{r}, t) \equiv \frac{k_0 \rho_0}{k_d}$$

Keller–Segel instability

Smoluchowski Equation

$$\dot{\rho} = -\nabla \cdot (\beta_D \rho \nabla c) + D\nabla^2 \rho$$

$$\dot{c} = D_c \nabla^2 c + k_0 \rho - k_d c$$

Linear stability analysis

$$(\rho, c) = (\rho_0, k_0 \rho_0 / k_d)$$

$$\rho = \rho_0 + \delta\rho,\ c = c_0 + \delta c\ \ (|\delta\rho| \ll \rho_0,\ |\delta c| \ll c_0)$$

$$\begin{aligned}
\dot{\delta\rho} &= -\beta_D \nabla \cdot (\rho \nabla \delta c) + D\nabla^2 \delta\rho \\
&= -\beta_D \nabla \cdot [(\rho_0 + \delta\rho)\nabla(c_0 + \delta c)] + D\nabla^2(\rho_0 + \delta\rho) \\
&= D\nabla^2 \delta\rho - \beta_D \rho_0 \nabla^2 \delta c - \beta_D \nabla \cdot \underbrace{(\delta\rho \nabla \delta c)}_{\approx 0} \\
&= D\nabla^2 \delta\rho - \beta_D \rho_0 \nabla^2 \delta c
\end{aligned}$$

$$\begin{aligned}
\dot{\delta c} &= D_c \nabla^2 \delta c + k_0 \delta\rho - k_d \delta c + \underbrace{k_0 \delta_0 - k_d c_0}_{=0} \\
&= D_c \nabla^2 \delta c + k_0 \delta\rho - k_d \delta c
\end{aligned}$$

Take the form of a plane wave:

$$\delta\rho = \delta\rho_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}},\ \ \delta c = \delta c_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}}$$

Symbol	Means
σ	growth rate
$\mathbf{k}$	wave vector (representing the oscillation mode in space)
$k = \lvert\mathbf{k}\rvert$	wave numbers (LSA usually focuses on the σ corresponding to different wave numbers)

For $\delta\rho = \delta\rho_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}}$

$$\text{left} = \dot{\delta\rho} = \sigma \delta\rho_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}}$$

$$\text{right} = D(-k^2)\delta\rho_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}} - \beta_D \rho_0 (-k^2) \delta c_0 \mathrm{e}^{\sigma t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}}$$

$$\sigma \delta\rho_0 = -Dk^2 \delta\rho_0 + \beta_D \rho_0 k^2 \delta c_0$$

$$\begin{cases}
\sigma \delta\rho_0 = -Dk^2 \delta\rho_0 + \beta_D \rho_0 k^2 \delta c_0 \\
\sigma \delta c_0 = -D_c k^2 \delta c_0 + k_0 \delta\rho_0 - k_d \delta c_0
\end{cases}$$

Keller−Segel instability

$$\begin{cases} \sigma\delta\rho_0 = -Dk^2\delta\rho_0 + \beta_D\rho_0 k^2\delta c_0 \\ \sigma\delta c_0 = -D_c k^2\delta c_0 + k_0\delta\rho_0 - k_d\delta c_0 \end{cases}$$

This can be written in matrix form

$$\begin{pmatrix} \sigma + Dk^2 & -\beta_D\rho_0 k^2 \\ -k_0 & \sigma + D_c k^2 + k_d \end{pmatrix}\begin{pmatrix} \delta\rho_0 \\ \delta c_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

In order to have non-zero solutions, the det of the coefficient matrix must be 0:

$$\det\begin{pmatrix} \sigma + Dk^2 & -\beta_D\rho_0 k^2 \\ -k_0 & \sigma + D_c k^2 + k_d \end{pmatrix} = 0$$

$$\Downarrow$$

$$\sigma^2 + [(D + D_c)k^2 + k_d]\sigma + DD_c k^4 + (Dk_d - \beta_D\rho_0 k_0)k^2 = 0$$

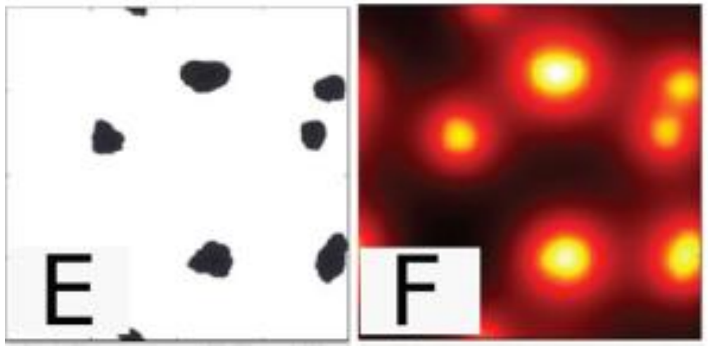
$$\forall k,\ \sigma < 0 \Rightarrow \forall k,\ \begin{cases} (D + D_c)k^2 + k_d > 0 \\ DD_c k^4 + (Dk_d - \beta_D\rho_0 k_0)k^2 > 0 \end{cases}$$

$$\Rightarrow\ Dk_d > \beta_D\rho_0 k_0$$

Keller−Segel instability:

$$\beta_D\rho_0 k_0 > Dk_d$$

The Keller−Segel instability leads to clusters of active particles and colocated clusters of the self-produced chemical that grow in the coarse of the time due to coarsening and cluster coalescence:



Chemotaxis Self-propelled Particles

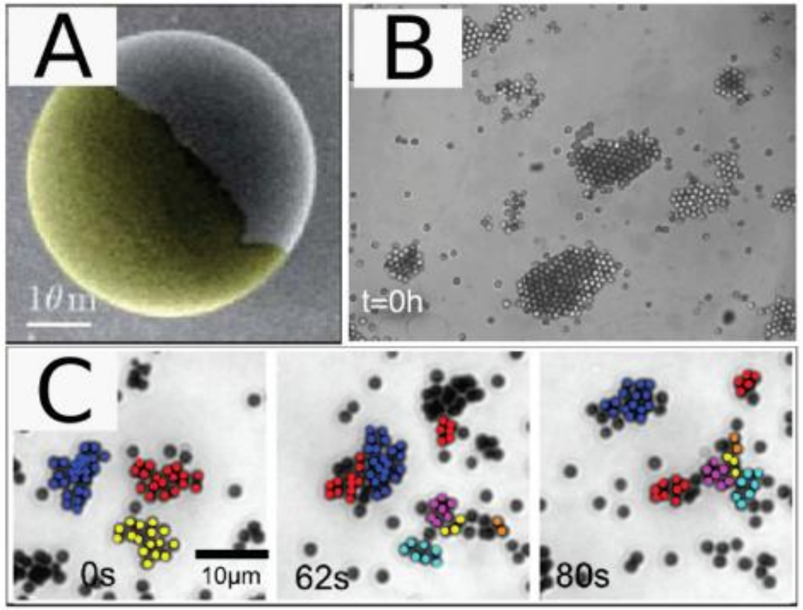
$$\dot{\mathbf{r}}(t) = \nu_0 \mathbf{p} + \beta_{D} \nabla c(\mathbf{r}(t), t) + \sqrt{2D}\,\boldsymbol{\xi}(t)$$

$$\dot{\theta}(t) = \beta \mathbf{p} \times \nabla c(\mathbf{r}(t), t) + \sqrt{2D_{\mathbf{r}}}\,\eta(t)$$

$$\dot{c}(\mathbf{r},t) = D_c \nabla^2 c(\mathbf{r},t) + k_0 \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) - k_d c(\mathbf{r},t)$$

$$\mathbf{p} = (\cos\theta,\ \sin\theta)$$

Janus colloid

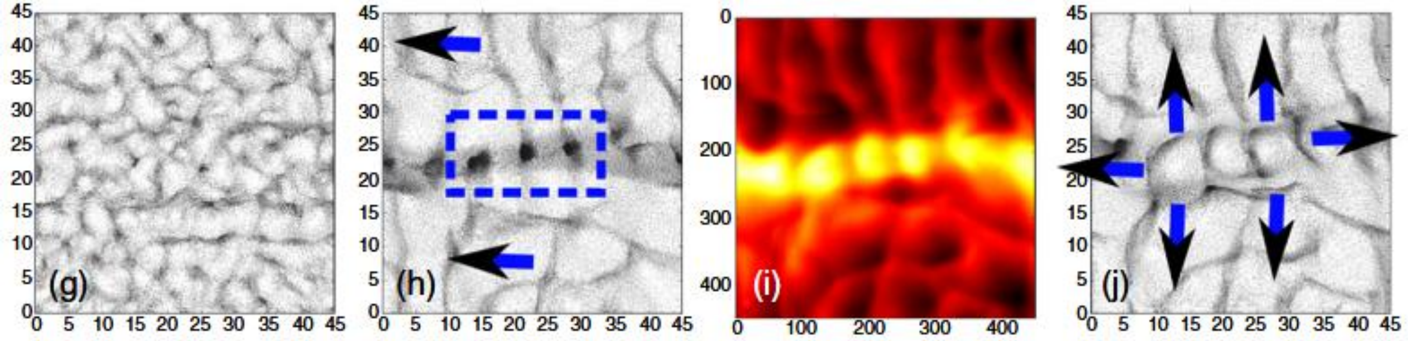


Phoretic Interactions Generically Induce Dynamic Clusters and Wave Patterns in Active Colloids:

$$\dot{\mathbf{r}}_i(t) = v\mathbf{p}_i, \tag{1}$$

$$\dot{\theta}_i(t) = \beta \mathbf{p}_i \times \boldsymbol{\nabla} c + \sqrt{2D_r}\eta_i(t). \tag{2}$$

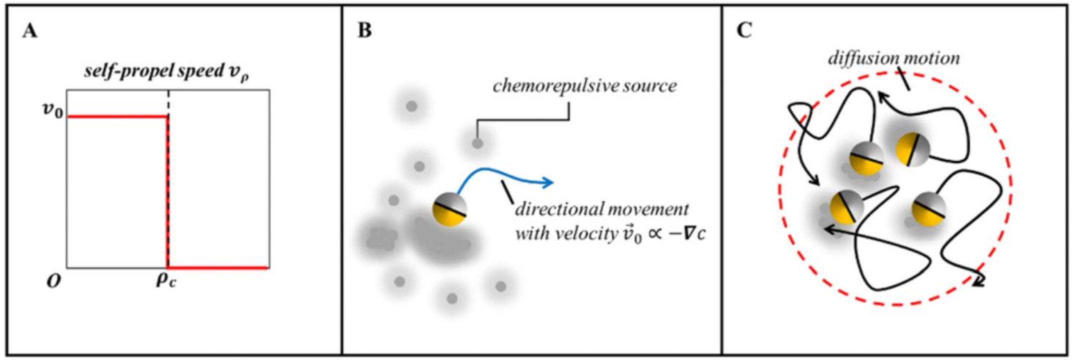
$$\dot{c}(\mathbf{r},t) = D_c \boldsymbol{\nabla}^2 c - k_d c + \sum_{i=1}^{N} \oint d\mathbf{x}_i \delta(\mathbf{r} - \mathbf{r}_i(t) - R_0 \mathbf{x}_i)\sigma(\mathbf{x}_i). \tag{3}$$



[1] B. Liebchen, D. Marenduzzo, and M. E. Cates, Phoretic Interactions Generically Induce Dynamic Clusters and Wave Patterns in Active Colloids, Phys. Rev. Lett. 118, 268001 (2017).

A Variety of Chemotaxis Particles

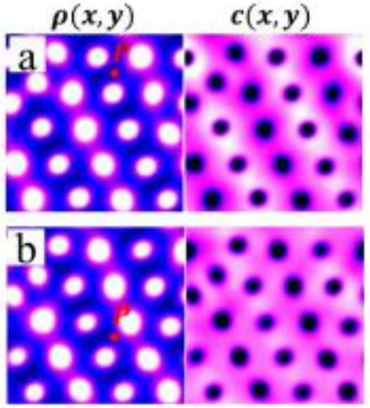
Quorum sensing-induced transition

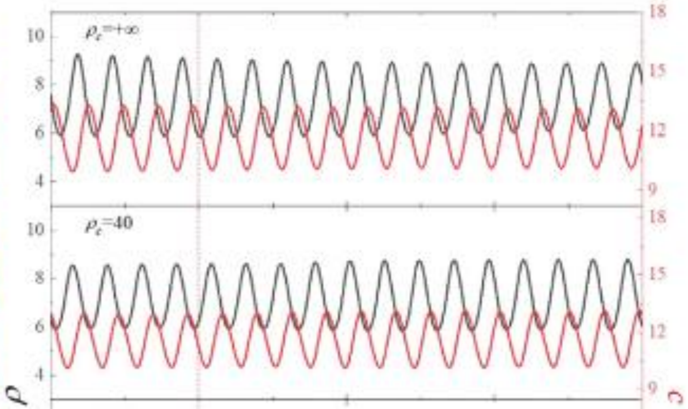


$$\dot{\rho} = -\nabla\cdot(\rho v_\rho \boldsymbol{P}) + D_\rho \nabla^2 \rho$$

$$\dot{\boldsymbol{P}} = -\gamma \boldsymbol{P} + D_{\mathrm{P}} \nabla^2 \boldsymbol{P} + \beta \nabla c - \gamma_2 |\boldsymbol{p}^2| \boldsymbol{P}$$

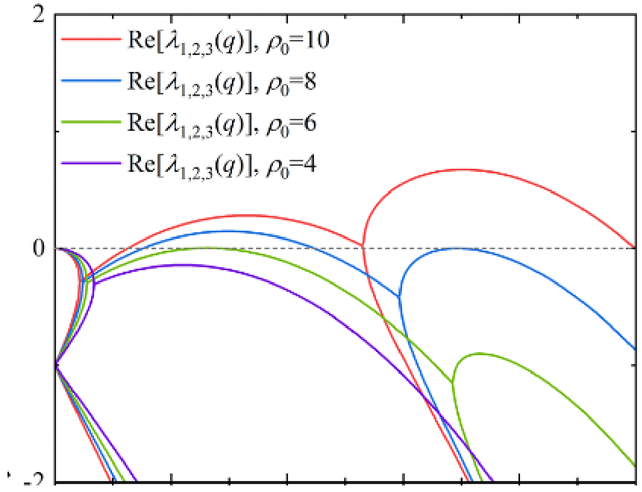
$$\dot{c} = D_{\mathrm{c}} \nabla^2 c + k_0 \rho - k_{\mathrm{d}} c + k_{\mathrm{a}} \nabla\cdot(\rho \boldsymbol{P})$$

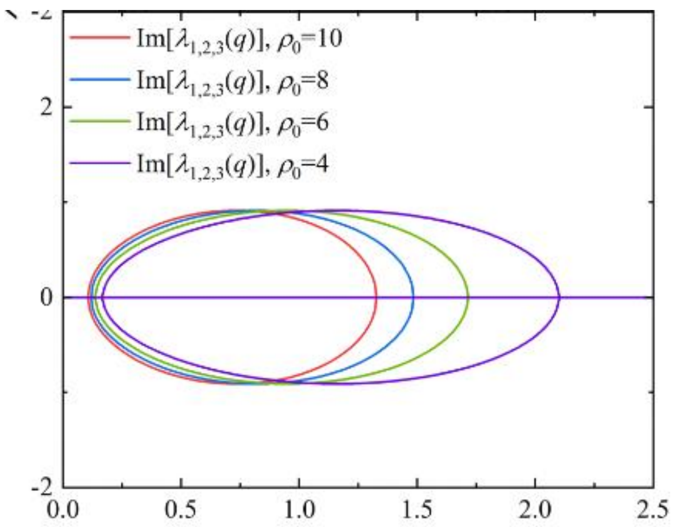




$$\begin{pmatrix} \dot{\delta\rho} \\ \dot{\delta P} \\ \dot{\delta c} \end{pmatrix} = M \begin{pmatrix} \delta\rho \\ \delta P \\ \delta c \end{pmatrix}; \quad M = \begin{pmatrix} \partial_x^2 & -\rho_0 \partial_x & 0 \\ 0 & -\Gamma + \mathscr{D}_{\mathrm{P}} \partial_x^2 & s\partial_x \\ 1 & \kappa \rho_0 \partial_x & \mathscr{D}_{\mathrm{c}} \partial_x^2 - 1 \end{pmatrix}$$

$$\begin{aligned} P(\lambda) &= \det(M - \lambda I) \\ &= (z^2 - \lambda)(z^2 \mathscr{D}_{\mathrm{c}} - \lambda - 1)(-\Gamma + z^2 \mathscr{D}_{\mathrm{P}} - \lambda) \\ &\quad - \rho_0 s z^2 (-\kappa\lambda + \kappa z^2 + 1) \end{aligned}$$

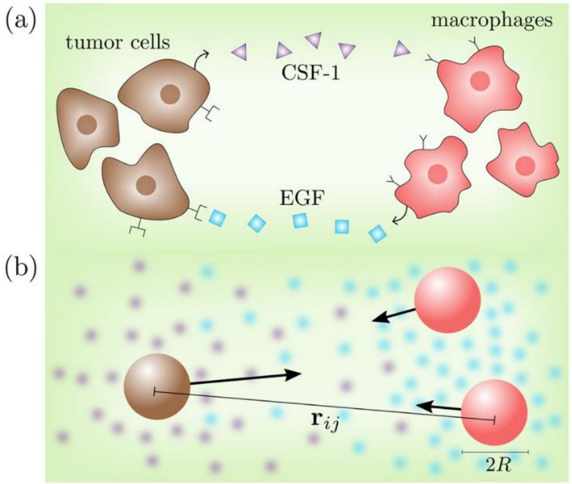




[1] J. Cao, J. Wu, and Z. Hou, Quorum sensing-induced transition from colloidal waves to Turing-like patterns in chemorepulsive active colloids, Phys. Chem. Chem. Phys. 26, 7783 (2024).

A Variety of Chemotaxis Particles

Swarm Hunting in chemically communicating Active Mixtures



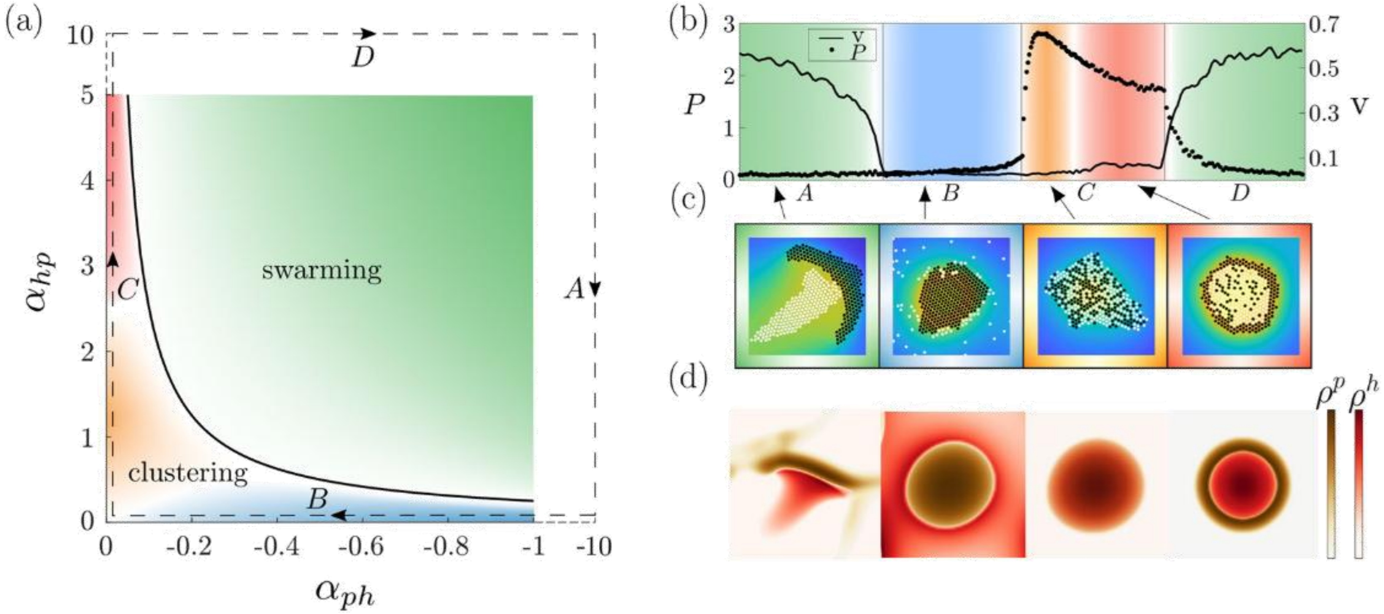
$$\partial_t \mathbf{r}_i^s(t) = \sum_{s' \in \{p,h\}} \alpha_{ss'} \nabla c^{s'} - \nabla_{\mathbf{r}_i} V + \sqrt{2D}\,\boldsymbol{\eta}_i^s$$

$$\partial_t c^s(\mathbf{r}, t) = (D_c \Delta - \mu) c^s + \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i^s)$$

$$\partial_t \delta\rho^p = D\Delta\delta\rho^p - \alpha_{pp}\rho_0^p \Delta\delta c^p - \alpha_{ph}\rho_0^p \Delta\delta c^h$$
$$\partial_t \delta\rho^h = D\Delta\delta\rho^h - \alpha_{hh}\rho_0^h \Delta\delta c^h - \alpha_{hp}\rho_0^h \Delta\delta c^p \ ,$$

$$\partial_t \delta c^s = D_c \Delta\delta c^s + \delta\rho^s - \mu\delta c^s \ .$$

$$\lambda \begin{pmatrix} \delta\hat{\rho}^p \\ \delta\hat{c}^p \\ \delta\hat{\rho}^h \\ \delta\hat{c}^h \end{pmatrix} = \begin{pmatrix} -D\mathbf{q}^2 & \alpha_{pp}\rho_0^p\mathbf{q}^2 & 0 & \alpha_{ph}\rho_0^p\mathbf{q}^2 \\ 1 & -D_c\mathbf{q}^2 - \mu & 0 & 0 \\ 0 & \alpha_{hp}\rho_0^h\mathbf{q}^2 & -D\mathbf{q}^2 & 0 \\ 0 & 0 & 1 & -D_c\mathbf{q}^2 - \mu \end{pmatrix} \begin{pmatrix} \delta\hat{\rho}^p \\ \delta\hat{c}^p \\ \delta\hat{\rho}^h \\ \delta\hat{c}^h \end{pmatrix}$$



(a) The steady state is stable, if the eigenvalues of the matrix all have real parts strictly less than zero.

(b) The steady state is unstable, if at least one of the eigenvalues of the matrix has a positive real part.

(c) Otherwise in the marginal case higher order terms determine the stability of the problem.

[1] J. Grauer, H. Löwen, A. Be'er, and B. Liebchen, Swarm Hunting and Cluster Ejections in Chemically Communicating Active Mixtures, Sci Rep 10, 5594 (2020).

Application of Chemotaxis Particles

Collective chemotactic search strategies

$$\dot{\mathbf{r}}_i(t) = v_0 \mathbf{e}_i(t) + \sum_{j=1}^{N} \frac{\mathbf{f}(r_{ij})}{\gamma_t} ,$$

$$\dot{\varphi}_i(t) = \frac{\kappa}{\gamma_{\mathbf{r}}} \left[\nabla c(\mathbf{r}_i(t),t) \times \mathbf{e}_i(t) \right]_z + \sqrt{2D_r}\, \eta_i(t) ,$$

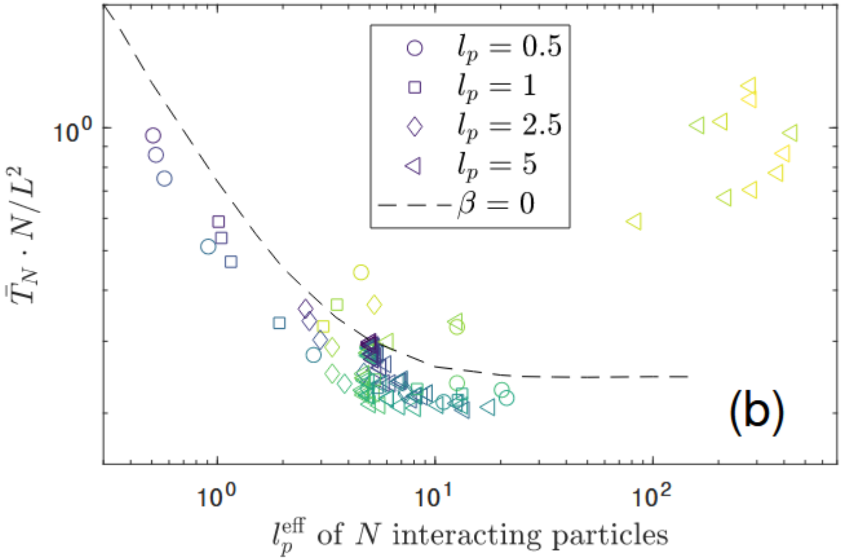
$$\dot{c}(\mathbf{r},t) = D_c \nabla^2 c(\mathbf{r},t) - k_c c(\mathbf{r},t) + h_c \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t)) .$$

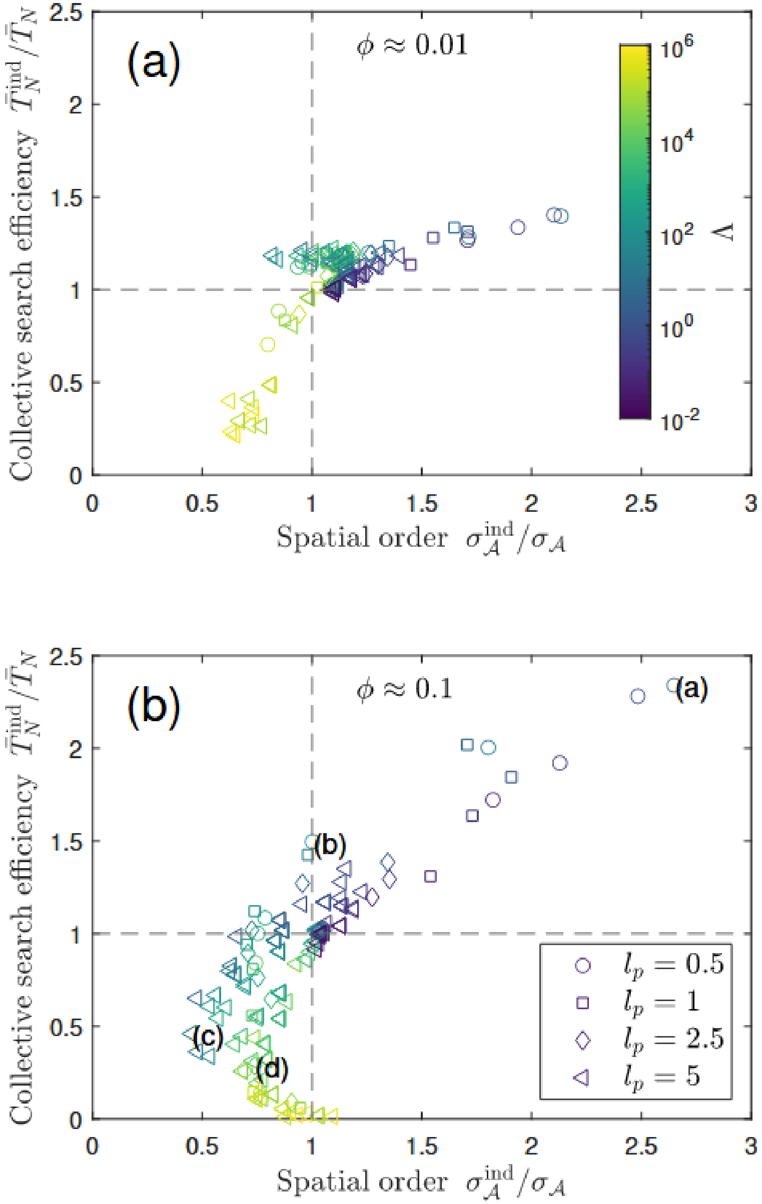
$$\mathbf{e}_i(t) = (\cos\varphi_i(t),\ \sin\varphi_i(t))^\top$$

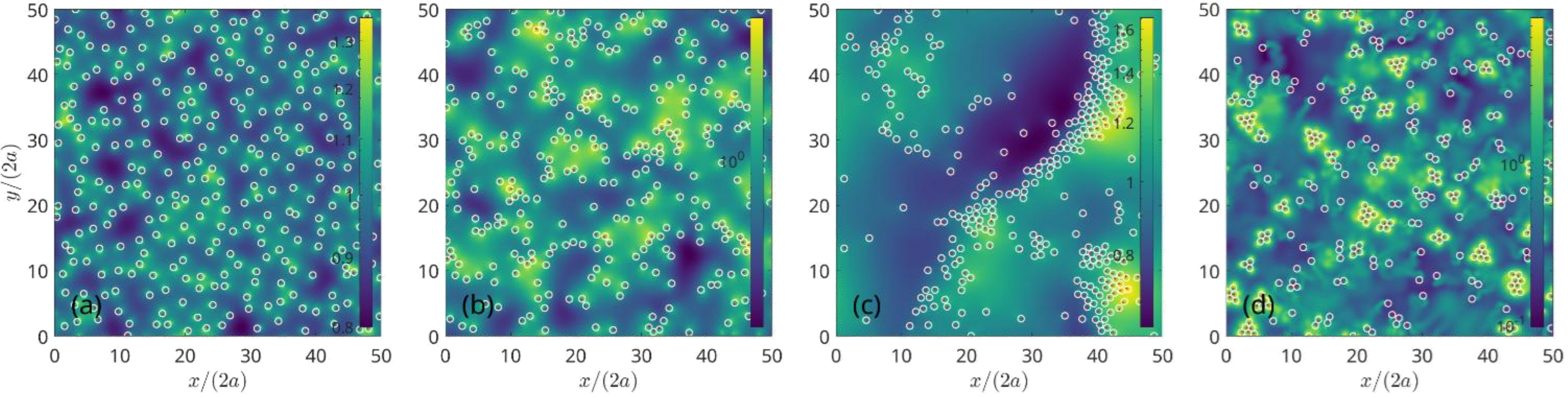
$$l_p = v_0/(aD_r),\ \Lambda = \kappa h_c a/\gamma_r D_c^2$$

$\sigma_{\mathcal{A}}^{ind}/\sigma_{\mathcal{A}} > 0$, more uniform

$\bar{T}_N^{ind}/\bar{T}_N$, collective more advantageous







[1] H. Meyer, A. Wysocki, and H. Rieger, Collective Chemotactic Search Strategies, arXiv:2409.04262.