Swarm Hunting and Cluster Ejections in Chemically Communicating Active Mixtures

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A large variety of microorganisms produce molecules to communicate via complex signaling mechanisms such as quorum sensing and chemotaxis. The biological diversity is enormous, but synthetic inanimate colloidal microswimmers mimic microbiological communication (synthetic chemotaxis) and may be used to explore collective behaviour beyond the one-species limit in simpler setups. In this work we combine particle based and continuum simulations as well as linear stability analyses, and study a physical minimal model of two chemotactic species. We observed a rich phase diagram comprising a “hunting swarm phase”, where both species self-segregate and form swarms, pursuing, or hunting each other, and a “core-shell-cluster phase”, where one species forms a dense cluster, which is surrounded by a (fluctuating) corona of particles from the other species. Once formed, these clusters can dynamically eject their core such that the clusters almost turn inside out. These results exemplify a physical route to collective behaviours in microorganisms and active colloids, which are so-far known to occur only for comparatively large and complex animals like insects or crustaceans.

Chemotaxis - the movement of organisms in response to a chemical stimulus - allows them to navigate in complex environments, find food and avoid repellants. It is involved in many biological processes where microorganisms (or cells) coordinate their motion; these include wound healing, fertilization, pathogenic invasion of a host, and bacterial colonization.1,2 In such cases, microorganisms are attracted (or repelled) by certain substances (chemoattractants/chemorepellents), but they are also attracted to chemicals produced by other microorganisms (or cells), such as CAMP in the case of Dictyostelium cells3 or autoinducers in signaling Escherichia coli4, which leads to chemical interactions (communication) among the microorganisms.

While many existing models studying microbiological chemotaxis (or chemical interactions) focus on a single species5–12, the typical situation in the microbiological habitat is that various different species simultaneously produce certain chemicals to which others respond via chemotaxis or based on quorum sensing mechanisms. One simple example involving chemical signaling across species is provided by macrophage-facilitated breast cancer cell invasion which has recently been modeled13. There, tumor cells attract macrophages, which are certain white blood cells normally playing a key role in the human immune system. They then control the physiological function of the macrophages and exploit their abilities. More specifically, the tumor cells produce the colony-stimulating factor (CSF-1) leading to the attraction and growth of macrophages which in turn release epidermal growth factors (EGF) resulting in the growth and mobility increase of the tumor cells (see Fig. 1).

Similarly to microorganisms, synthetic inanimate colloids, coated with a material which catalyzes a certain reaction on (a part of) their surface, show chemical interactions as well14–16. There, the colloids act as sources of the chemical field, which shows a 1/r-steady-state far-field profile in 3D (if the chemical does not ‘decay’ e.g. through bulk reactions), leading to long-ranged chemical interactions between the colloids. For active colloids17–21, these interactions have been explored in single-species systems22–27, and more recently also in mixtures28–34, where chemical interactions can be non-reciprocal and break action-reaction symmetry28,35,36. This allows for the formation of active molecules28–30, where self-propulsion spontaneously emerges when the underlying nonmotile ‘colloidal atoms’ bind together. Similarly as for their microbiological counterparts, in all these studies on mixtures of synthetic colloids it has been assumed that the different species interact via a single chemical substance.

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In the present work, we propose and explore a physical minimal model for two species of chemically interacting particles, both of which produce an individual chemical substance. Such a situation occurs for example in tumor–macrophage systems involving the EGF/CSF-1 paracrine signalling loop between two cell types mentioned above. By comparing numerical simulations of Langevin equations describing the particle dynamics (Fig. 2(a–d)) with numerical solutions of deterministic continuum equations describing the dynamics of their density fields (Fig. 2(e–h)) and a linear stability analysis, we systematically explore and analyze the phase diagram of this system. As our key result, we discover a "hunting-swarm phase" (see Fig. 2(a,e)), where both species segregate and form individual swarms, one of them closely pursuing the other one. This phase resembles a group of hunters chasing a group of prey trying to stay together, not allowing the hunters to split up the group. It is interesting to note that a phenomenologically similar form of swarm hunting also occurs in much larger systems, e.g. in insects and systems of larvae hunting crustaceans (Daphnia), where collective predation phenomena and escape strategies have already been analyzed, but not for microorganisms or synthetic colloids. Physically this phase occurs, if one species ("the hunters") is attracted by the chemicals produced by the other species ("the prey") and the prey is in turn repelled by the chemicals produced by the hunters. Note that a different form of moving clusters has recently been observed also in simulations involving only one chemical species. Unlike the hunting swarms which we present here, the moving clusters in do not involve a species segregation into two individual swarms, but rather consist of a single aggregate of asymmetrically distributed predator and prey particles. By systematically exploring the parameter space underlying our model, we find that hunting swarms in fact occur generically if the chemical interactions are strong enough and have opposite sign. However, if the response of hunters and prey to the chemicals produced by the respective other species is strongly asymmetric, we instead find dense clusters of one species surrounded by a diffusive or rigid corona of particles from the other species (see Fig. 2(b,d,f,h)). These core-shell clusters can show a complex dynamics, ejecting their interior once they have formed. This behaviour hinges on model-ingredients which have not been considered in previous models of chemically interacting particle mixtures. These are (i) a finite relaxation time of the chemicals leading to delay or memory effects in the absence of which the cluster ejections do not occur and (ii) the presence of two chemicals, which can lead e.g. to a coexistence of instantaneous and non-instantaneous interactions and in general also to coexisting attractions and repulsions with different ranges. The setup considered in the present work allows us to exemplify that a phenomenologically similar ejection may in principle originate from a remarkably simple mechanism hinging on a systematic invasion of the hunters into a cluster of prey particles, as we will later discuss in detail.

Model

We consider an ensemble of two species of overdamped colloids (synthetic or biological), which we call prey and hunters, , each of which contains particles which produce a chemical field with a rate . We assume that each particle responds to the chemical fields either via synthetic chemotaxis, which leads to a coupling in far-field, similar as for apolar colloids, or via biological chemotaxis which is sometimes modeled using an analogous form of the coupling. To model the particle dynamics we use Langevin equations:

\[ \gamma \partial_t \mathbf{r}_i^s(t) = \sum_{j \in \{p,h\}} \alpha_{ij} \nabla c^s - \nabla V + \sqrt{2D} \gamma \eta_i^s \]  

(1)
represents unit-variance Gaussian white noise with zero mean. The chemotactic, and zero else. Here \(kR\) where \(s_i \sigma_{ss}\) leads to chemoattraction, and \(s_i \sigma_{ss}\) are produced by particles of hunters and prey, respectively. The dynamics is the particle diameter. \(2rr\) is denoted as \(\rho^h\) and \(4r^2\) results in chemorepulsion (negative chemotaxis). In addition, \(\eta_s\) and box length \(L_\text{box}\) are identical for both species.

indicates a cutoff radius beyond which the potential energy is zero. Here \(\epsilon\) determines the strength of the potential, \(\eta_s\) denotes the distance between particles \(i\) and \(j\). \(2^{1/6}\sigma\) indicates a cutoff radius beyond which the potential energy is zero and \(\sigma = 2R\) is the particle diameter.

The chemical fields \(c^h(\mathbf{r}, t)\), \(c^p(\mathbf{r}, t)\) are produced by particles of hunters and prey, respectively. The dynamics of these fields, follows a diffusion equation (diffusion coefficient \(D_i\)), with additional (point) sources. We also use a sink term whose coefficient may be zero or nonzero if chemical reactions or other processes degrading the chemical occur in bulk. For simplicity we focus on the case where \(D_h, k_v, k_d\) are identical for both species.

\[
\partial_t c^i(\mathbf{r}, t) = D_i \Delta c^i - k_d c^i + k_b \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j^n)
\]  

(2)

To reduce the parameter space, we choose \(x_0 = R\) and \(t_0 = \frac{1}{k_0}\) as the units of length and time. The resulting dimensionless parameters are \(\delta_{kl} = \frac{\alpha_{ss}}{2^{1/6} \sigma} \epsilon\), \(\alpha_{ss} = \frac{1}{k_0}\), \(\eta_j\) and \(\mu = \frac{k_d}{k_b}\) (see the Supplementary Material (SI) for details) and Eqs. (1), (2) reduce to (omitting tildes)

\[
\partial_t c^i(\mathbf{r}, t) = \sum_{j \in \{p, h\}} \alpha_{ss} \nabla c^j - \nabla_i V + \sqrt{2D_i} \eta_i
\]  

(3)

\[
\partial_t c^i(\mathbf{r}, t) = (D_i \Delta - \mu) c^i + \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j^n)
\]  

(4)

Figure 2. Hunting swarms and core-shell clusters: Simulation snapshots of Eqs. (3), (4) for \(2N = 2000\) chemically interacting particles (white dots represent hunter–particles; black dots show prey–particles) coupled to self-produced chemical fields at time \(t = 1500\) (a), \(5000\) (b–d)]. Panels (a–d) show particle based simulations, where colours show the chemical field produced by the prey \(c^p\), panels (e–h) show simulations of the associated continuum equations at time \(t = 5000\) (e), \(10000\) (f–h), where colours show the density of hunters \(\rho^h\) and prey \(\rho^p\). (a,e) show hunting swarm patterns, (c,g) show mixed clusters, (b,f) show core-shell clusters with diffusive and (d,h) with rigid corona. Dimensionless parameters (tildes omitted); \(\alpha_{pp} = 1, \alpha_{ph} = 0, \mu = 0.001, D_h = 1, D = 0.001\) (a–d), \(D = 0.01\) (e–h) for reasons of stability, \(\epsilon = 1\) and box length \(L_\text{box}\) = 250 (a–d), \(L_\text{box} = 100\) (e–h). See supplementary material for simulation details and the stabilization method used for the field equations underlying panels (e–h).
Hunting Swarms and Core-Shell Clusters

To explore the collective behaviour of many chemotactic agents, we now solve Eqs. (3) and (4) using Brownian dynamics simulations for the particle dynamics coupled to a finite difference scheme to calculate the dynamics of the self-produced chemical fields. We solve the diffusion equation in 2D for numerical efficiency and do not expect that our results would change qualitatively when solving the 3D diffusion equation (see the exemplaric simulation snapshot Fig. 2 in the SI and notice that the linear stability analysis which does not depend on the dimensionality of the diffusion equation is also in very good agreement with the particle based simulations). We use a quadratic simulation box with periodic boundary conditions (see SI for details) and observe the following patterns or nonequilibrium phases:

(i) A hunting swarm phase (see Fig. 2(a,e) and movies 1, 5), where both species segregate and form moving swarms which hunt each other.

(ii) A clustering phase (see Fig. 2(c,g) and movies 3, 7), where both species form a cluster and the different species are mixed.

(iii,iv) Two phases showing core-shell clustering, where one species forms the inner core and the other one forms a corona which may be diffusive (b,f) or rigid and which is strongly localized around the core (d,h).

Let us now characterize these phases and the dynamics leading to their emergence in detail.

To see in which parameter regimes each of these patterns prevails, in Fig. 3 we show a slice through the state diagram in the plane spanned by the chemotactic cross-species coupling coefficients $\alpha_{ph}$ and $\alpha_{hp}$ for fixed $\alpha_{pp} = 1$; $\alpha_{hh} = 0$. The green domain represents hunting swarms, which are characterized by their ballistic motion and their emergence from an oscillatory instability (the black line shows the analytical prediction of the transition line), whereas colours for the remaining cluster phases are defined via the value of the mixing parameter shown in panel (b) (see text). The state diagram was created with more than 200 evaluated state points. (b) Mixing parameter $P$, counting the average number of black next neighbors per white particle and mean particle velocity $v$ at late times discriminating between the individual states: Each point corresponds to a parameter set on the dashed line in the parameter plane of panel a. The labels $A$, $B$, $C$, $D$ correspond to those shown on the dashed line in panel (a). (c,d) Extracts from the simulations underlying Fig. 2 (see movies 1–8).

**Figure 3.** (a) State diagram in the plane spanned by the chemotactic cross coupling coefficients $\alpha_{ph}$ and $\alpha_{hp}$ for fixed $\alpha_{pp} = 1$; $\alpha_{hh} = 0$. The green domain represents hunting swarms, which are characterized by their ballistic motion and their emergence from an oscillatory instability (the black line shows the analytical prediction of the transition line), whereas colours for the remaining cluster phases are defined via the value of the mixing parameter shown in panel (b) (see text). The state diagram was created with more than 200 evaluated state points. (b) Mixing parameter $P$, counting the average number of black next neighbors per white particle and mean particle velocity $v$ at late times discriminating between the individual states: Each point corresponds to a parameter set on the dashed line in the parameter plane of panel a. The labels $A$, $B$, $C$, $D$ correspond to those shown on the dashed line in panel (a). (c,d) Extracts from the simulations underlying Fig. 2 (see movies 1–8).
Figure 3(b) shows, whereas red means (see SI for details) at

Crossover regions between the individual patterns are marked by white domains in

with 500 prey-particles and 2000 hunter-particles.

Figure 4. Sequence of simulation snapshots showing a cluster ejection which occurs due to chemical delay effects. Dimensionless parameters: $\alpha_{pp} = 100, \alpha_{ph} = 0, \alpha_{ph} = -1000, \alpha_{hp} = 10, \mu^p = 0.1, \mu^h = 0.01, D^p = 0.5, D^h = 10, D = 0.001, \epsilon = 10$ with 500 prey-particles and 2000 hunter-particles.

din classification. Let us define an “order parameter” $\gamma$ that is associated with an oscillatory instability, as discussed further below, can be clearly distinguished from the stationary cluster phases of hunting swarms exceeds that in other regimes. While the hunting swarm phase, which emerges from late times for parameters chosen along the dashed line in Fig. 3(a), where one can easily see how the velocity in simulations underlying Fig. 2, the hunters invade even small prey-clusters, for appropriate initial conditions, we can see a proper inside out reversal of comparatively large clusters (movie 9) (species reversal). In each case, the result is a counterintuitive pattern consisting of a dense cluster containing mostly hunters surrounded by ring of prey-particles.

Dynamical ejections of particle clusters. We have investigated the dynamics of these core-shell clusters more precisely. Assuming the diffusion of $c^p$ is considerably lower than that of $c^h$ and $c^h$ is produced very slowly, this results in a certain delay effect. A typical course of this process is shown in Fig. 4 (see also movie 10). The prey-particles that attract each other initially accumulate and form clusters (Fig. 4(a)). Due to a resulting higher concentration of $c^h$, the hunters are also attracted. These hunter-particles then form a surrounding shell, but cannot immediately invade the prey-cluster as $\alpha_{ph} > \alpha_{pp}$ (Fig. 4(b)). Although slowly, the concentration of $c^h$ increases with time as more hunter-particles join. At some point a significant concentration of $c^h$ is exceeded and since $\alpha_{ph} > \alpha_{pp}$ the prey-particles are ejected outwards from the center of the cluster (Fig. 4(c)). Since the chemicals $c^p$ produced by the prey diffuses on a much smaller timescale, the hunter-particles still move towards each other, form a dense cluster which persists for a while (Fig. 4(d)), before the hunter-cluster dissolves slowly and the whole process starts all over again.

Irregular aggregation. Finally, when $\alpha_{ph}, \alpha_{pp}$ are both small, with $|\alpha_{ph}| < |\alpha_{pp}|$ (orange regime in Fig. 3(a,b) and movies 3, 7), prey and hunter particles form clusters containing a seemingly irregular mixture of hunter and prey particles (Fig. 3(c), orange). These clusters emerge because we have a chemically mediated prey-prey attraction and a hunter-by-prey attraction which exceeds the prey-by-hunter-repulsion, so that effectively prey particles similarly strongly attract all other particles, leading to a rather irregular aggregation.

Classification. In contrast to the static clusters, structures in the green region of Fig. 3(a) move ballistically and hence show a non-vanishing velocity. Figure 3(b) depicts the mean particle velocity $v(t)$ (see SI for details) at late times for parameters chosen along the dashed line in Fig. 3(a), where one can easily see how the velocity in regions of hunting swarms exceeds that in other regimes. While the hunting swarm phase, which emerges from an oscillatory instability, as discussed further below, can be clearly distinguished from the stationary cluster phases, let us define an “order parameter” $P$ to distinguish the remaining cluster phases. We define $P$ as the average number of black next neighbors (prey) per white particle (hunter), where we denote a neighbor as a particle within a distance $\rho < 2 + 0.1$. Figure 3(b) shows $P$ for parameters chosen along the dashed line in Fig. 3(a). This parameter would have a value of $3$ for completely irregular and infinitely large dense clusters. For the orange domain, where particles aggregate almost irregularly, it has a value $P > 2.5$, whereas red means $1.5 < P < 2.3$ and blue means $P < 0.5$. Crossover regions between the individual patterns are marked by white domains in Fig. 3(a).
Linear Stability Analysis – Emergence and Dynamics of Patterns at Early Times

To understand the structure of the state diagram we now introduce a continuum description for the particle dynamics and perform a linear stability analysis.

Continuum model. The Smoluchowski equation, describing the dynamics of the (non-normalized) probability \( \rho^s (\mathbf{r}, t) \) to find a particle of species \( s \) at position \( \mathbf{r} \) at time \( t \) reads as follows (\( s \in \{ p, h \} \)):

\[
\partial_t \rho^s = D \Delta \rho^s - \sum_{s' \in \{p,h\}} \alpha_{ss'} \nabla \cdot (\rho^s \nabla \rho^{s'}).
\]  
(5)

These deterministic equations are equivalent to the Langevin Equation (1) for point particles \( (V = 0) \). We can now also rewrite the evolution equation for the chemical fields as follows:

\[
\partial_t c^s = (D \Delta - \mu) c^s + \rho^s.
\]  
(6)

Before carrying out a linear stability analysis, let us solve these equations numerically to test them: Integrating Eqs. (5), (6) for a uniform initial state (plus small fluctuations) on a square box of size \( L_{\text{box}} = 100 \), we indeed find the same patterns as in our particle based simulations (Figs. 2(e–h) and 3) (see SI for details regarding these simulations and the used method to stabilize them).

Linear stability analysis. We now linearize these four coupled equations around the stationary solution \( (\rho, c) = (\rho_0, p_0/h_0) \) which represents the uniform disordered phase, and solve them in Fourier Space, to understand the dynamics of a small plane wave perturbation with wavenumber \( q \) around the uniform phase. We denote the dispersion relation of these fluctuations as \( \lambda(q) \). If \( \lambda \) has a positive real part for some \( q \) value, the uniform phase is unstable. Calculating \( \lambda \) (see Supplementary Material for details), we find that the uniform phase looses stability if

\[
2D\mu < \rho_0 \text{Re} \alpha_{pp} + \sqrt{4\alpha_{ph}\alpha_{hp} + \alpha_{pp}^2},
\]  
(7)

where we have chosen \( \alpha_{ph} = 0 \) as in our simulations. While Fig. 3 shows only parameter regimes where the uniform phase is unstable, we have performed additional simulations (see SI) which are in close quantitative agreement with the prediction of the onset of the instability due to Eq. (7). This holds true both in the regime where the instability is stationary and where it is oscillatory. The instability criterion shows that chemo-attractions among the prey particles support the emergence of a pattern in competition with diffusion and the potential decay of the chemical, whereas cross interactions only support the emergence of a pattern if they, \( \alpha_{ph} \) and \( \alpha_{hp} \), have the same sign.

To understand the transition between static clusters and hunting swarms, we also derive a criterion discriminating between stationary instability (static clusters, \( \lambda \) is real) and oscillatory instabilities (moving structures, complex \( \lambda \)) which reads as follows (see SI):

\[
2\sqrt{-\alpha_{ph}\alpha_{hp}} > \alpha_{pp}.
\]  
(8)

This criterion defines the solid black line in Fig. 3(a), which quantitatively agrees with our simulations. It shows that an oscillatory instability and hence moving patterns can appear only if \( \alpha_{ph}\alpha_{hp} \) have opposite sign, i.e. if one species effectively hunts the other one whereas the other one tries to escape. In this parameter regime where it is oscillatory, we have numerically tested the instability criterion (Eq. (7)) to see if it is shifted due to “perturbation convection”, see\(^{42}\). We did not find any shift, suggesting that the advective and absolute instability are very close to each other in the present case.

In Fig. 5 we show the complete dispersion relation \( \lambda(q) \) (real and imaginary part) of small plane wave fluctuations around the uniform phase. Here the location of the maxima in \( \text{Re} \{\lambda(q)\} > 0 \) define the fastest growing mode, typically determining the length scale of the pattern at early times.

Having understood the transition line between the cluster phases and the hunting swarms, let us also explore if we can understand how fast the swarms move. To do this, in Fig. 6, we compare the imaginary part of \( \lambda \) (the expected speed of the hunting swarm) is \( \nu(q) = \frac{\text{Im} \{\lambda(q)\}}{q} \rightarrow \left\langle v \right\rangle \approx \frac{\text{Im} \{\lambda(q_{\text{max}})\}}{q_{\text{max}}} \) with the velocity of the hunting swarms in our particle based simulations at early times and find close agreement.

Structure and Growth at Late Times

Having explored how the patterns emerge and behave at early times, we now want to explore their structure and dynamics also at late times. To do this, we introduce the instantaneous pair-correlation function \( g(\mathbf{r}) \) defined as

\[
g(\mathbf{r}) = \frac{1}{\rho_{id}} \left\langle \sum_{i=0}^{\frac{2N}{L_{\text{box}}} - 1} \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle,
\]  
(9)

for an average number density \( \rho_{id} = \frac{2N}{L_{\text{box}}} \) with box length \( L_{\text{box}} = 250 \), total number of particles \( 2N \) and \( \langle \cdot \rangle \) denoting the ensemble average. The radially averaged and time averaged pair-correlation function \( \langle g(\mathbf{r}) \rangle \), where \( r = |\mathbf{r}| \), shown in Fig. 7 describes how the density varies as a function of distance from a reference particle at which we averaged over all particles of hunters and prey.
As one can see in the inset of Fig. 7, there is a large peak around $r_2$, which is the typical distance between two particles ($R_1$ in dimensionless units). We can also find peaks around $r_{23}$ and $r_4$ caused by the next two neighbors. This reflects the fact that the static clusters (blue, orange, red) show a hexagonal packing.

**Late-stage dynamics.** Once the patterns have emerged, they reach a state where their morphology changes only slowly. However, even at late stages the size of the individual structures still increases in time. The swarms move ballistically and frequently collide with each other often leading to their break up. They still grow on average, ultimately leading to a single swarm at late times. This is because after each collision a new swarm forms rapidly, i.e. on timescales before the individual particles which were part of the ‘old’ swarm significantly diffuse away. The newly forming swarm rapidly reaches a size exceeding that of its “ancestors”, because it involves particles from both swarms which were involved in the collision. To quantify this growth, we consider the time evolution of the radial distribution function $g_r(t)$ and define the length scale $L(t)$ of clusters as the smallest value where $g_r(t) \leq 1$, for all $r > L(t)$. Thus, the $g_r(t)$ shown in Fig. 7 corresponds to a length scale of $\approx 201$ (dimensionless units). At late-times, we find that $L(t) \propto t^{1/3}$ follows a power law with an exponent of $\beta \approx 0.35$ (Fig. 8) for the (nonmoving) cluster phases, which is close to the value of $\beta = 1/3$ as expected for diffusive growth (in the absence of hydrodynamic interactions)\(^43-47\). We find a much larger exponent, of $\beta \approx 0.56$ (Fig. 8), for the patterns in the green region, which is close to $\beta = 0.5$ as expected for ballistic aggregation. This is a consequence of the fact that the individual structures move ballistically, collide and merge with each other much faster (but also break up).

As a second measure for the growth of the clusters, we measure the distance between them. To do this, we consider the structure factor of the system:

$$S(k) = 1 + \rho_d \int_V \text{d} \mathbf{r} e^{-ik \cdot \mathbf{r}} [g_r(t) - 1]$$

and calculate the distance between clusters as the inverse of the first moment of the structure factor\(^48\), i.e. as:

$$L_2(t) = 2\pi \left[ \frac{\int_{k=1}^{k_{\text{cut}}} k S(k, t) dk}{\int_{k=1}^{k_{\text{cut}}} S(k, t) dk} \right]^{-1},$$

where we choose the cutoff wavelength $k_{\text{cut}}$ as the first local minimum of $S(k)$\(^48\). Figure 9 shows the structure factor for a cluster in the red region of Fig. 3(a) at time $t = 250$ for small values of $k$. The peaks that can be seen in the inset of Fig. 9 correspond to the distance of two possible lattice planes of the hexagonal structure. The peak at $k = 3.3$ results from the minimum distance between two particles ($\pi \approx 2$). One finds a huge peak around $k = 0.11$ with which we can estimate a typical length, $l \approx \frac{2\pi}{k} \approx 57.1$; the enormous size of the peak hinges on the fact that each of the contributing clusters contains a large number of particles. The $k$-value where this peak occurs

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**Figure 5.** Real and imaginary part of the dispersion relation $\lambda$, for hunting swarms (green) and static clusters (red). Parameters as in Fig. 2(a,d).

**Figure 6.** Mean particle velocity in the hunting swarm phase, extracted from the simulations underlying Fig. 3(a) at early times (red) and reduced imaginary part of $\lambda$ at the wavenumber corresponding to the fastest growing mode, i.e. $\text{Im}(\lambda(q_{\text{max}}))/q_{\text{max}}$ (blue) as a function of $-a_{ph} = a_{hp}$. 
corresponds to the mean cluster distance, which corresponds to the value of $r$ where $g(r)$ approaches 1 from below (see Fig. 7). This distance grows basically with the same power law as the cluster sizes, as shown in Fig. 8, i.e. calculating cluster sizes via $L_1(t)$ and calculating cluster-distances $L_2(t)$ basically leads to the same growth law (Fig. 8)\textsuperscript{49}. Thus, there is only one independent macroscopic length scale in the system.

Conclusions
Inspired by the generic presence of multi-species chemotaxis in microbiological communities, e.g. in macrophage-tumor cell systems, we have proposed and explored a physical minimal model to study the collective behaviour beyond the commonly considered one-species limit. We have found that the novel key ingredient of our model - the species selective chemical production - leads to interesting behavior: patterns that comprise a "hunting swarm" phase consisting of a crowd of particles of one species pursuing the other species, and a phase where the two-species self-aggregate in a core-shell structure, which then dissolves abruptly in a dynamic process by ejecting the inner particles.

All these patterns could be observed both on the level of a particle-based description (Eqs. (3), (4)) and in a continuum model (Eqs. (5), (6)), allowing to analytically understand the transition line between cluster phases, which originate from a stationary instability of the uniform phase, and hunting swarms, emerging from an oscillatory instability. As a further characteristic difference between these phases, we find that clusters (and the

Figure 7. Pair–correlation function $g(r)$ (radial average of $g(r)$) of a system of $2N = 2000$ particles at time $t = 250$. The data are averaged over 100 independent ensembles. The dashed line shows a threshold to extract a characteristic length scale. Parameters as in Fig. 2(d).

Figure 8. Time-dependent characteristic length scale (a) obtained from the pair-correlation function and (b) from the structure factor for structures in the red region (red dotted line) and in the green region (green dotted line of Fig. 3(a)). The dashed lines indicate the fitted exponents. Parameters as in Fig. 2(a,d). Panel (c) shows a sequence of snapshots from a representative simulation of the hunting swarms which continuously collide, split up and grow to a larger size.
distance between them) grow diffusively \((L(t) \propto t^{0.35})^{43–47,49}\), whereas hunting swarms grow significantly faster \((L(t) \propto t^{0.56})^{50}\).

While the key aim of the present work was to explore a minimal framework illustrating how chemical cross-interactions may lead to complex behavior, it should in principle be possible to realize the present model also with (autophoretic) colloidal mixtures, e.g., based on a combination of nonreciprocal repulsive thermo-phoretic and attractive chemo-phoretic interactions, which have been confirmed to be non-reciprocal in recent experiments\(^{59}\). Future work might include more specific biological details and could address the effect of confining boundaries or obstacles\(^{51–55}\). Other topics concern additional aligning interactions and their impact on the cluster structure\(^{55–57}\) and ternary systems describing species of a longer biological food chain.

**Data availability**

All relevant data are available from the authors upon reasonable request.

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**Figure 9.** Small wavenumber regime of the structure factor \(S(k)\) for a system of \(2N = 2000\) particles at time \(t = 250\). Inset shows \(S(k)\) for a larger wavenumber regime. The wavenumber \(k\) is given in dimensionless units \((k_0 = \frac{2\pi}{a})\). Parameters as in Fig. 2(d).
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H.L. and B.L. have planned and designed the research project; J.G. has performed most of the research; all authors have discussed the results; J.G. and B.L. have written the manuscript; H.L. and A.B. have edited it.

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The authors declare no competing interests.

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