RESEARCH STATEMENT

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Introduction. I am an applied mathematician who specializes in solving problems originating at the interface of mathematics, biology, and physics. By taking advantage of the tools and data present in each field, I am able to develop models with the ability to capture the essential physics of a system yet be amenable to mathematical analysis. The unifying theme among all my research topics is interactions (interparticle, molecular, fluid-mediated, etc.) leading to the emergence of natural phenomena. My work consists of developing differential equations based models for biosystems and materials that predict the emergence of collective behavior and result in dramatic changes in the system’s effective properties. Techniques from applied analysis, PDEs, and scientific computation are used to uncover deeper understanding of the systems under consideration.

After the completion of my Ph. D. in Mathematics at Penn State University in August 2014 under the direction of Leonid Berlyand, I began a position as a Postdoctoral Research Associate with a dual appointment in the Department of Mathematical Sciences and Liquid Crystal Institute at Kent State University working with Peter Palffy-Muhoray and Xiaoyu Zheng. I have been fortunate enough to publish articles in leading peer-reviewed journals in both mathematics and physics such as SIAM Multiscale Analysis and Simulation, Journal of Mathematical Biology, and Scientific Reports. Throughout the past 7+ years, I have worked closely with physicists and mathematicians at Kent State, PSU, and Argonne National Laboratory to help explain experimental observation using mathematical analysis. I enjoy learning new techniques as well as facing new challenges in hopes of applying my results to better understand the world around us.

First, I will discuss my ongoing research in Mathematical Biology and Materials Science. Next, I will briefly introduce my thesis research on developing models for studying collective motion and effective properties in bacterial suspensions. Then I will conclude with a outline of my future directions of study and an overview of my long and short term goals to ensure the development of a successful research program. Most of all I want to convey my desire to be a leader in the field of applied analysis and take an active role in advancing the reputation of my future department.

Active Research. My current research can be divided into three main projects: (i) Dynamics of foam materials and liquid crystals, (ii) superconductivity and vortex patterns, (iii) chemically driven motion in microorganisms and social insects.

The first area involves work on two projects with Xiaoyu Zheng (KSU Math) and Peter Palffy-Muhoray (KSU LCI) concerning the developing a kinematic model for the evolution of a foam on the sphere (recently submitted [16]) and the development of a novel computational algorithm for studying the effect of an external chemical dye on the liquid crystal director field. The first project focuses on studying the dynamics of cells (foam bubbles) on the surface of a sphere. In the planar case the von Neumann-Mullins Law, \( \frac{dA}{dt} = K_0(n - 6) \), reveals a beautiful relation for how the cell area evolves based solely on the number of sides it possesses. Recently cited as a “historical touchstone” of material science [15] this relationship illustrates that the only stable solution will be composed of hexagonal cells. However, recent theory and experiments suggest that the dynamics are quite different on the surface of a three-dimensional object such as a sphere of radius \( R \) where there is an extra
component to the dynamics due to the surface curvature. Starting from first principles we obtain an effective von Neumann Law $\frac{dA_n}{dt} = K_0 [(n - 6) + \frac{12A_n}{4\pi R^2}]$ containing an additional term. In stark contrast to the planar case exhibiting linear behavior, the additional term leads to exponential growth and decay of the cells. This is verified by our novel computational algorithm accounting for curvature driven motion of the cell boundaries (see Fig. 1(a)). In addition, by accounting for topological changes such as cell removal and cell boundary exchanges, our model is capable of simulating the longtime dynamics of the cell from any number of initial cells until finally one remaining cell envelops the entire sphere. The second project is in its infancy and we will use the computational model for the foam on the sphere to handle the evolution of the director field ($\mathbf{n} \in S^2$) in the presence of harmful chemicals.

The second area of ongoing research focuses on a project with collaborators outside KSU studying the interplay between physics and mathematics in superconducting materials (with L. Berlyand (PSU), V. Mityushev (U. Krakow), and V. Vinokur (Argonne)). In particular, this project is concerned with the distribution of vortices (points where superconductivity is lost) in a composite superconductor with small holes. The main focus is to study how the distributions of degrees varies (indicating trapped vortices). Our analysis confirms that nested subdomains of like degree form in the case of a periodic array of holes (see Fig. 1(b)). The main result was that our model predicted that the interface between the subdomains becomes more fractal with increasing randomness in the array of holes [13, 12]. This fundamentally changed the way we look at the standard magnetic field temperature plot for type-II superconductors in the presence of holes and is currently being considered experimentally at Argonne National Lab.

The final area consists of two projects. The first involves the study of collective motion induced by chemical signaling in bacterial suspensions (with C. Xue (OSU)). We have developed a first principle model for a bacteria suspension which takes into account the numerical efficiency of the point dipole approach developed within my Ph. D. dissertation (described later) and adds an additional contribution due to chemical signaling. The result is the formation of mesoscopic aggregates of bacteria which move with the fluid. The ultimate goal is
Figure 2. Left: Pushers like E. coli bundle flagella to propel forward (outward force dipole). Pullers like the algae Chlamydomonas swim via a breast stroke type motion. (a) Effective viscosity vs. concentration [1]. (b) Effective viscosity vs. volume fraction for interacting dipoles [2]. Simulations performed on GPUs at Argonne National Laboratory.

to study the case of a strong external signal at the center of the domain in hopes of finding spiral formations of aggregates that match recent experimental observation [20].

The second project involves a single author project interested in investigating the collective dynamics observed during ant foraging and raiding. In nature ants perform a random walk in search of food. Once food is found ants returning to the nest with food begin to lay a trail consisting of a chemical gradient to direct other ants toward the food. Upon returning to the nest they become foragers once again, but now follow the chemical trail to efficiently recover the needed resources. This entire cycle of foraging and returning is referred to as a raid. The basic idea is to start with an individual based ODE model derived from first principles (balance of forces) coupled to a reaction-diffusion PDE for pheromone deposition that has shown striking collective features similar to recent experiment observation [17]. Namely, self-organization of the ants into a collective state exhibiting local traffic flow consisting of the formation of three lanes: two outside lanes for foragers and one central lane for ants returning with food (see Fig. 1(c)) [18]. Currently, I am investigating the macroscopic behavior using a continuum PDE model for the ant density derived via a kinetic theory approach [19]. The novel feature in the derivation is that each population (foragers and returners) obeys different dynamic equations resulting in the presence of two coupled continuum PDEs for each density instead of one for the entire population. The immediate plan is to perform numerical simulations on the macroscopic model to compare it with the individual based model. If the results are favorable, I will then proceed to use techniques from PDE theory to analyze the existence, uniqueness, and regularity of the system.

Thesis Research. Throughout this section I will briefly review my thesis work on developing novel models for bacterial suspensions in order to explain experimental observations of effective changes in the rheological properties of a suspension due to the onset of collective behavior. Such suspensions of self-propelled microscopic particles, such as swimming bacteria Bacillus subtilis, exhibit collective motion leading to remarkable experimentally-observable macroscopic properties.
Effective viscosity of bacterial suspensions. The first stage of this project involved developing and analyzing a coupled PDE / ODE model for a suspension of interacting bacteria to identify the physical mechanisms responsible for the experimentally observed decrease in viscosity (see Fig. 2(b)) [2]. To account for pairwise hydrodynamic interactions as well as excluded volume type interactions a simple model is employed where a bacterium is represented as a point force dipole with size (introduced through the use of a short-range Lennard-Jones type repelling potential) and shape. Direct particle simulations were performed in parallel on GPUs, which allowed for the computation of the viscosity as a longtime average of the instantaneous viscosity for many realizations (see Fig. 2(a)). The numerical results showed good qualitative agreement with experiment through a full range of concentrations.

Formal analysis on a corresponding continuum (Liouville) equation for the evolution of the particle distribution function for bacterial positions and orientations uncovers an explicit asymptotic formula for the effective viscosity due to interactions in terms of known physical parameters [11]. This formula reveals the physical mechanisms responsible for the striking effective viscosity experimental observation. Namely, self-propulsion, elongated shape, and hydrodynamic interactions are required to observe the dramatic decrease in the effective viscosity. In a subsequent work [3], it is shown that the coupled PDE/ODE system introduced admits unique particle trajectories for all time given non-overlapping initial data.

The final portion of my thesis involved understanding the nontrivial spatiotemporal correlations emerging in the course of collective swimming in suspensions of swimming bacteria [7]. Specifically, we were able to capture the qualitative effects on the correlation length and correlation time of a bacterial suspension. Our experiments and simulations suggest that self-organization in bacterial suspensions is governed by two competing mechanisms: short-range collisions and long-range hydrodynamic interactions. While collisions tend to increase the correlation length of collective motion, hydrodynamic interactions result in its decrease in the local order. This work exemplifies the delicate balance between various physical mechanisms governing collective motion in bacterial suspensions and provides important insights into its mesoscopic nature.

Figure 3. Mean particle velocity vs. concentration (blue) and correlation length vs. concentration (green) in (a) experiment [5] and (b) simulation [7]. (c) Velocity/vorticity field for different swimming speeds, \( V_0 \). a-b experiment and c-d simulation.
Research Plan (Next 3 years). Self-organization is a fascinating process manifested in biological systems that results in interesting physical phenomena such as enhanced movement/mixing, efficient foraging, and striking effective properties in materials. While these striking features can readily be observed, a complete understanding of the physical interactions at the microscale leading to their emergence is lacking. My research going forward concerns the theoretical development and analysis of novel models for biosystems and biomaterials capable of exhibiting collective phenomena. All forms of collective motion found in nature (e.g., swarming, swimming, insect foraging, etc.) exhibit multiple characteristic scales requiring a multilevel approach to develop a basic understanding of the underlying chemical/physical mechanisms needed for the onset of self-organization.

The proposed research will follow the general strategy of first introducing minimal individual based (PDE/ODE) models taking into account interactions at the microscale. Using simulations to develop intuition, I will show each system results in a phase transition to a collective state. Once established, I will derive the limiting kinetic PDE equations amenable to analysis that govern the evolution of the probability density of the system at the macroscale. The proposed research consists of two central themes:

Area (A) Active bioystems. The focus of this area is to understand the fundamental chemical and physical mechanisms at the microscale that contribute to the formation of mesoscopic structures and the resulting benefits to the system. The two fundamental systems under consideration are (i) bacterial suspensions and (ii) social insects. The goal of the first project is to rigorously show that while chemotaxis can bring bacteria together, self-organization occurs primarily due hydrodynamic interactions and collisions. The second project seeks to analyze the effects of the environment, competition between colonies, and predators on the formation of trails and the resulting local lane formation.

Area (B) Biomaterials. The objective of this area consists of using knowledge of relevant chemical/physical mechanisms for self-organization obtained from Area (A) to provide insight into materials that benefit from interaction with biological systems. Two primary applications will be considered: transport in microtubule networks present in all eukaryotic cells and so-called living liquid crystals consisting of bacteria submerged in a non-toxic liquid crystal environment. These systems have wide ranging applications including vascular network transport and the living liquid crystal can be used to detect the presence of harmful chemicals in a system.

This research will address fundamental questions arising in biology and biomaterials. Having studied Mathematical Biology and PDEs for my Ph.D. research and Materials Science during my postdoc I am positioned to develop models for biomaterials from a unique perspective. Potential applications of the proposed work include insight into the physical mechanisms responsible for self-organization as well as studying novel materials exhibiting enhanced functionality due to the interaction between the material and a biological system. The proposed work will also have a direct impact on the education of students. This research is accessible to both undergraduate and graduate students allowing for mentoring opportunities and student support from grants. Since this work is accessible, I would also like to
continue to organize math exploration days for local high school students to ignite their passion to pursue mathematics in their future studies. In addition, I would like to develop a special topics undergraduate course introducing the fundamentals of mathematical biology and materials science. This will consist of developing intuition for modeling biosystems as well as learning the computational skills needed to study complex systems with many interacting components. This proposed research has been submitted in the form of a grant proposal for consideration of the National Science Foundation Division of Mathematical Sciences.

REFERENCES


