RESEARCH STATEMENT
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Areas of interest: Aggregation, Chemotaxis, Asymptotic methods, Singularly perturbed problems, Similarity

Introduction

Modeling and solving physically-based problems has always been my main research interest. I am particularly partial to problems whose solution involves analytical tools such as asymptotic expansions, multiple scales, or similarity solutions. While the analysis cannot usually be entirely free of numerical solutions, I think that by striking a balance between the analysis and the numerical, better-resolved and more informative results are obtained.

Prior to working on my PhD thesis, I had worked on two similar shape-optimization problems in elastic theory [7, 6]. These problems involve an ODE eigenvalue problem with a singular boundary condition that makes it difficult to solve using standard methods. Using an analytic solution the system can be reduced so that even simple shooting works. I would seem that solving similarly singular problems with this method is possible and could be interesting.

For my PhD thesis, I worked on homogeneous aggregation[5]. I derived a physical model that encompasses two previously accepted, but contradictory models of cluster growth. I then solved the resulting system using distinguished limits that correspond to three phases of the solution. Modeling homogeneous aggregation and solving the resulting equations has both interesting mathematical content and important industrial motivations and applications, from the deposition of monolayers on silicon wafers to the precipitation of acid out of fumes in furnaces, to name two examples. I would like to continue working on these problems in the next few years.

Recently, I have derived a new particle-based numerical solver for solving conservation PDE [9, 8]. This new method uses a similarity solution to construct an interpolation between the particles that "carry" the solution and uses this interpolation to guarantee exact conservation of the numerical solution. This method could be extended to higher-order systems and higher space dimensions. I am interested in using the method for exploring physical problems that need the combination of its unique benefits. One such problem is Burger's equation with a convolution source term for which it is conjectured that the solution space forms a fractal set.

I have currently been looking at problems related to bacterial chemotaxis, the way in which bacteria react to local chemistry and alter their motion. I would like to gain insight and understanding on the diversity in chemotactic methods: Different bacteria use qualitatively different mode of locomotion. For example, E. Coli makes use of the "run-and-tumble" mechanism, whereas many marine bacteria use "run-and-reverse" without "tumbling" at all. Similarly, there is evidence that some bacteria's run-lengths have a Poisson distribution others have "fat-tailed" distribution of run-lengths. Are these differences arbitrary? Do they point to different degrees of adaptation? Or are they each best suited for the specific habitat of the bacteria? I would like to learn more about these and other related problems.

In the following sections these topics are presented in greater detail.

1 Bacterial Chemotaxis

The understanding of bacterial motion is crucial for our understanding of diseases and the carbon cycle in the ocean, to name two immediate examples. In the seminal Berg and Brown paper [1] they introduce the notion of "run-and-tumble" in the context of the motion of E. Coli. This type of motion consists of two phases: a "run" phase in which the motion is nominally straight, followed by a "tumble" phase in which the direction is randomized. What makes the motion interesting is that the *lengths* of the runs are increased when nutrient concentration is increasing. Therefore, on average, bacteria will move towards higher nutrient concentration.

A number of papers in the literature have studied the motion of E. Coli, with various configurations, but most of them maintain the run-and-tumble model. Marine bacteria often have a different locomotion model: run-and-reverse. This is not as counter-productive as it might seem at first: These bacteria are much smaller than E. Coli and therefore the thermal fluctuations in direction are much larger. In addition, the nutrients in the oceans are small and transient. Reversing when the conditions are deteriorating is a fast way to return to the localized nutrients.

Together with Professor Roman Stocker (Environmental Engineering, MIT) I am currently looking at ways of quantifying the difference between run-and-tumble and run-and-reverse using both analysis and experiment. While Stocker is setting up experiments for measuring the particulars of the chemotactic motion of the bacteria, I will provide the mathematical basis for the modeling of the process. Using a population-based model, run-and-reverse can be written as a Fokker-Plank equation for the density of bacteria $n(x, \theta, t)$ at location x, traveling in direction θ, at time t:

$$n_t - D\Delta_\theta n = -v\theta \cdot \nabla_x n - \frac{1}{T}n + \frac{1}{T}n(x, -\theta, t). \tag{1}$$

Here, D is a rotational diffusion constant, Δ_θ is the diffusion operator on the direction vector θ, v is the (constant) speed of motion, and T controls the distribution of reversals. The Fokker-Plank equation above is written for run-lengths distributed according to a Poisson process.

The problem is well-suited for multiple-scale methods and asymptotics. At first, I will find a prediction for the average "foraging" rate of a bacterium given the parameters of its chemotaxic motion. I then intend to compare efficiencies of different bacteria in different environments to determine whether the models are optimized for their environment.

2 Particle methods for Conservation Laws

Conservation PDEs are natural models for the evolution of continuum quantities, which can describe shocks and rarefaction behavior. Their mathematical properties include global and local conservation, the presence of similarity solutions, and the existence of characteristic curves.

I have developed a particle-based numerical method for solving one-dimensional, scalar conservation PDE of the form

$$u_t + f(u(x))_x = 0, \tag{2}$$

for a broad class of functions f. Like all particle-based methods, the data is located on a moving cloud of points, the "particles", which moves with their characteristic velocity. The method interpolates between neighboring particles with a similarity solution, and uses the interpolation to add or remove particles in a conservative manner. The resulting method is variation diminishing, entropy non-increasing, and, naturally, exactly conservative. Even after shocks are formed, it had second-order accuracy.

I am currently interested in an application of the method in its current form: Burger's equation with a convolution term

$$u_t + uu_x = u * \sin x, \quad x \in [0, 2\pi] \tag{3}$$

and periodic boundary conditions is a simple model for pressure waves in a thin tapered tube. Professor Ruben Rosales (MIT, Mathematics) has conjectured that the stable solutions of equation (3) form a fractal set due to

KAM theory. I am looking for numerical evidence for this by examining the stability of solutions along different segments of function space. The analytical solution has constant energy, except in shocks where it is decreasing. Other numerical methods that can deal with shocks introduce numerical dissipation, and spectral methods fail when shocks arise. The properties of my particle method make it well-suited for examining the long-term solutions of (3). Finding numerical evidence for a fractal solution set of such a basic physical problem would be unusual and exciting, which explains why I find this problem appealing.

3 Homogeneous Aggregation

The coalescence of small particles (monomers) into large aggregates (clusters) is a fundamental natural process. First-order phase transitions associated with condensation in a gas/liquid system [16, 17], solidification of melts, and precipitation out of a liquid solution [11, 13, 14, 15] are basic examples.

Under certain assumptions, the aggregation process can be approximated as an advection PDE with an integral term:

$$\partial_t r + \partial_n(\eta n^{\frac{1}{3}} - 1)r = 0 \text{ in } n > 0, \qquad \eta n^{\frac{1}{3}} r \to \mathrm{e}^{-\frac{1}{\eta^2}} \text{ as } n \to 0^+,$$
$$\eta(t) = \eta(0) - \int_0^\infty n r(n,t)\,\mathrm{d}n.$$

For the sake of clarity, all the physical constants and numerical factors have been set to 1. Remaining are the important variables: $r(n,\, t)$ is the density of clusters of size n at time t, and $\eta(t)$ is the super-saturation, the scaled amount by which the monomer density is greater than the saturation density. The usual model is valid for small values of the super-saturation. This smallness of η is used extensively in the asymptotic solution. In my PhD thesis [5], I derive a physical model that encompasses both the Becker-Döring model of cluster growth (which is based on surface reactions) and the Lifshitz-Slyozov growth rate (which is based on diffusion limited growth). The resulting PDE is then solved asymptotically using three distinguished limits which correspond to three "eras" of the solution: *creation*, during which most of the clusters are formed; *growth*, wherein the clusters all grow in a narrow distribution of sizes and no new cluster form; and *coarsening*, in which the larger clusters grow at the expense of the smaller ones and the distribution converges to a similarity solution.

There are several interesting and challenging related problems that I would like to solve in the near future. An example of such a problem is that of homogeneous aggregation with a *decreasing* temperature. A preliminary result [4] shows that after a time-lag, a short burst of nucleation lowers the super-saturation, which has risen due to the cooling. Further cooling only causes the resulting clusters to grow.

The solution of the simple quench will provide insight for another possible direction: aggregation in a flow of hot, humid gas onto a cold surface. This problem is inspired by the creation of Na_4SO_2 droplets in coal-fired power stations [2, 3]. One goal of this project is to find the amount of condensation that lands on the cold surface by the combined effects of direct condensation and droplet transport. In the boundary layer near the surface, droplets nucleate and grow, removing monomers from the vapor. The problem will involve examining the thermal and viscous boundary layer near the stagnation point and solving the coupled problem for flow speed, temperature, super-saturation and cluster size.

One last example is aggregation in a 2D medium. This problem is important for the silicon-industry (to name one), and is interesting mathematically due to the logarithmic solutions that arise in 2D diffusion. Experiments suggest that even when the "far field" super-saturation is kept constant, the growth of clusters stagnates long before the clusters encroach on one another [12, 10]. The logarithmic solutions that surround every cluster could explain the long-range interaction, and provide a path for solving this problem.

References

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