Pattern Formation in Active Suspensions

Sara Yacoub*

Advisor: Laurel Ohm

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Courant Institute of Mathematical Sciences, New York University.

Abstract

Active suspension systems are large-scale collections of self-propelled interacting particles called swimmers, or active swimmers. They are common in nature where bacteria and other micro-organisms form large colonies. They also have technological, for example engineers develop artificial swimmers for various researched applications. These particles propel themselves through fluid inducing disturbance perturbations causing complex nonlinear patterns to form.

In this writeup, we will build a kinetic model describing an active suspension system using a conservation of particles equation coupled with Navier-Stokes equation describing the fluid in the lower limit of Reynold's number due to the micro size of the swimmers causing the time derivative expressions to approach zero. We will then perform a linear stability analysis to find ranges of the eigenvalue parameters where the instabilities occur. We will use MATLAB to build the model and allow it to simulate the behavior of the particles in these stability regions as time progress to observe the different patterns forming and measure the change in the system.

1 Introduction

Active suspension systems have been observed to produce turbulence patterns [1-3]. These systems consisting of large collections of rod-like articles called swimmers are present in nature, as well as engineered applications for various reasons as cited by Saintillan and Shelly, 2008[1]. In their paper, they develop a kinetic 3-dimentional model using governing equations of particle density conservation and momentum and mass conservation, perform a linear stability analysis using an eigenvalue problem and simulate the nonlinear model to observe pattern formation as time progresses. In this writeup, we will follow their methodology for our 2-dimentional model.

We will consider a kinetic model of the dynamics arising from the large-scale collections of self-propelled interacting particles called active swimmers immersed in a viscous fluid in systems known as active suspensions. Many studies have noted that the swimming particles induce disturbance flows as they propel themselves through the fluid, causing them to interact hydrodynamically and resulting in collective motions in large suspensions. Large, concentrated suspensions give rise to interesting patterns and 'bacterial turbulences' in certain parameter regimes from plane wave perturbations to the uniform isotropic steady state. The aim is to predict the critical parametric conditions over which the uniform isotropic steady state loses stability to plane wave perturbations, and the onset of pattern formation and turbulence.

2 Model

The kinetic model for the suspension system is based on some governing equations describing how the self-propelled rod-like particles interact with each other dynamically. Each particle is described by the configuration variables: its center of mass position $\boldsymbol{x}$ and orientation vector $\boldsymbol{p}$ such that $\boldsymbol{p} \cdot \boldsymbol{p} = 1$

2.1 Particles Density

The time-dependent probability distribution function, $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{p}, t)$ represents the number density with position $\boldsymbol{x} \in \mathrm{T}^d$ and orientation $\boldsymbol{p} \in S^{d-1}$, where *d* is the dimension of the space the fluid occupies. This model will be considered in 2-dimensional space, i.e., *d = 2*. $\boldsymbol{\psi}$ evolves by the conservation Smoluchowski equation:

$$\partial_t \boldsymbol{\psi} = -\nabla_x \cdot (\dot{\boldsymbol{x}} \boldsymbol{\psi}) - \nabla_p \cdot (\dot{\boldsymbol{p}} \boldsymbol{\psi}); \qquad \nabla_p := (\boldsymbol{I} - \boldsymbol{p}\boldsymbol{p}^T)\partial_t \tag{1}$$

The translational and rotational fluxes are given by:

$$\dot{\boldsymbol{x}} = V_0\boldsymbol{p} + \boldsymbol{u} + D_T\nabla_x(\log\boldsymbol{\psi}) \tag{2}$$

$$\dot{\boldsymbol{p}} = (\boldsymbol{I} - \boldsymbol{p}\boldsymbol{p}^T)(\nabla_x\boldsymbol{u}\boldsymbol{p}) - D_R\nabla_p(\log\boldsymbol{\psi}) \tag{3}$$

The translational velocity is a linear combination of the swimming speed V_0 in the direction $\boldsymbol{p}$, local fluid velocity $\boldsymbol{u}$ induced by other swimmers, and the translational diffusion where D_T is the coefficient of translational diffusion. The rotational velocity is a linear combination of Jeffery's term for the rotation of a rod by a linear flow and the rotational diffusion where D_R is the coefficient of rotational diffusion.

2.2 Navier-Stokes Equations for Fluid Velocity and Pressure

The local velocity of the fluid induced by other swimmers $\boldsymbol{u}(\boldsymbol{x}, t)$ and the fluid pressure q, are related through the Navier-Stokes equations at the low limit of Reynold's Number:

$$-\mu\nabla_x^2\boldsymbol{u} + \nabla_x q = \nabla_x \cdot \Sigma^a, \qquad \nabla_x \cdot \boldsymbol{u} = 0; \tag{4}$$

$$\Sigma^a = \sigma_0 \int_{S^{d-1}} \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{p}, t) \left(\boldsymbol{p}\boldsymbol{p}^T - \frac{1}{d}\boldsymbol{I}\right) d\boldsymbol{p} \tag{5}$$

Where μ is the fluid viscosity. Σ^a $(\boldsymbol{x}, t)$ is the active stress exerted by the particles on the fluid, and it's the orientational average of the force dipoles exerted by the particles on the fluid, where the sign of the coefficient σ_0 is the sign of the dipoles: $\sigma_0 > 0$ for pullers and $\sigma_0 < 0$ for pushers.

Note that Reynold's number, the dimensionless parameter $Re = \frac{V_0 l}{\gamma}$ where γ is the kinematic viscosity of the fluid at the appropriate temperature, and l is the characteristic length of each of the rod-like particles. Since l is infinitesimally small, then Re goes to the lower limit and gets rid of the time-derivative term of the Navier-Stokes equation for our model.

2.3 Linear Stability Analysis

The stability of the system is studied under small perturbations from uniform isotropy. A method of normal modes is employed to study the oscillations and instabilities of the dynamical system.

2.3.1 Nondimensionalization

The common variables used in the previous set of governing equations are nondimensionalized to produce a reduced number of dimensionless parameters crucial to the following analysis. Letting N denote the number of particles in the system and L the characteristic length of the periodic box in which the particles are suspended. The nondimensionalized variables are:

$$\boldsymbol{\psi}' = \frac{L^d}{N}\boldsymbol{\psi}, \qquad \boldsymbol{x}' = \frac{2\pi}{L}\boldsymbol{x}, \qquad t' = \frac{|\sigma_0|N}{L^d\mu}t, \qquad \boldsymbol{u}' = \frac{2\pi\mu L^{d-1}}{|\sigma_0|N}\boldsymbol{u}$$

Using the chain rule, to find all the new expressions, the set of governing equations becomes:

$$\partial_{t'}\boldsymbol{\psi}' = -\nabla_{x'}(\partial_{t'}\boldsymbol{x}'\boldsymbol{\psi}') - \nabla_p(\partial_{t'}\boldsymbol{p}\boldsymbol{\psi}') \tag{6}$$

$$\partial_{t'}\boldsymbol{x}' = \beta\boldsymbol{p} + \boldsymbol{u}' - D_T{}'\nabla_{x'}(\log\boldsymbol{\psi}) \tag{7}$$

$$\partial_{t'}\boldsymbol{p} = (\boldsymbol{I} - \boldsymbol{p}\boldsymbol{p}^T)(\nabla_{x'}\boldsymbol{u}'\boldsymbol{p}) - D_R{}'\nabla_p(\log\boldsymbol{\psi}) \tag{8}$$

$$-\nabla_{x'}^2\boldsymbol{u}' + \nabla_{x'}q' = \pm\int_{S^{d-1}}\nabla_{x'}\boldsymbol{\psi}'(\boldsymbol{x},\boldsymbol{p},t)\left(\boldsymbol{p}\boldsymbol{p}^T - \frac{1}{d}\boldsymbol{I}\right)d\boldsymbol{p}, \quad \nabla_{x'}\cdot\boldsymbol{u}' = 0; \tag{9}$$

The parameters of interest have been reduced to three dimensionless parameters: Translational diffusion, rotational diffusion and the swimming speed, respectively:

$$D_T' = \frac{4\pi^2\mu L^{d-2}}{|\sigma_0|N}D_T, \qquad D_R' = \frac{\mu L^d}{|\sigma_0|N}D_R, \qquad \beta = \frac{2\pi\mu L^{d-1}}{|\sigma_0|N}V_0$$

This nondimensionalization varies slightly from that which is commonly used in literature, but it is more desirable since it allows us to examine the swimming speed in the case for which ($V_0 = 0$) while maintaining continuity. The parameter β also contains information regarding the ratio of swimming speed to the active stress magnitude and particle concentration. Also, note that in (9) the active stress coefficient has been dropped and replaced with a unit magnitude that retains the sign of the force dipole exerted by the particles on the fluid: +1 for puller particles and -1 for the pusher particles

Dropping the prime notation, our system (6)-(9) can be expressed more concisely by the equations:

$$\partial_t\boldsymbol{\psi} = -\beta\boldsymbol{p}\cdot\nabla_x\boldsymbol{\psi} - \boldsymbol{u}\cdot\nabla_x\boldsymbol{\psi} - \nabla_p[(\boldsymbol{I} - \boldsymbol{p}\boldsymbol{p}^T)(\nabla_x\boldsymbol{u}\boldsymbol{p})\boldsymbol{\psi}] + D_T\nabla_x^2\boldsymbol{\psi} + D_R\nabla_p^2\boldsymbol{\psi} \tag{10}$$

$$-\nabla_x^2\boldsymbol{u} + \nabla_x q = \pm\int_{S^{d-1}}\nabla_x\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{p},t)\left(\boldsymbol{p}\boldsymbol{p}^T - \frac{1}{d}\boldsymbol{I}\right)d\boldsymbol{p}, \qquad \nabla_x\cdot\boldsymbol{u} = 0; \tag{11}$$

2.3.2 Linearization

In order to linearize the last system of equation to measure deviations about the swimmer density $\boldsymbol{\psi}$ from the uniform steady state, first we consider the normalization of the distribution function as follows:

$$\int_{\mathrm{T}^d} d\boldsymbol{x} \int_{S^{d-1}} d\boldsymbol{p}\, \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{p}, t) = 1 \tag{12}$$

The system's isotropic steady state, $\boldsymbol{\psi_0} = \frac{1}{2^{d-1}\pi}$ and $\boldsymbol{u_0} = 0$ will serve as uniform equilibrium for linearization. Applying a similar analysis of the relative entropy of the system to that of Saintillan and Shelly, 2008[1] to our model, we can see that for the puller particles ($\sigma_0 > 0$) the entropy is driven down by both diffusive processes and the negative of the active stress exerted by particles. We expect puller suspensions to always decay to isotropy. Pusher suspensions have been simulated [1]-[3] to show that complex nonlinear patterns and fluctuations in particle alignment and concentration arise in certain parameter regimes. Hence, we focus our analysis on pusher suspensions ($\sigma_0 < 0$).

We further simplify (10) by considering $\nabla_x \cdot \boldsymbol{u} = 0$, $|\boldsymbol{p}|^2 = 1$ and vector calculus methods to simplify the expression:

$$\nabla_p[(\boldsymbol{I} - \boldsymbol{pp}^T)(\nabla_x \boldsymbol{up})\boldsymbol{\psi}] = -d\boldsymbol{\psi}\boldsymbol{p}^T \nabla_x \boldsymbol{up} + (\nabla_x \boldsymbol{up}) \cdot (\nabla_p \boldsymbol{\psi}) \tag{13}$$

We then consider solutions ($\boldsymbol{\psi}$, $\boldsymbol{u}$) very close to the isotropic steady state; for very small ϵ, we substitute $\boldsymbol{\psi} = \boldsymbol{\psi_0} + \epsilon\boldsymbol{\psi}$ and $\boldsymbol{u} = \boldsymbol{u_0} + \epsilon\boldsymbol{u}$ into our system of equations (10)-(11) after the simplification (13), take the first derivative of all expressions of the PDEs with respect to ϵ, and take $\epsilon = 0$. This results in getting rid of nonlinear terms, linearizing our system about the isotropic steady state (recall $d = 2$):

$$\partial_t \boldsymbol{\psi} = -\beta \boldsymbol{p} \cdot \nabla_x \boldsymbol{\psi} + 2\boldsymbol{p}^T \nabla_x \boldsymbol{up} + D_T \nabla_x^2 \boldsymbol{\psi} + D_R \nabla_p^2 \boldsymbol{\psi} \tag{14}$$

$$-\nabla_x^2 \boldsymbol{u} + \nabla_x q = -\frac{1}{2\pi} \int_{S^1} \nabla_x \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{p}, t) \left(\boldsymbol{pp}^T - \frac{1}{2}\boldsymbol{I}\right) d\boldsymbol{p}; \qquad \nabla_x \cdot \boldsymbol{u} = 0 \tag{15}$$

2.3.3 Eigenproblem

We set up the eigenproblem by using the Fourier transform of our dependent variables in the conservation equation (14). The general solution to arrive at should be a linear combination of exponential eigenfunctions, and through examining the eigenvalues of the solution we can find parameter ranges through a dispersion relation that guarantee the exponentials won't decay, thus causing instabilities. If the solution takes the general form $\sum_d C_k \boldsymbol{\psi}_k e^{\lambda_k t}$. Considering the stability in $e^{\lambda_k t}$, if Re $(\lambda_k) > 0$ the perturbations in the system grow, while the imaginary component stays bounded by the unit circle causing instabilities in the system and formation of patterns. If Re $(\lambda_k) < 0$ the perturbations decays and the system enters the isotropic steady state where the change in the system with respect to time, or in the case of our system the fluid velocity norm, stabilizes to zero and the particles exhibit no directional preference. Denoting the Fourier transform in $\boldsymbol{x}$ by $\hat{g}(\boldsymbol{k}, \boldsymbol{p}, t) \coloneqq \int_{\mathrm{T}^2} g(\boldsymbol{k}, \boldsymbol{p}, t) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$ and defining $\overline{\boldsymbol{k}} \coloneqq \frac{\boldsymbol{k}}{|\boldsymbol{k}|}$ where $\boldsymbol{k}$ is the spatial mode (or wave number) for each of the components for $\boldsymbol{x}$ (i.e., $\boldsymbol{k} = ke_x$ for the x component and $\boldsymbol{k} = ke_y$ for the y component). Choosing coordinates $\boldsymbol{k} = ke_x$ and $\boldsymbol{p} = cos\theta e_x + sin\theta e_y$ and substituting $\widehat{\boldsymbol{\psi}}$ in (14) we get:

$$\partial_t \widehat{\boldsymbol{\psi}} = -ik\beta cos\theta \widehat{\boldsymbol{\psi}} + \frac{1}{\pi} cos\theta sin\theta \int_0^{2\pi} \widehat{\boldsymbol{\psi}} cos\theta sin\theta d\theta + D_T k^2 \widehat{\boldsymbol{\psi}} + D_R \partial_{\theta^2} \widehat{\boldsymbol{\psi}} \qquad (16)$$

Consider the ansatz $\widehat{\boldsymbol{\psi}} = \psi(k, \boldsymbol{p}) e^{\sigma t}$, where $\sigma \in \mathbb{C}$ and is called the growth rate. Defining $\lambda_k \coloneqq \sigma + D_T k^2$, equation (16) becomes an eigenvalue problem in the general form of $\lambda_k \psi_k = A\psi_k$. We assume that $D_R = 0$ for this analysis, and through manipulating the eigenproblem arrive at the dispersion relation for Re $(\lambda_k) \neq 0$:

$$\frac{\lambda_k \beta^2 k^2 + 2\lambda_k^3 - 2\lambda_k^2 \sqrt{\beta^2 k^2 + \lambda_k^2}}{\beta^4 k^4} = 1 \qquad (17)$$

Solving for the numerical relation between parameters σ and β is demonstrated in Figure 1. A similar calculation for $\boldsymbol{k} = ke_y$ shows that the y-direction eigenmodes are a $\frac{\pi}{2}$ in θ of the x-direction eigenmodes. In particular, the eigenfunctions are given by:

$$\boldsymbol{\psi}(\boldsymbol{x}, \theta, t) = c_x \psi_x(k, \theta) e^{ikx + \sigma t} + c_y \psi_y(k, \theta) e^{iky + \sigma t}; \qquad \sqrt{c_x^2 + c_y^2} = 1 \qquad (18)$$

Where $\psi_x = \frac{cos\theta sin\theta}{\sigma + D_T k^2 + ik\beta cos\theta}$ and $\psi_y = \frac{cos\theta sin\theta}{\sigma + D_T k^2 + ik\beta sin\theta}$

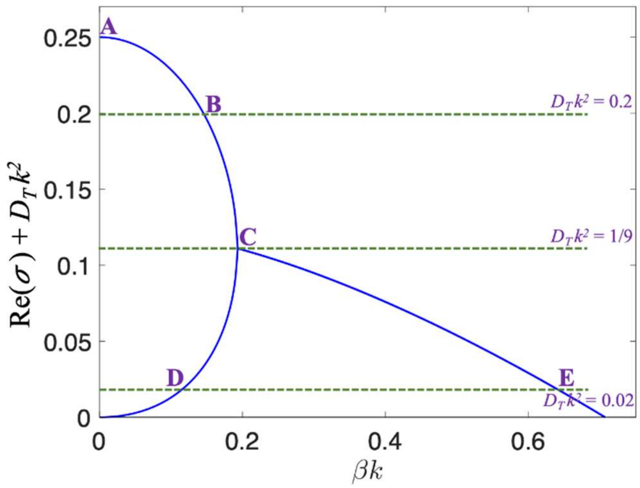


Figure 1: Dispersion relation in (17) between parameters $\mathrm{Re}(\sigma) + D_T k^2$ vs βk showing areas of the parameter regions where the instabilities occur, and wave perturbations grow over time. In the next section we will discuss results of the simulated nonlinear model within certain parameter regions of this plot and how particles density behaves over time.

3 Results

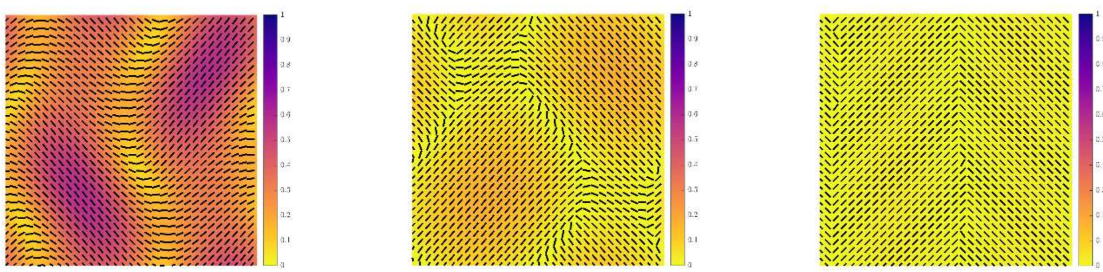
3.1 Simulation Method

In this section, we perform numerical simulations of the nonlinear kinetic model on MATLAB. The scalar order parameter (SOP) is the highest eigenvalue of the particle orientation tensor of the particles with position in the characteristic box of length L where the particles are suspended in a 2-dimensional area; the concentration of the SOP correlates to how much of the particles' orientation at said position agree with the mean orientation plotted. We evaluate the SOP in different regions in the parameter space provided by the dispersion relation in Figure 1.

For this section, we will focus on points around the bifurcation C in Figure 1. In particular, this simulation will focus on sufficiently small $|k|$ and rotational diffusion D_R; their values were set to $|k| = 1$ and $D_R = 0.001$. The bifurcation at C occurs on the intersection of two curves at the values of $\beta = \frac{\sqrt{3}}{9} \approx 0.19$ and $D_T = \frac{1}{9} \approx 0.11$. The simulation will be estimating these points since rotational diffusion, D_R is present in this model. For each phase while running the simulation, one of these two parameters will be fixed while the other varies to observe how the patterns change given sufficient time to estimate the state of the system as $t \rightarrow \infty$.

3.2 Swimming patterns

On the curve on the right-hand side of bifurcation C in Figure 1, as D_T increases the turbulence of swimming patterns dissipate as they approach the curve and enter the isotropic steady state as they pass the curve. Below the curve as shown in the SOP plotted in Figure 2(a) turbulence nonlinear patterns occur due to the instable state of the system. Regardless of the swimming speed β, the presence of the active stress coefficient σ_0 in the Navier-Stokes' equation (11) assumes the particles to change alignment and perpetuate the turbulence. Figure 2(b) shows the SOP of the particles as D_T increases and the system approaches bifurcation C. The concentration of the SOP decreased. The system stabilizes in Figure 2(c) as $D_T > \frac{1}{9}$ showing no change in fluid velocity and no directional preference.



(a) (b) (c)

Figure 2: Scalar order parameter plot (SOP) exerts with parameters $\beta = \frac{\sqrt{3}}{9}$, $D_R = 0.001$ and D_T increases with every $300t$ (a) $t = 490$ and $D_T = 0.07$ (b) $t = 1010$ and $D_T = 0.11$ (c) $t = 1414$ and $D_T = \frac{1}{9}$

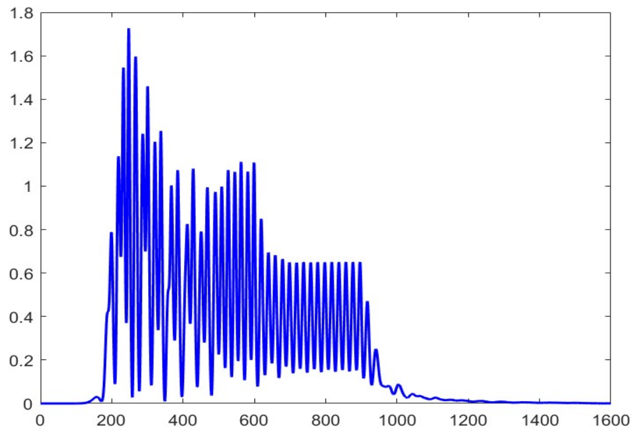
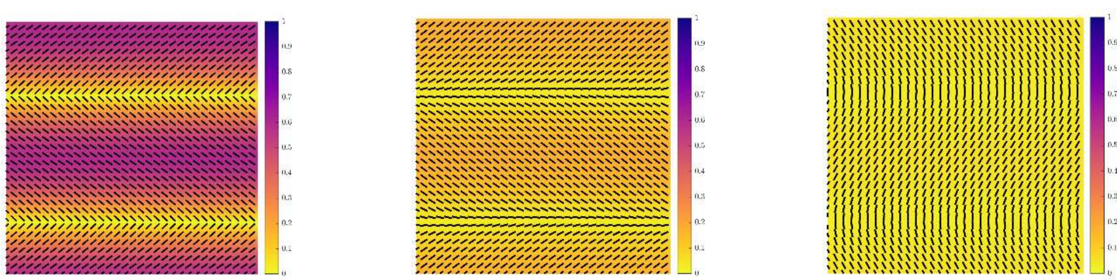


Figure 3: Nondimensionalized fluid velocity norm is plotted against the dimensionless time corresponding to the simulation run of Figure 2

3.3 Patterns of aligned stripes

On the curve on the left-hand side of bifurcation C in Figure 1, as β decreases patterns of aligned stripes start to form. Similar to that of the simulation run shown in Figure 2, the system in the simulation run of Figure 4 enters the isotropic steady as the parameter ranges passes the curves to the right of point C in Figure 1. Figure 4(a) shows aligned stripe-like patterns with high concentration in the SOP plot and regardless of the weaker swimming speed β the active stress coefficient σ_0 in the system ensures the particles align. By Figure 4(b) their alignment concentration becomes weaker and completely dissipates in the isotropic steady state.



(a) (b) (c)

Figure 4: Scalar order parameter plot (SOP) exerts with parameters $D_T = \frac{1}{9}$, $D_R = 0.001$ and β increases with every 300t (a) $t = 247$ and $\beta = 0.1$ (b) $t = 400$ and $\beta = 0.19$ (c) $t = 640$ and $\beta = 0.2$

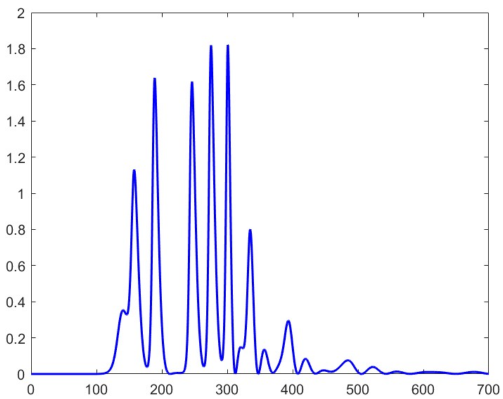


Figure 5: Nondimensionalized fluid velocity norm is plotted against the dimensionless time corresponding to the simulation run of Figure 4

4 Conclusion

In this paper, we developed a 2-dimensional kinetic model describing active suspension systems of rod-like swimmer particles and simulated it using MATLAB. The system was observed to form aligned stripe-like patterns and turbulence patterns in different parameter regions. These patterns formed in instable regions and as the model approached isotropic steady state, the change in the system with respect to time stabilized to zero with no directional preference.

For future work, I would hope to produce the continuation of the linear stability analysis, eigenproblem and simulation runs with variation of the rotational diffusion. I would also like to use the simulation to locate boundaries between alignment strips and swimming patterns and to explore zero swimming bifurcation and other boundaries of interest.

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References

[1] David Saintillan and Michael J. Shelley, Instabilities, pattern formation and mixing in active suspensions, *Physics of Fluids* 20 (123304), 2008.

[2] Christel Hohenegger and Michael J. Shelley, Stability of active suspensions, *Physical Review* 81 (046311), 2011

[3] David Saintillan and Michael J. Shelley, Active Suspensions and their nonlinear models, *C. R. Physique* 14 (2013): 497-517, 2013.