Multiscale Analysis of Pattern Formation in Active Biological Systems

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Summary

Active biological systems exhibit new forms of order, self-organization and phase transitions that are only now beginning to be understood by scientists. These systems, such as biopolymer networks, bacterial suspensions, operate far from equilibrium and actively dissipate energy to shape and maintain large-scale coherent structures. We have been studying these phenomena mathematically with a focus on the multiscale nature of the self-organization process.

Understanding self-organization in active systems is of paramount importance for basic science and technology. For the past year we have been studying a range controlled biological systems through quantitative methods of physics and applied mathematics. The unifying feature of all of these systems is the interaction of different spatiotemporal scales that spontaneously conspire to produce long-range persistent order.

Phase transitions in biopolymers.

Our initial focus was on the understanding of the spontaneous transition to order in mixtures of microtubules and molecular motors. These transitions, observed *in vitro,* were for the first time convincingly explained by a stochastic model proposed by Igor Aronson (ANL/MSD) and Lev Tsimring (UCSD). This model is based on a master equation describing the probability distribution of biofilaments with a given orientation. The crucial component is the interaction kernel that captures the dynamics of filament *alignment* via irreversible "collisions" mediated by molecular motors. The kernel is constructed from a microscopic model of filament-motor interactions that accounts for their

anisotropy. This anisotropy is ultimately responsible for the range of coherent patterns these mixtures exhibit.

In the past year we have furthered the understanding of the biofilament self-organization process. We have extended our analysis to systems of actin filaments – the building block of the cellular cytoskeleton. Through this work we have illuminated the role of passive cross-linkers (e.g., inactive motors) in the formation of *bundle* states in actin networks (Fig. 1) that were previously observed experimentally. Furthermore, we have shown that a microscopic model of actin-motor interactions predicts the onset of buckling instability in the filaments, whose role in the large-scale structure of the cytoskeleton is yet to be understood.

Clustering dynamics.

The systems of equations describing the behavior of biofilament systems are highly nonlinear, nonlocal (integro-differential) and singular. We overcome these challenges by developing new applied mathematical techniques. In particular, in the study of the limiting case of the spatially homogeneous master equation we have developed a systematic perturbative technique that

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reduces the corresponding stationary equation to a Hamiltonian system, whose solutions can be explicitly obtained in terms of classical *Abelian functions*.
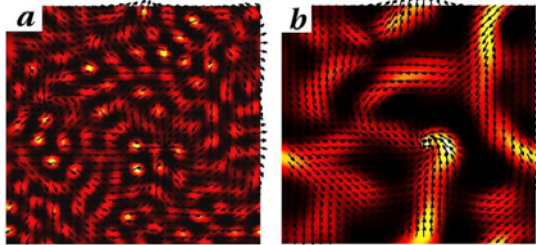

Fig. 1: Simulation: filamentation (right) occurs in the presence of crosslinkers, coupling motion of polymer rods to the order parameter (orientation).

Even this homogeneous master equation exhibits nontrivial dynamical behavior – clustering and bifurcation. We feel that the use of the deep analytical apparatus of function theory can shed significant light on this process. Recently, Los Alamos researchers applied the same model to describe social opinion dynamics, making our results relevant in an altogether different area of self-organization.

Bacterial suspensions.
Our initial results in protein alignment led us to investigate similar behavior in suspensions of swimming bacteria. These bacteria align via hydrodynamic interactions due to the flows their motion induces. They form clusters and other patterns, such as vortices, exhibiting rich multiphase behavior reminiscent of turbulent flow.

Experimental studies on bacterial populations in a thin liquid layer were conducted in collaboration with the Material Sciences Division. The observed alignment process is illustrated in Fig. 2.
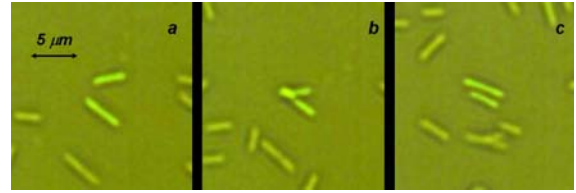

Fig. 2: Photographs of alignment of a bacterial pair (highlighted) via hydrodynamic interactions.

These experimental results prompted us to investigate mathematical models of hydrodynamic alignment and the reduced effective viscosity of suspensions of self-propelled particles. These efforts have already led to interesting results, such as a generalization of Einstein's classical result on the effective viscosity of a suspension of passive inclusions. This work also involves several students, fulfilling an important educational aspect of our project.

Future: mathematics of biomaterials.
We believe that the study of biomaterial systems is a fruitful arena for collaboration between physicists and mathematicians. In the end, it leads to new mathematics and new science.

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