Clusters, confinement, and collisions in active matter

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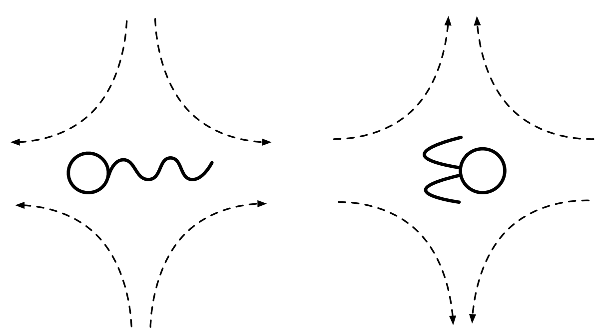
Abstract

Building upon the work of active suspensions by Saintillan and Shelley [12], we investigate the dynamics of clusters (localized concentrations of active matter) and the effects of confinement by considering active matter in a droplet. In addition, we show that the physics of binary collisions is absent from the Smoluchowski equation.

1 Introduction

Active matter consists of particles which consume energy to undergo motion or perform mechanical work. Examples of active matter include flocking, bacterial swarms, microtubules and kinesin, fish schools — just to name a few. In this work, we look at suspensions of 'pusher' and 'puller' swimmers (see figure 1) which model bacterial and microtubule-kinesin systems. There are many modeling approches to self-propelled matter [7, 9, 15, 16], but we will focus on one approach introduced by Saintillan and Shelley [11–13]. We will investigate (1) clusters, localized concentrations of active matter in a droplet, (2) the effects of confinement on active matter, and (3) the assumptions made about binary collisions on the microscopic level to determine its impact on the Smoluchowski equation.



(A) Pusher (B) Puller

Figure 1: Flow field about (A) pushers and (B) pullers can be approximated as a flow generated by a force dipole.

2 Model

Following Saintillan and Shelley [12], we describe a suspension of N self-propelled rod-like particles within a fluid by the particle distribution function $\Psi(\mathbf{x}, \mathbf{p}, t)$ that evolves in time t through the Smoluchowski equation

$$\Psi_t + \nabla_{\mathbf{x}} \cdot (\dot{\mathbf{x}}\Psi) + \nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}}\Psi) = 0 \tag{1}$$

where $\mathbf{x}$ is the position, $\mathbf{p}$ is the particle orientation, and $\nabla_{\mathbf{p}} = (\mathbf{I} - \mathbf{pp}) \cdot \partial/\partial\mathbf{p}$. The fluxes $\dot{\mathbf{x}}$ and $\dot{\mathbf{p}}$ are given by

$$\dot{\mathbf{x}} = V_0\mathbf{p} + \mathbf{u}(\mathbf{x}) - d_t \nabla_{\mathbf{x}} (\ln \Psi) \tag{2}$$

$$\dot{\mathbf{p}} = (\mathbf{I} - \mathbf{pp}) \cdot (\mathbf{p} \cdot \nabla\mathbf{u}) - d_r \nabla_{\mathbf{p}} (\ln \Psi) \tag{3}$$

where d_t is the translational diffusion, d_r is the rotational diffusion, V is the swimming speed, and $\mathbf{u}(\mathbf{x}, t)$ is the fluid velocity. Equation (1) conserves the total number N of particles; More precisely, (1) implies

$$\int_{\Omega} \Psi(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x} = N$$

for all time t. The fluid moves as a Stokes flow described by

$$-\nabla q + \mu\nabla^2\mathbf{u} + \nabla \cdot \mathbf{\Sigma}_a = \mathbf{0} \tag{4}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{5}$$

where q is the fluid pressure, μ is the dynamic viscosity, and the active stress $\mathbf{\Sigma}_a$ imparted on the fluid by the suspended particles is given by the following mean-field approximation:

$$\mathbf{\Sigma}_a(\mathbf{x}) = \alpha \int_{\Omega} \Psi(\mathbf{x}, \mathbf{p}, t) \left(\mathbf{pp} - \frac{1}{3}\mathbf{I} \right) d\mathbf{p} \tag{6}$$

with $\alpha > 0$ for pullers and $\alpha < 0$ for pushers. We used the same scaling as that described by Saintillan and Shelley [12]. The local fluid motion about pullers and pushers are illustrated in figure 1. The flow about a single individual swimmer can be approximated as a flow generated by a force dipole (see figure 1). This approximation is used in the derivation [11] of (6).

3 Numerics

We wish to solve equation (1) in the 2-dimensional case. In terms of phase space, this equation must be solved over 3 dimensions (2 spatial coordinates plus the orientation angle θ). Equation (1) becomes

$$\Psi_t + \nabla_x \cdot (\dot{\mathbf{x}}\Psi) + \partial_\theta(\dot{\theta}\Psi) = 0. \tag{7}$$

The flux conditions become

$$\dot{\mathbf{x}} = V_0\mathbf{p} + \mathbf{u} - d_t \nabla_{\mathbf{x}} \ln \Psi \tag{8}$$

$$\dot{\mathbf{p}} = \dot{\theta}\hat{\theta} = [\hat{\theta} \cdot (\mathbf{p} \cdot \nabla_{\mathbf{x}}\mathbf{u}) - d_r \partial_\theta \ln \Psi]\hat{\theta} \tag{9}$$

where $\mathbf{p} = (\cos\theta, \sin\theta)^T$, $\hat{\theta} = (-\sin\theta, \cos\theta)^T$, and the flow $\mathbf{u}$ is described by equations (4) - (6). Using (5), (8), and (9), note that, in two dimensions, we have

$$\mathbf{p}^{\perp} \cdot \dot{\mathbf{p}} = \mathbf{p}^{\perp} \cdot (\mathbf{I} - \mathbf{pp}) \cdot (\mathbf{p} \cdot \nabla \mathbf{u}) \Rightarrow \tag{10}$$

$$\dot{\theta} = -u_x \sin(2\theta) + \frac{v_x}{2}(1 + \cos(2\theta)) - \frac{u_y}{2}(1 - \cos(2\theta)), \tag{11}$$

(using $u_x + v_y = 0$). Then equation (7) becomes (using $\nabla_x \cdot \dot{\mathbf{x}} = 0$ via continuity),

$$\begin{aligned} &\Psi_t + (V_0 \cos\theta + u)\Psi_x + (V_0 \sin\theta + v)\Psi_y - d_t(\Psi_{xx} + \Psi_{yy}) \\ &\quad + \partial_\theta \left[\left(-u_x \sin(2\theta) + \frac{v_x}{2}(1 + \cos(2\theta)) - \frac{u_y}{2}(1 - \cos(2\theta)) \right) \Psi \right] - d_r \Psi_{\theta\theta} = 0. \end{aligned} \tag{12}$$

The equation (12) will be solved on a periodic domain in each phase space coordinate $x_1 \in [0, \ell_1), x_2 \in [0, \ell_2)$, and $\theta \in [0, 2\pi)$. We will use a pseudospectral method for each phase space coordinate. For time-stepping we will use the following method which solves the linear problem exactly and uses a second-order Adams-Bashforth method of updating the nonlinear terms. Let

$$\Psi(\mathbf{x}, \theta, t) = \sum_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}}(t) e^{2\pi i (k_1 x/\ell_1 + k_2 y/\ell_2) + i k_3 \theta}. \tag{13}$$

Discretizing time uniformly as $t_n = n\Delta t$, for $n \in \{0, 1, 2, ...\}$, and denoting $\hat{\Psi}(t_n)$ by $\hat{\Psi}^n$, we write for each mode $\mathbf{k}$:

$$\hat{\Psi}_{\mathbf{k}}^{n+2} = e^{-\alpha_{\mathbf{k}} \Delta t} \left[\hat{\Psi}_{\mathbf{k}}^{n+1} + \frac{\Delta t}{2} \left(3 \hat{\mathcal{N}}_{\mathbf{k}}[\Psi^{n+1}, u^{n+1}] - e^{-\alpha_{\mathbf{k}} \Delta t} \hat{\mathcal{N}}_{\mathbf{k}}[\Psi^n, u^n] \right) \right], \tag{14}$$

where

$$\alpha_{\mathbf{k}} = (d_t([2\pi k_1/\ell_1]^2 + [2\pi k_2/\ell_2]^2) + d_r k_3^2) \tag{15}$$

and

$$\begin{aligned} \mathcal{N}[\Psi^n, u^n] = &-(V_0 \cos\theta + u^n)\Psi_x^n - (V_0 \sin\theta + v^n)\Psi_y^n \\ &+ \partial_\theta \left[\left(u_x^n \sin(2\theta) - \frac{v_x^n}{2}(1 + \cos(2\theta)) + \frac{u_y^n}{2}(1 - \cos(2\theta)) \right) \Psi^n \right]. \end{aligned} \tag{16}$$

3.1 Velocity field

The computation of the velocity field is performed as follows in this first approach. Define the velocity and pressure fields (with time dependence suppressed since they are determined instantaneously at any given time), as

$$\mathbf{u}(\mathbf{x}) = \sum_{k_1, k_2} \hat{\mathbf{u}}_{\mathbf{k}} e^{2\pi i (k_1 x/\ell_1 + k_2 y/\ell_2)}, \tag{17}$$

$$p(\mathbf{x}) = \sum_{k_1, k_2} \hat{p}_{\mathbf{k}} e^{2\pi i (k_1 x/\ell_1 + k_2 y/\ell_2)}. \tag{18}$$

Define also the active forcing

$$\mathbf{f}_a = \nabla \cdot \mathbf{\Sigma}_a(\mathbf{x}) = (f_a, g_a). \tag{19}$$

The Stokes equations with continuity yield:

$$-2\pi i(k_1/\ell_1)\hat{p}_{\mathbf{k}} + \mu\left[(2\pi i k_1/\ell_1)^2 + (2\pi i k_2/\ell_2)^2\right]\hat{u}_{\mathbf{k}} + (\hat{f}_a)_{\mathbf{k}} = 0, \tag{20}$$

$$-2\pi i(k_2/\ell_2)\hat{p}_{\mathbf{k}} + \mu\left[(2\pi i k_1/\ell_1)^2 + (2\pi i k_2/\ell_2)^2\right]\hat{v}_{\mathbf{k}} + (\hat{g}_a)_{\mathbf{k}} = 0, \tag{21}$$

$$(2\pi i k_1/\ell_1)\hat{u}_{\mathbf{k}} + (2\pi i k_2/\ell_2)\hat{v}_{\mathbf{k}} = 0. \tag{22}$$

Multiplying the first equation by (k_1/ℓ_1), the second by (k_2/ℓ_2), and adding, and using the third equation, we find that

$$\hat{p}_{\mathbf{k}} = \frac{(k_1/\ell_1)(\hat{f}_a)_{\mathbf{k}} + (k_2/\ell_2)(\hat{g}_a)_{\mathbf{k}}}{2\pi i[(k_1/\ell_1)^2 + (k_2/\ell_2)^2]}, \tag{23}$$

and the velocity field satisfies

$$\hat{u}_{\mathbf{k}} = \frac{(\hat{f}_a)_{\mathbf{k}} - 2\pi i(k_1/\ell_1)\hat{p}_{\mathbf{k}}}{\mu\left[(2\pi k_1/\ell_1)^2 + (2\pi k_2/\ell_2)^2\right]}, \quad \hat{v}_{\mathbf{k}} = \frac{(\hat{g}_a)_{\mathbf{k}} - 2\pi i(k_2/\ell_2)\hat{p}_{\mathbf{k}}}{\mu\left[(2\pi k_1/\ell_1)^2 + (2\pi k_2/\ell_2)^2\right]}. \tag{24}$$

Or, letting $\mathbf{q} = (k_1/\ell_1, k_2/\ell_2)$, we may write this in a more familiar form,

$$\hat{p}_{\mathbf{k}} = \frac{\mathbf{q}\cdot(\hat{\mathbf{f}}_a)_{\mathbf{k}}}{2\pi i|\mathbf{q}|^2}, \quad \hat{\mathbf{u}}_{\mathbf{k}} = \frac{1}{(2\pi)^2\mu}\left(\frac{\mathbf{I}-\mathbf{q}\mathbf{q}}{|\mathbf{q}|^2}\right)\cdot(\hat{\mathbf{f}}_a)_{\mathbf{k}}. \tag{25}$$

3.2 Active stress

Inserting the Fourier representation for Ψ, we have:

$$\mathbf{\Sigma}_a(\mathbf{x}) = \alpha\int_\Omega \Psi(\mathbf{x},\mathbf{p},t)\left(\mathbf{p}\mathbf{p} - \frac{1}{2}\mathbf{I}\right)d\mathbf{p} \tag{26}$$

$$= \frac{\alpha}{N_{xgrid}N_{ygrid}N_{\theta grid}}\sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}(t)\int_\Omega e^{2\pi i(k_1x/\ell_1 + k_2y/\ell_2) + ik_3\theta}\begin{pmatrix}\cos^2\theta - 1/2 & \sin\theta\cos\theta\\ \sin\theta\cos\theta & \sin^2\theta - 1/2\end{pmatrix}d\theta \tag{27}$$

$$= \frac{\alpha}{N_{xgrid}N_{ygrid}N_{\theta grid}}\sum_{k_1,k_2}\begin{pmatrix}\frac{\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right) & \frac{i\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right)\\ \frac{i\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right) & -\frac{\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right)\end{pmatrix}e^{2\pi i(k_1x/\ell_1 + k_2y/\ell_2)}. \tag{28}$$

The 2D case is given by

$$\hat{\mathbf{\Sigma}}_a = \frac{\alpha}{N_{xgrid}N_{ygrid}N_{\theta grid}}\begin{pmatrix}\frac{\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right) & \frac{i\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right)\\ \frac{i\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right) & -\frac{\pi}{2}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right)\end{pmatrix}, \tag{29}$$

and then (omitting the N_xN_y since they are included with $\hat{f}$)

$$(\hat{\mathbf{f}}_a)_{\mathbf{k}} = (\nabla\cdot\hat{\mathbf{\Sigma}}_a)_{\mathbf{k}} = \frac{\alpha}{N_{\theta grid}}\begin{pmatrix}\frac{\pi^2 ik_1}{\ell_1}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right) - \frac{\pi^2k_2}{\ell_2}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right)\\ \frac{-\pi^2k_1}{\ell_1}\left(\hat{\Psi}_{k_1,k_2,2} - \hat{\Psi}_{k_1,k_2,-2}\right) - \frac{i\pi^2k_2}{\ell_2}\left(\hat{\Psi}_{k_1,k_2,2} + \hat{\Psi}_{k_1,k_2,-2}\right)\end{pmatrix}. \tag{30}$$

4 Cluster dynamics

4.1 Single cluster

We consider four simple initial configurations of a single cluster: an isotropic cluster, a polarized cluster of pullers, a polarized cluster of pushers, and an elongated polarized cluster of pushers

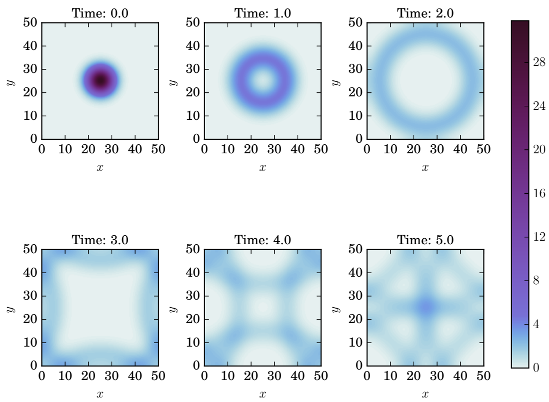


Figure 2: Concentration field during the spreading of an isotropic cluster with a swimming speed of $V = 10\mu m/s$ and $\alpha = -1$. We choose the following other parameters: $l_x = 50$, $l_y = 50$, $l_\theta = 2\pi$, $a = 5$, $d_r = 0.0$, $d_t = 0.0$, $x_0 = l_x/2$, and $y_0 = l_y/2$. (Colormap developed by Thyng *et al* [14])

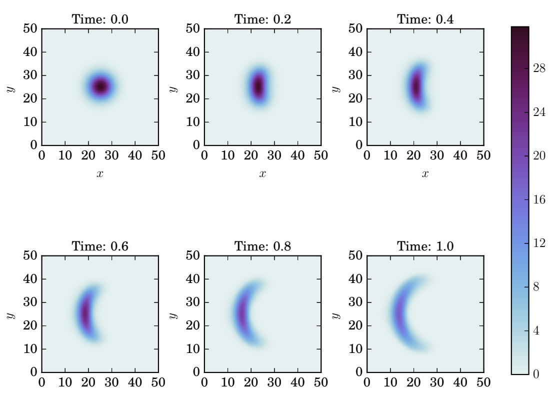


Figure 3: Concentration field during the spreading of a polarized cluster of pullers with a swimming speed of $V = 10\mu m/s$ and $\alpha = 1$. We choose the following other parameters: $l_x = 50$, $l_y = 50$, $l_\theta = 2\pi$, $a = 5$, $b = 0.5$, $d_r = 0.001$, $d_t = 0.001$, $x_0 = l_x/2$, $y_0 = l_y/2$, and $\theta_0 = \pi$.

1. (Isotropic cluster) Consider a cluster of characteristic width a located at the origin with uniformly distributed initial orientation, so that we have

$$\Psi(\mathbf{x}, \theta, t = 0) = Ae^{-((x-x_0)^2+(y-y_0)^2)/a^2} \tag{31}$$

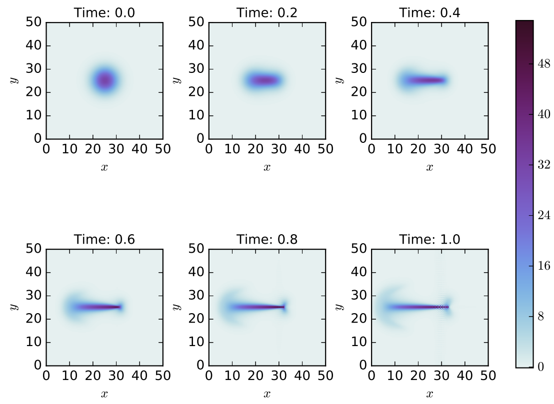


Figure 4: Concentration field during the spreading of a polarized cluster of pushers with a swimming speed of $V = 10 \mu m/s$ and $\alpha = -1$. We choose the following other parameters: $l_x = 50$, $l_y = 50$, $l_\theta = 2\pi$, $a = 5$, $b = 0.5$, $d_r = 0.001$, $d_t = 0.001$, $x_0 = l_x/2$, $y_0 = l_y/2$, and $\theta_0 = \pi$.

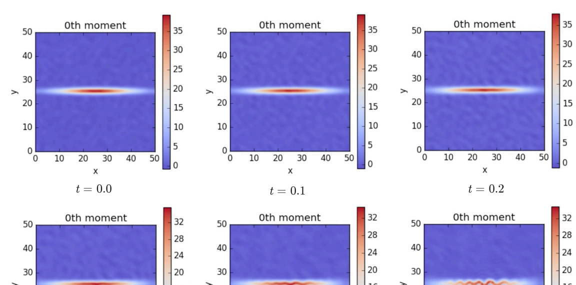


Figure 5: Concentration field of an initially elongated polarized cluster of pushers with a swimming speed of $V_0 = 5 \mu m/s$ and $\alpha = -1$ with a small perturbation across Fourier modes. An instability arises which is most visible in the final frame above. We chose the following other parameters: $l_x = 50$, $l_y = 50$, $l_\theta = 2\pi$, $b = 0.5$, $d_r = 0.001$, $d_l = 0.001$, $x_0 = l_x/2$, $y_0 = l_y/2$, $\theta_0 = \pi + \pi/20$, $x_w = l_x/3$, and $y_w = l_y/40$.

with A is a normalization factor to ensure that mean density is $\frac{1}{2\pi}$. We noticed that the dynamics did not depend on α. We think this is due to the symmetry of the problem. We plan to investigate this further in future work.

2. (Polarized cluster of pullers) Consider a cluster at the origin, but now with *polarized* initial orientation to left, so that we have

$$\Psi(\mathbf{x}, \theta, t=0) = Ae^{-((x-x_0)^2+(y-y_0)^2)/a^2-(\theta-\theta_0)^2/b^2}. \tag{32}$$

Recall that α is negative for pushers; We chose $\alpha = 1$ for the simulation shown in figure 3. We observed splaying of the initial distribution of swimmers and an overall collective radial motion which moved roughly at the individual swimming speed of 10.

3. (Polarized cluster of pushers) Consider a cluster at the origin so that we have

$$\Psi(\mathbf{x}, \theta, t=0) = Ae^{-((x-x_0)^2+(y-y_0)^2)/a^2-(\theta-\theta_0)^2/b^2}. \tag{33}$$

We have made only one parameter change here relative to the last example — α is now positive for pullers. We observed a 'squeezing' effect lateral to the swimming direction which is consistent with our understanding of the local dynamics surrounding an individual pusher (see figure 1).

4. (Elongated polarized cluster of pushers)

$$\Psi(\mathbf{x}, \theta, t=0) = Ae^{-(x-x_0)^2/x_w^2-(y-y_0)^2/y_w^2-(\theta-\theta_0)^2/b^2}, \tag{34}$$

We observed an instability in this case (see figure 5). We perturbed the initial condition with small random perturbations across fourier modes with$k_x < 15\frac{2\pi}{l_x}$ or $k_y < 15\frac{2\pi}{l_y}$. As a result, this perturbation excited an instability in this configuration. This suggests that the configuration shown in figure 4 at later times is a singular and unstable situation.

4.2 Dynamics of two colliding point particles

In this section, we will first take a look at a simple two point particle collision to see if it can capture the key features observed in the upcoming section when considering the collision of two patches.

Suppose that the motion of a single point particle at location $\mathbf{x}$ with direction $\mathbf{p}$ is governed by

$$\begin{aligned} \dot{\mathbf{x}} &= V_0\mathbf{p} + \mathbf{u} & (35)\\ \dot{\mathbf{p}} &= (\mathbf{I} - \mathbf{pp}) \cdot \nabla\mathbf{u} \cdot \mathbf{p} & (36) \end{aligned}$$

where the point particle supplies a point force in a Stokes flow. We consider the collision of two such point particles as shown in figure 6 and investigate their dynamics. The surrounding fluid obeys

$$-\nabla q + \mu\nabla^2\mathbf{u} + \sum_{n=1,2} S(\mathbf{p}_n) \cdot \nabla\delta(\mathbf{x} - \mathbf{x}_n) = \mathbf{0}, \tag{37}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{38}$$

where $S(\mathbf{p}_n) = \sigma\mathbf{p}_n\mathbf{p}_n$. The solution is given by

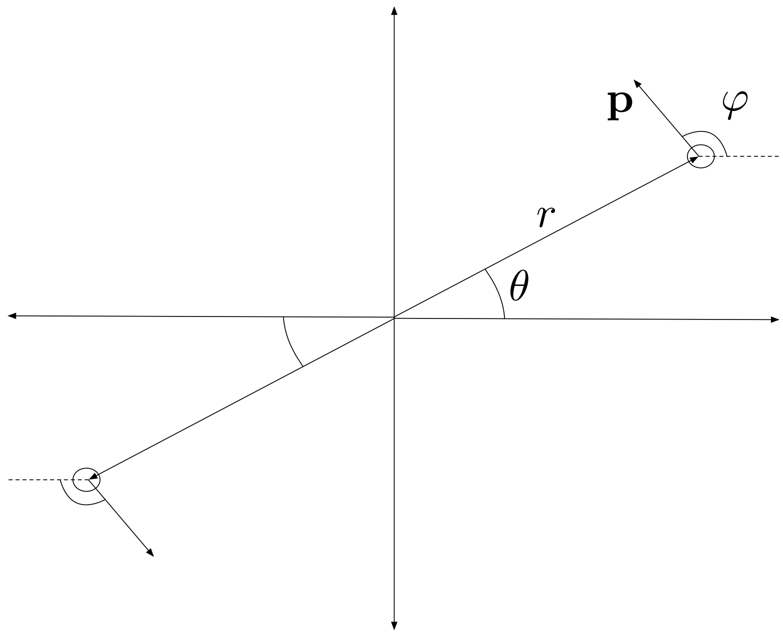


Figure 6: A symmetric collision of two point particles

$$\mathbf{u}(\mathbf{x}) = \sum_{n=1,2} S(\mathbf{p}_n) : \nabla J(\mathbf{x} - \mathbf{x}_n) \tag{39}$$

where $J(\mathbf{r}) = \frac{1}{8\pi\mu}(I - \hat{\mathbf{r}}\hat{\mathbf{r}})\frac{1}{|\mathbf{r}|}$ and $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$. Given the symmetry of the collision, the state of the system is completely determined by three dynamic variables r, θ, and φ. We find that

$$\begin{aligned} \dot{r} &= V_0 \cos(\varphi - \theta) + u^r && (40) \\ r\dot{\theta} &= V_0 \sin(\varphi - \theta) + u^\theta && (41) \\ \dot{\varphi} &= -u_x \sin(2\varphi) + \frac{v_x}{2}(1 + \cos(2\varphi)) - \frac{u_y}{2}(1 - \cos(2\varphi)). && (42) \end{aligned}$$

or equivalently,

$$\begin{aligned} \dot{r} &= V_0 \left(\cos(\varphi - \theta) - \frac{\alpha \cos(2(\theta - \varphi))}{8\pi r} \right) && (43) \\ \dot{\theta} &= \frac{V_0}{r} \sin(\varphi - \theta) && (44) \\ \dot{\varphi} &= \alpha V_0 \left(\frac{\sin(4\theta - 4\varphi) - \sin(2\theta - 2\varphi)}{16\pi r^2} \right). && (45) \end{aligned}$$

Figure 7 shows a series of collision trajectories across a range of the impact parameter y. Interestingly, as you decreased the impact parameter, you eventually surpass a threshold for which the trajectories are trapped in circular orbit at a fixed radius which has a $\sqrt{|\alpha|}$ dependence.

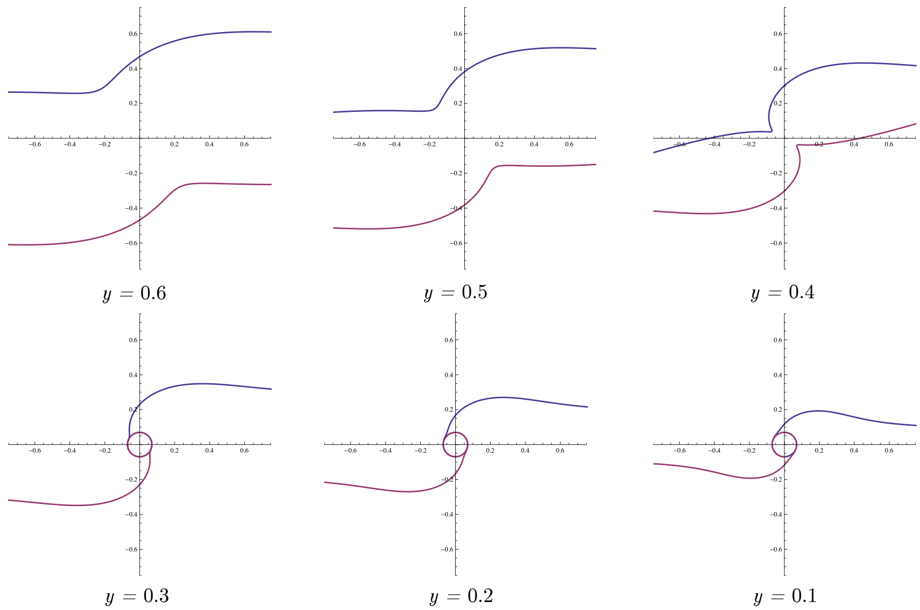


Figure 7: Trajectories of a symmetric collision of two point particles. The horizontal and vertical axes ranges from -0.75 to 0.75. y_0 measures the impact parameter relative the horizontal axis. We chose the following parameters: $\alpha = -5.0$, $V_0 = 1.0$, and the initial x-coordinate $x_0 = 1.0$.

4.3 Dynamics of cluster collision

$$\Psi(\mathbf{x}, \theta, t = 0) = A\left(e^{-((x-x_0)^2+(y-y_0)^2)/a^2-\theta^2/b^2} + e^{-((x+x_0)^2+(y+y_0)^2)/a^2-(\theta-\pi)^2/b^2}\right), \tag{46}$$

Figure 8 shows how the dynamics change with decreasing impact parameter. Given the point particle analysis of the last section, we expected to see the clusters orbit around each other for small enough impact parameter. This however was not the case. Instead, we saw a 'curling' effect emerge from the interaction of the two clusters. It appears that the collision is exciting the instability discussed earlier when examing the single polarized puller cluster.

5 Droplet Dynamics

Now, we model a droplet with active matter. To do this numerically, we implemented a immersed boundary method [8]. We modeled the boundary by two different methods: a lagrangian point method and a levelset method.

The Smoluchowski equation (1) remains the same. We add new terms to the flux conditions. The translation flux $\dot{\mathbf{x}}$ now has a new term that is responsible for making the boundary nearly impenetrable; the rotational flux $\dot{\mathbf{p}}$ has a new term that causes the swimmers to turn when encountering the interface. Specifically, the fluxes $\dot{\mathbf{x}}$ and $\dot{\mathbf{p}}$ change to (new terms are in blue)

$$\dot{\mathbf{x}} = V\mathbf{p} + \mathbf{u}(\mathbf{x}) - d_t\nabla_{\mathbf{x}}(\ln\Psi) - V_0\mathbf{p}\cdot\hat{n}\hat{n}\delta_\epsilon(\mathbf{x})1_{\{\mathbf{p}\cdot\hat{n}>0\}} \tag{47}$$

$$\dot{\mathbf{p}} = (\mathbf{I} - \mathbf{pp})\cdot(\mathbf{p}\cdot\nabla\mathbf{u}) - d_r\nabla_{\mathbf{p}}(\ln\Psi) - \beta\mathbf{p}\cdot\hat{n}\mathbf{p}^\perp\cdot\hat{n}\hat{n}\delta_\epsilon(\mathbf{x})1_{\{\mathbf{p}\cdot\hat{n}>0\}} \tag{48}$$

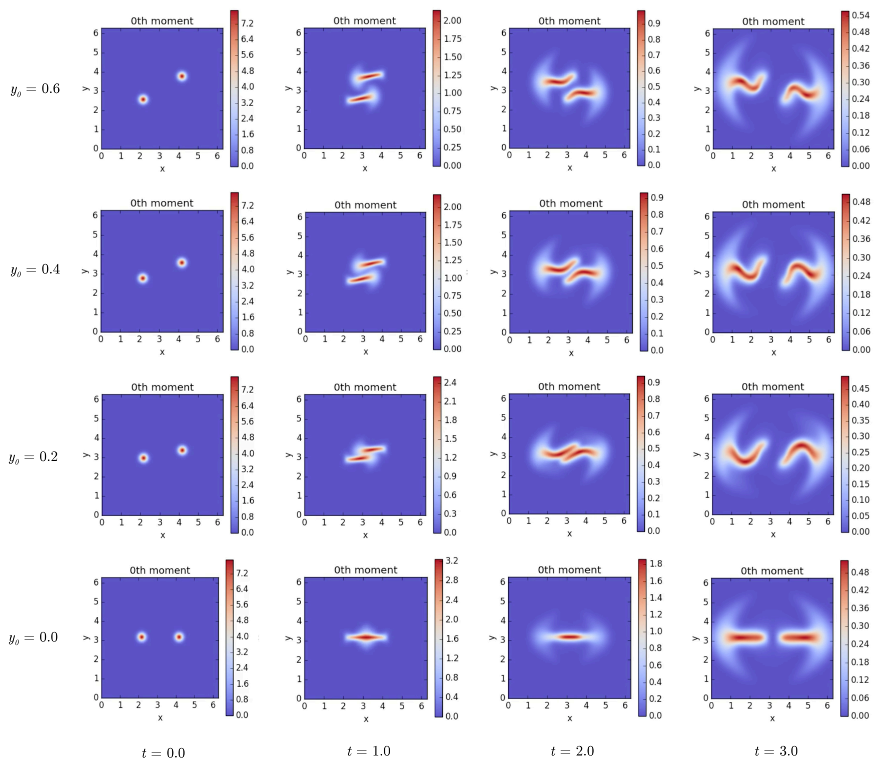


Figure 8: A symmetric collision of two polarized puller ($\alpha = -1$) clusters with varying impact parameter y as function of time t. We chose the parameters: We chose the following other parameters: $l_x = 2\pi$, $l_y = 2\pi$, $l_\theta = 2\pi$, $a = 0.2$, $b = 0.2$, $d_r = 0.01$, $d_l = 0.01$, $x_0 = 1.0$.

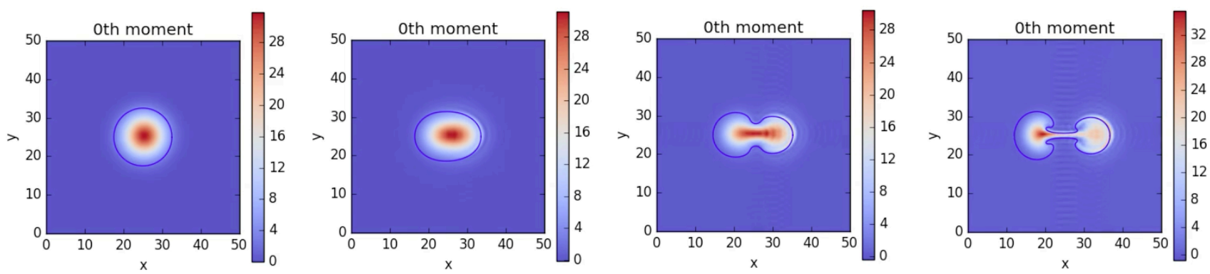
where $\hat{n}$ is the surface normal, β is a tunable parameter to set the degree influence the interface has on the rotation of a swimmer, and $\delta_\epsilon(\mathbf{x})$ is a numerical 'delta' function with width ϵ. We add a term for the normal stress due to surface tension in the Stokes equation:

$$-\nabla q + \mu \nabla^2 \mathbf{u} + \nabla \cdot \mathbf{\Sigma}_a - \gamma(\nabla \cdot \hat{n})\hat{n}\delta_\epsilon(\mathbf{x}) = \mathbf{0} \tag{49}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{50}$$

where γ is the surface tension. We used two alternative methods for evolving the boundary:

1. (Lagrangian method) We evolved the surface Lagrangian points by $\frac{dx_j}{dt}$ for $j = 1, 2, 3, \ldots, M$ where x_j is the position of the jth Lagrangian point and M is the total number of Lagrangian points.
2. (Level-set method) We evolved a level-set function ϕ according to $\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$ where $\phi = 0$ defines the interface, ϕ is positive in the interior, and ϕ is negative in the exterior.



$t = 0.0$ $t = 1.0$ $t = 2.0$ $t = 3.0$

Figure 9: Droplet simulation with $l_x = l_y = 50$, $\alpha = -0.1$, $\beta = 1.0$, $V_0 = 1.0$, $d_t = 0.1$, $d_r = 0.1$ and $\gamma = 50000$. The active matter in the interior is a polarized cluster of pushers oriented to the right.

Figure 9 shows a simulation with $l_x = l_y = 50$, $\alpha = -0.1$, $\beta = 1.0$, $V_0 = 1.0$, and $\gamma = 50000$. Recall from earlier that we observed an elongation effect for the case without the droplet interface (see figure 4). This effect still seems to be present when the cluster is place in the interior of the droplet. But now, this elongation process causes the droplet to pinch in the center and creates a small filament between two newly formed daughter droplets (as seen in the last frame of figure 9). We were unable to get the two daughter droplets to completely separate. The problem of separation is two-fold: (1) the simulation used the Lagrangian method which by construction does not allow for splitting of the droplet interior domain (this can be solved by using the level-set method) and (2) we believe that we are neglecting physics about phase separation and may consider using a Cahn-Hillard potential for this purpose.

6 Is binary collision physics captured by the Smoluchowski equation?

After observing such rich dynamics in the binary collision of point particles (as seen in section 4.2), we asked the following "Is this physics captured in the Smolukowski equation?" This may remind some of the Boltzmann equation which accounts for binary collisions of rarefied gases. On the other

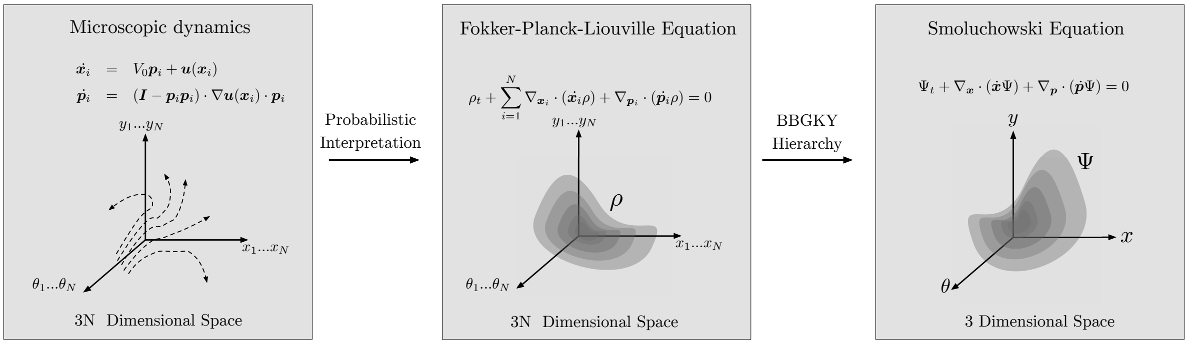


Figure 10: Microscopic description turns from a description in $3N$-dimensional space to a 3-dimensional space through the BBGKY hierarchy.

hand, a related equation, used mostly for describing plasmas, is the Vlasov equation which neglects the effects of binary collions. So to state our question another way, we ask "Is the Smolukowski equation Boltzman-like or Vlasov-like?" To answer this question, we will start with a microscopic description for N particles and derive the Smolukowski equation by using statistical assumptions and the BBGKY hierarchy approach [1–6, 17] a. This procedure, illustrated in figure 10, provides a way to reduce the dimension of phase space from $3N$ to 3 coordinates and provides a link between microscopic particle dynamics and the Smolukowski equation.

We begin by considering a periodic box with N particles. The particle motion is governed by (while ignoring random thermal forcing)

$$
\begin{aligned}
\dot{\mathbf{x}}_1 &= V_0\mathbf{p}_1 + \mathbf{u}(\mathbf{x}_1) && (51)\\
\dot{\mathbf{p}}_1 &= (\mathbf{I} - \mathbf{p}_1\mathbf{p}_1)\cdot\nabla\mathbf{u}(\mathbf{x}_1)\cdot\mathbf{p}_1 && (52)\\
\dot{\mathbf{x}}_2 &= V_0\mathbf{p}_2 + \mathbf{u}(\mathbf{x}_2) && (53)\\
\dot{\mathbf{p}}_2 &= (\mathbf{I} - \mathbf{p}_2\mathbf{p}_2)\cdot\nabla\mathbf{u}(\mathbf{x}_2)\cdot\mathbf{p}_2 && (54)\\
&\vdots && (55)\\
\dot{\mathbf{x}}_N &= V_0\mathbf{p}_N + \mathbf{u}(\mathbf{x}_N) && (56)\\
\dot{\mathbf{p}}_N &= (\mathbf{I} - \mathbf{p}_N\mathbf{p}_N)\cdot\nabla\mathbf{u}(\mathbf{x}_N)\cdot\mathbf{p}_N && (57)
\end{aligned}
$$

where

$$
\mathbf{u}(\mathbf{x}_i) = \sum_{j=1, j\neq i}^{N} \mathbf{u}_j(\mathbf{x}_i|\mathbf{x}_j, \mathbf{p}_j) \tag{58}
$$

and $\mathbf{u}_j(\mathbf{x})$ is the velocity field generated by the force-dipole particle j satisfying

$$
\begin{aligned}
\mu\Delta\mathbf{u}_j - \nabla q + \sigma\mathbf{p}_j\mathbf{p}_j\cdot\nabla\delta(\mathbf{x}-\mathbf{x}_j) &= 0 && (59)\\
\nabla\cdot\mathbf{u}_j &= 0. && (60)
\end{aligned}
$$

The corresponding n-particle Fokker-Planck-Louiville equation associated with equations (51)-(57) is

$$\frac{\partial\rho}{dt} + \sum_{i=1}^{N} \nabla_{\mathbf{x}_i} \cdot \{[V_0\mathbf{p}_i + \mathbf{u}(\mathbf{x}_i)]\rho\} + \sum_{i=1}^{N} \nabla_{\mathbf{p}_i} \cdot \{[(\mathbf{I} - \mathbf{p}_i\mathbf{p}_i) \cdot \nabla_{\mathbf{x}_i}\mathbf{u}(\mathbf{x}_i) \cdot \mathbf{p}_i]\rho\} = 0 \tag{61}$$

The s-particle probability density is defined as

$$\rho_s(\mathbf{x}_1, \mathbf{p}_1, \ldots, \mathbf{x}_s, \mathbf{p}_s, t) = \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \rho(\mathbf{x}_1, \mathbf{p}_1, \ldots, \mathbf{x}_N, \mathbf{p}_N, t) \tag{62}$$

where the definition assumes symmetry with respect to permutation of the particles. The time evolution of ρ_s is given by

$$\begin{aligned}
\frac{\partial\rho_s}{\partial t} &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{N} \nabla_{\mathbf{x}_j} \cdot \{[V_0\mathbf{p}_j + \mathbf{u}(\mathbf{x}_j)]\rho\} - \sum_{j=1}^{N} \nabla_{\mathbf{p}_i} \cdot \{[(\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \nabla_{\mathbf{x}_j}\mathbf{u}(\mathbf{x}_j) \cdot \mathbf{p}_j]\rho\} \right) \\
&= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{N} \nabla_{\mathbf{x}_j} \cdot \{[V_0\mathbf{p}_j + \sum_{k=1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k)]\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{N} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \nabla_{\mathbf{x}_j} \left(\sum_{k=1,k\neq j} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k) \right) \cdot \mathbf{p}_j]\rho\} \right)
\end{aligned}$$

First, let's us break up this expression into the three following parts:

$$\frac{\partial\rho_s}{\partial t} = G_s + G_{N-s} + G' \tag{63}$$

1. a term representing the interaction among a group of s particles

$$\begin{aligned}
G_s &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \{[V_0\mathbf{p}_j + \sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k)]\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \nabla_{\mathbf{x}_j} \left(\sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k) \right) \cdot \mathbf{p}_j]\rho\} \right)
\end{aligned}$$

2. a term representing the interaction among the remaining group of $N - s$ particles

$$\begin{aligned}
G_{N-s} &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{x}_j} \cdot \{[V_0\mathbf{p}_j + \sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k)]\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \nabla_{\mathbf{x}_j} \left(\sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k) \right) \cdot \mathbf{p}_j]\rho\} \right)
\end{aligned}$$

3. and a term representing the interaction between the s-group and the $(N-s)$-group

$$
\begin{aligned}
G' &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \{ \sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k)\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{x}_j} \cdot \{ \sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k)\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j]\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j]\rho\} \right)
\end{aligned}
$$

Let us evaluate each integral separately.

$$
\begin{aligned}
G_s &= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ \left[V_0\mathbf{p}_j + \sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right] \left(\int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \rho \right) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ \left[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j \right] \left(\int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \rho \right) \right\} \\
&= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ \left[V_0\mathbf{p}_j + \sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right] \rho_s(\mathbf{x}_1,\ldots,\mathbf{p}_s) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ \left[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=1,k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j \right] \rho_s(\mathbf{x}_1,\ldots,\mathbf{p}_s) \right\}
\end{aligned}
$$

G_{N-s} vanishes due to the divergence theorem and periodic boundary conditions.

$$
\begin{aligned}
G_{N-s} &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{x}_j} \cdot \{[V_0\mathbf{p}_j + \sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k)]\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=s+1}^{N} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j]\rho\} \right) = 0
\end{aligned}
$$

Finally, we simplify G'.

$$
\begin{aligned}
G' &= \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \{ \sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k)\rho\} \right) \\
&+ \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \left(-\sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \{[(\mathbf{I}-\mathbf{p}_j\mathbf{p}_j)\cdot\nabla_{\mathbf{x}_j} \left(\sum_{k=s+1,k\neq j}^{N} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k,\mathbf{p}_k) \right)\cdot\mathbf{p}_j]\rho\} \right)
\end{aligned}
$$

where we have again used the divergence theorem and periodic boundary conditions to eliminate the 2nd and 4th terms from the original expression.

$$
\begin{aligned}
G' &= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ \sum_{k=s+1, k\neq j}^{N} \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k)\rho \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ (\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \left[\sum_{k=s+1, k\neq j}^{N} \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \nabla_{\mathbf{x}_j} \left(\mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k)\right) \rho \right] \cdot \mathbf{p}_j \right\}
\end{aligned}
$$

Assuming symmetry with respect to particle permutations, we have that

$$
\begin{aligned}
G' &= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ (N-s) \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1})\rho \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ (\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \left[(N-s) \int \prod_{i=s+1}^{N} d\mathbf{x}_i d\mathbf{p}_i \nabla_{\mathbf{x}_j} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1})\right) \rho \right] \cdot \mathbf{p}_j \right\}
\end{aligned}
$$

Then, we have

$$
\begin{aligned}
G' &= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ (N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1}) \left[\int \prod_{i=s+2}^{N} d\mathbf{x}_i d\mathbf{p}_i \rho \right] \right) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ (\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \left[(N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left\{ \nabla_{\mathbf{x}_j} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1})\right) \left[\int \prod_{i=s+2}^{N} d\mathbf{x}_i d\mathbf{p}_i \rho \right] \right\} \right] \cdot \mathbf{p}_j \right\} \\
&= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ (N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1}) \rho_{s+1}(\mathbf{x}_1, \ldots, \mathbf{p}_{s+1}) \right) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ (\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \left[(N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left\{ \nabla_{\mathbf{x}_j} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1})\right) \rho_{s+1}(\mathbf{x}_1, \ldots, \mathbf{p}_{s+1}) \right\} \right] \cdot \mathbf{p}_j \right\}
\end{aligned}
$$

Finally, we have that

$$
\begin{aligned}
&\frac{\partial \rho_s}{\partial t}(\mathbf{x}_1, \ldots, \mathbf{p}_s, t) \\
&= -\sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ \left[V_0 \mathbf{p}_j + \sum_{k=1, k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k) \right] \rho_s(\mathbf{x}_1, \ldots, \mathbf{p}_s) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ \left[(\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \nabla_{\mathbf{x}_j} \left(\sum_{k=1, k\neq j}^{s} \mathbf{u}_k(\mathbf{x}_j|\mathbf{x}_k, \mathbf{p}_k) \right) \cdot \mathbf{p}_j \right] \rho_s(\mathbf{x}_1, \ldots, \mathbf{p}_s) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{x}_j} \cdot \left\{ (N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1}) \rho_{s+1}(\mathbf{x}_1, \ldots, \mathbf{p}_{s+1}) \right) \right\} \\
&- \sum_{j=1}^{s} \nabla_{\mathbf{p}_j} \cdot \left\{ (\mathbf{I} - \mathbf{p}_j\mathbf{p}_j) \cdot \left[(N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \left\{ \nabla_{\mathbf{x}_j} \left(\mathbf{u}_{s+1}(\mathbf{x}_j|\mathbf{x}_{s+1}, \mathbf{p}_{s+1})\right) \rho_{s+1}(\mathbf{x}_1, \ldots, \mathbf{p}_{s+1}) \right\} \right] \cdot \mathbf{p}_j \right\}.
\end{aligned}
$$

Note that the evolution of ρ_1 depends on ρ_2 and ρ_2 depends on ρ_3 and so forth. Therefore to make use of the above expression, one must create a closure to truncate the hierarchy. Let us examine the first equation of the hierarchy.

$$\begin{aligned}
&\frac{\partial \rho_1}{\partial t}(\mathbf{x}_1, \mathbf{p}_1, t) + V_0 \mathbf{p}_1 \cdot \nabla_{\mathbf{x}_1} \rho_1(\mathbf{x}_1, \mathbf{p}_1) \\
= \;& -\nabla_{\mathbf{x}_1} \cdot \left\{ (N-1) \int d\mathbf{x}_2 d\mathbf{p}_2 \left(\mathbf{u}_2(\mathbf{x}_1 | \mathbf{x}_2, \mathbf{p}_2) \rho_2(\mathbf{x}_1 \mathbf{p}_1, \mathbf{x}_2, \mathbf{p}_2) \right) \right\} \\
- \;& \nabla_{\mathbf{p}_1} \cdot \left\{ (\mathbf{I} - \mathbf{p}_1 \mathbf{p}_1) \cdot \left[(N-1) \int d\mathbf{x}_2 d\mathbf{p}_2 \left\{ \nabla_{\mathbf{x}_1} \left(\mathbf{u}_2(\mathbf{x}_1 | \mathbf{x}_2, \mathbf{p}_2) \right) \rho_2(\mathbf{x}_1 \mathbf{p}_1, \mathbf{x}_2, \mathbf{p}_2) \right\} \right] \cdot \mathbf{p}_1 \right\}.
\end{aligned}$$

Now we choose the closure $\rho_2(\mathbf{x}_1, \mathbf{p}_1, \mathbf{x}_2, \mathbf{p}_2) = \rho_1(\mathbf{x}_1, \mathbf{p}_1)\rho_1(\mathbf{x}_2, \mathbf{p}_2)$, this physically means that the interaction among the particles is long range rather than short range (only mediated via two particle interactions) as seen in the Boltzmann equation. Furthermore, if we introduce the s-particle density functions,

$$\Psi_s(\mathbf{x}_1, \ldots, \mathbf{p}_s) = \frac{N!}{(N-s)!} \rho_s(\mathbf{x}_1, \ldots, \mathbf{p}_s),$$

then one finds that the 1-particle density function evolves as

$$\begin{aligned}
&\frac{\partial \Psi_1}{\partial t}(\mathbf{x}_1, \mathbf{p}_1, t) + V_0 \mathbf{p}_1 \cdot \nabla_{\mathbf{x}_1} \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \\
= \;& -\nabla_{\mathbf{x}_1} \cdot \left\{ \int d\mathbf{x}_2 d\mathbf{p}_2 \left(\mathbf{u}_2(\mathbf{x}_1 | \mathbf{x}_2, \mathbf{p}_2) \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \Psi_1(\mathbf{x}_2, \mathbf{p}_2) \right) \right\} \\
- \;& \nabla_{\mathbf{p}_1} \cdot \left\{ (\mathbf{I} - \mathbf{p}_1 \mathbf{p}_1) \cdot \left[\int d\mathbf{x}_2 d\mathbf{p}_2 \left\{ \nabla_{\mathbf{x}_1} \left(\mathbf{u}_2(\mathbf{x}_1 | \mathbf{x}_2, \mathbf{p}_2) \right) \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \Psi_1(\mathbf{x}_2, \mathbf{p}_2) \right\} \right] \cdot \mathbf{p}_1 \right\}.
\end{aligned}$$

If we define

$$\mathbf{u}'(\mathbf{x}_1) = \int d\mathbf{x}_2 d\mathbf{p}_2 \mathbf{u}_2(\mathbf{x}_1 | \mathbf{x}_2, \mathbf{p}_2) \Psi_1(\mathbf{x}_2, \mathbf{p}_2), \tag{64}$$

we arrive at the Vlasov-like equation

$$\begin{aligned}
&\frac{\partial \Psi_1}{\partial t}(\mathbf{x}_1, \mathbf{p}_1, t) + V_0 \mathbf{p}_1 \cdot \nabla_{\mathbf{x}_1} \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \\
= \;& -\nabla_{\mathbf{x}_1} \cdot \left\{ \mathbf{u}'(\mathbf{x}_1) \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \right\} \\
- \;& \nabla_{\mathbf{p}_1} \cdot \left\{ (\mathbf{I} - \mathbf{p}_1 \mathbf{p}_1) \cdot \nabla_{\mathbf{x}_1} \mathbf{u}'(\mathbf{x}_1) \cdot \mathbf{p}_1 \Psi_1(\mathbf{x}_1, \mathbf{p}_1) \right\}
\end{aligned}$$

which is exactly the diffusion-less Smoluchowski equation used in our model. Therefore, we have arrived at an answer to the question posed — the Smoluchowski equation is Vlasov-like and does *not* include binary-collision physics.

7 Discussion

In this work, we studied the model introduced by Saintillan and Shelley [10]. In particular, we investigated the dynamics of active matter clusters, studied the confinement of active matter within a droplet, and discovered the absence of binary collision physics in the Smoluchowski equation.

The isotropic cluster expanded out in a 'ring' as expected due to the uniform distribution over orientation angle θ. Due to the symmetry of the problem we saw that the dynamics were independent of α. A polarized cluster of pullers showed splaying into a crescent shape with near radial motion at later times. On the other hand, A polarized cluster of pushers exhibited an elongation along its polarized axis and thinning in the lateral directions. We then considered an initially elongated cluster of pushers with a slight perturbation which excited an instability. Thus, this shows that the final stages of the elongation effect seen in figure 4 may not be stable. We then considered the binary collision of point particles as a reduced model of the collision of two polarized clusters. We found that the dynamics of the polarized clusters did not match this reduced model since the clusters did not retain its coherent structure and quickly deformed. In fact, we observed a 'curling' effect which we suspect to be the result of the instability described earlier.

We then explored the effects of confinement by placing a cluster of active matter in the interior of a droplet. We included new terms to the flux conditions to enforce nearly impenetrable droplet walls. In addition, we endowed the interface with surface tension. We observed that a cluster of pusher particles elongated as seen without the interface. As a consequence, the droplet surface deformed in response to produce a dumbbell-like shape. We surmise that by including further physics of phase separation (by possibly considering the Cahn-Hillard potential), the dumbbell will turn into two separate daughter droplets.

We observed rich dynamics in a single binary collision, this prompt the following question, "Is the physics of binary collisions included in the Smoluchowski equation?" We discovered that the answer is 'No' by performing a derivation of the Smoluchowski equation by using the BBGKY hierarchy approach. Furthermore, we identified the Smoluchowski equation as Vlasov-like rather than Bolzmann-like. If the situation is at all similar to the kinetic theory of rarefied gases, we hypothesize that the inclusion of binary collisions will result in the addition of a new diffusive term, different than the diffusive term already included representing the effect of thermal fluctuations.

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