Patrick S. Eastham
Research Statement

Overview and Motivation

My research interests are applied and computational mathematics, fluid-structure interactions, particularly in biological, chemical and geo-physical applications, and complex fluids, particularly examining the effect of non-uniform viscosity on phoretic locomotion. I have skills in applying asymptotic and numerical methods for approximate solutions to problems too difficult to solve exactly.

My dissertation research is modeling precipitation reactions with a multiphase fluid-structure framework. Modeling efforts, motivated by experiments conducted by our collaborators, assist and inform experimental design. One large benefit of using this multiphase formulation is that structures can be generated dynamically, and the fluid-structure interaction effects are captured without any external input about locations of fluid-structure interfaces. There are several applications that I am looking into, including precipitate membranes, biofilms, and ultrasound-induced drug delivery.

My work on locomotion through complex fluids has stemmed from my time as a Research Assistant for Dr. Kourosh Shoele in FAMU-FSU's College of Engineering. We consider the case of a transported scalar field which affects a fluid's rheology. One way to model this is to have the fluid viscosity explicitly defined as a function of this scalar field, e.g. representing nutrient concentration or temperature. The particular application we are exploring is how ciliated swimming dynamics are affected by variable-viscosity fluids. More generally, this work can be applied to locomotion of heated active particles, where the temperature affects the viscosity. Our current research direction on this project is to investigate the influence of variable viscosity on different sources of drag on a particle, which is particularly important for particles in the Stokes limit, where inertial effects are negligible and all drag comes from viscous stress.

Finally, in a collaboration with a fellow graduate student, I am developing a numerical package to simulate wet granular material with the eventual goal of simulating sinkhole formation and collapse. We take a multiphase approach where a fluid phase and porous media phase (wet sand) interact. The fluid simulation is done with a finite element method, while the sand is simulated using discrete particles due to ambiguity in the literature for wet sand's constitutive law.

To assist in the above research goals, I have developed my own finite element package in the Julia programming language, called eFEMpart. It is developed with the intent to assist modelers, providing simple interfaces to define PDE systems. It is open-source, and accessible on Github.

In summary, I am interested in modeling and solving problems in complex fluids, in particular problems that involve dynamic coupling between physical processes, such as chemistry and fluid-structure interaction. To solve these problems, I employ several methods, both analytic and numerical. Where possible, model reductions to exactly-solvable cases are ideal, as they can provide inside into the more general cases. In cases where exact solution are not obtainable, asymptotic methods paired with numerical simulation can provide insight into specific parameter regimes. Wherever possible, I emphasize physical explanation obtained through mathematical analysis.

Multiphase modeling of precipitation reactions

One hypothesis for the "origin of life" is that the first biomolecules were formed in undersea hydrothermal vents. In this theory, passive, anisotropic diffusion across a membrane supports the transmembrane gradients necessary for the first biochemical molecules. An experimental approach to study this theory examines simpler systems in microfluidic reactors which allows for the controlled study of the prebiotic chemistry in hydrothermal vent chimneys. My research in this area has been to develop a multiphase model of precipitation reactions in microfluidic chambers.

The modeling challenges presented by this experiment involve a confluence of topics that have been studied before, namely ionic reactions, precipitation, passive diffusion through a membrane, and fluid-structure interaction. The particular combination of these aspects provided the opportunity for a new model that captures them all. One key challenge is that the "structure" in this problem is generated dynamically according to equations governing the chemistry. To address this, we chose to model the fluid-structure combination as a single multiphase material: one component "fluid" or solvent and one component "structure" or precipitate membrane. Such multiphase models have proven useful in a variety of complex-fluid applications, such as bacterial biofilms, tumor-growth, and biological membranes; their formulation is based on averaging momentum and stresses in separated, multi-component fluids.

Physically, the precipitating solid introduces additional forces on the fluid and eventually forms a membrane that is fixed in the flow due to adhesion with a substrate. A key challenge is that, in general, the location of the immobile membrane is unknown *a priori*. To model this situation, we use a multiphase framework with fluid and membrane phases; the aqueous chemicals exist as scalar fields that react within the fluid to induce phase change. To verify that the model exhibits desired fluid-structure behaviors, we make simplifying assumptions to obtain a reduced form of the equations that is amenable to exact solution. This analysis demonstrates no-slip behavior on the developing membrane without requiring fluid-membrane interface boundary conditions. The model has applications towards precipitate reactions where the precipitate greatly affects the surrounding flow, a situation appearing in many laboratory and geophysical contexts including the hydrothermal vent theory for the origin of life. More generally, this model can be used to address fluid-structure interaction problems that feature the dynamic generation of structures.
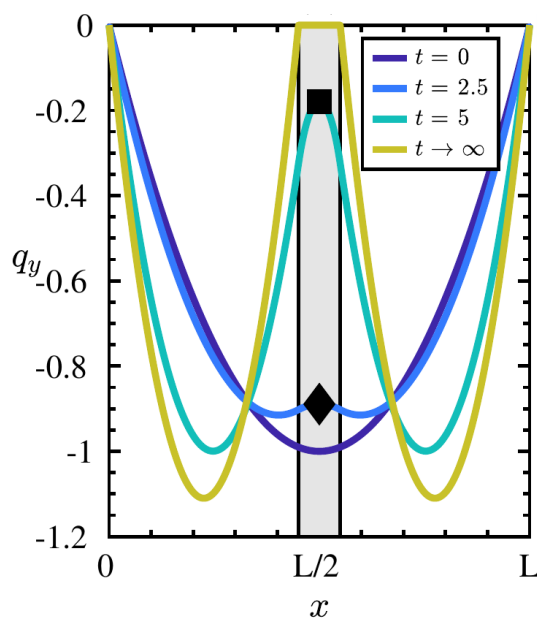

Figure 1: Developing 1D fluid flow where reaction region (gray) becomes more and more impermeable to fluid flow. The result is a dynamic transition from one- to two-channel flow[1]

Our results provide the expected fluid transition from single-channel flow without membrane, to a smooth transition to two-channel flow as the precipitation occurs (see Figure 1)[1] . Our current efforts are aimed at developing a robust numerical framework in order to simulate the governing equations in realistic geometries. These simulations will then be used directly to inform experiments, and aid experimental design, in particular with regards to interesting geometric effects.

Phoretic propulsion in complex fluids

The rate of nutrient intake at the surface of a swimmer not only affects the growth and reproduction rate of a microorganism, it can also modify the swimming speed of the organism or even enables an originally nonmotile system to start moving. The depletion of certain chemical agents from the surface of a microorganism or cell can also modify the material properties of fluid near the body by varying its effective viscosity and/or viscoelasticity; experimentalists have primarily used two compounds, methyl cellulose and Foxin, to systematically change the bulk viscosity of a medium. These are long-chain polymers and, while not being digestible, do suggest that other long-chained nutrients, such as complex sugars and proteins, could have a similar effect on bulk viscosity. This work assumes that nutrient-dependent bulk viscosity can be extended to a theoretical pointwise-dependence.
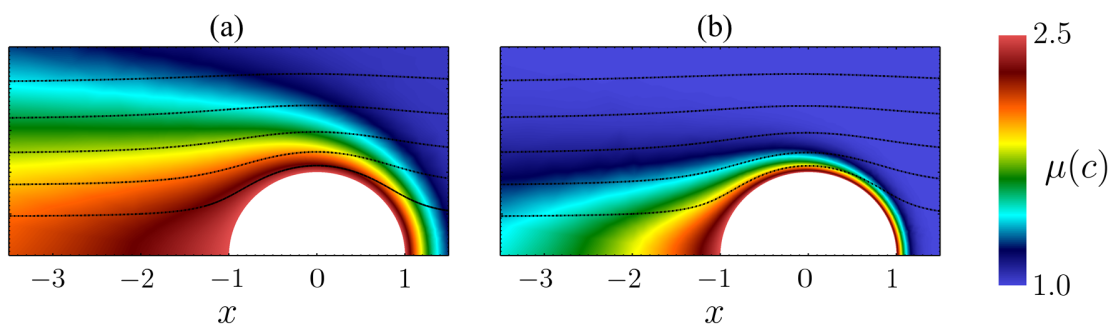

Figure 2: Viscosity field with two different nutrient-viscosity relationship parameters. The nutrient field is governed by advection-diffusion process past a squirmer particle. Because of the different viscosity fields, the above squirmers will have different swimming speeds.

The first step in analyzing this system was to employ the generalized Lorentz reciprocal theorem. This related the problem with nonuniform viscosity to the counterpart problem with uniform viscosity. Using a reciprocal theorem is a popular technique which has been successfully used in other fluids problems. By solving for the nutrient concentration in an advection-diffusion process around a free swimmer inside a fluid with uniform viscosity, we quantify the changes in the swimming velocity of the body when it moves in a fluid domain with nonuniform viscosity. To obtain the fluid velocity and stress, we also need to model the Stokes flow near the swimmer. This problem is primarily affected by viscous effects and the locomotion performance of the system only depends on the sequence of shapes used by the swimmer and not on the rate of shape changes. Solving for rate-independent flow field around a general free-swimming cell is challenging, especially when the swimmer shape is complex with many appendages like flagella or cilia. Different techniques have been proposed to study these kinds of systems. The most common are the boundary element method, simplified techniques like regularized Stokeslets, slender boundary theory, or the use of fundamental singularities to impose boundary conditions on the surface of a swimmer. Because they consider general shapes, these methods are inherently complicated to implement and generally are computationally expensive. One may use an alternative approach and approximate the geometry of a swimmer with a simplified canonical shape and solve the Stokes equation exactly in the uniform viscosity domain. This approach allows exploring the effects of a wide range of

controlling parameters on the hydrodynamics of force-free bodies at the limit of zero-Reynolds-number flow. This approach has been used successfully to study different mechanisms related to the hydrodynamics of ciliated swimmers.

To study systems with substantial nonlinearity, e.g resulting from a strong nutrient-viscosity coupling, one often requires to employ numerical techniques. To solve the problem considered here – a coupled variable-coefficient Stokes and Advection-Diffusion system – the Finite Element Method (FEM) is employed. The generality of this method allows us to examine complex domains that would be difficult to achieve with other methods such as Finite Differences. Although boundary integral methods have been employed to study ciliated swimmers, the presence of variable coefficients in our problem undermines their computational efficiency. The canonical model of a spheroidal squirmer allows us to explore the feedback mechanisms between passive and active swimming methods and their relation with the geometry of the swimmer in a computationally efficient manner.

This computational method allowed us to examine questions unexplored in our initial asymptotic results,[2] such as the effect of this nutrient-dependent viscosity on nutrient uptake, differences in the pressure field, and nonlinear effects from a strong coupling.[3] An interesting phonemonon that we are currently exploring is that the velocity field is robust to nonuniform viscosity, while the pressure field is modified greatly. This has a large influence on the resulting drag on the squirmer body, which leads to modifications in locomotion.

Sinkhole Formation and Collapse

Sinkhole are caused when water from the surface (either from rain, rivers, or underground aquifers) seeps through cracks in the bedrock. This flow of water gently erodes the bedrock over time. When the bedrock is weakened to the point that it cannot support the earth above it, a collapse occurs, which we see as a small (or large!) cavity on the earth's surface. A model to study this phenomenon could drive the study of fundamental mechanics of sinkhole formation and collapse.

Our model consists of a two-phase material consisting of fluid and porous rock (wet sand). Because the constitutive law of wet sand is not generally agreed upon, we have chosen a hybrid approach by modeling the fluid as a continuum Darcy flow, while the porous material is modeled using discrete particles where the particle-particle forces are described individually.

The particle-particle forces are chosen to be Lennard-Jones type forces, which includes both cohesion and repulsion. The permeability through

Figure 3: Visualization of point-particles (drawn as circles) overlaying a finite element mesh to simulate sinkhole formation and collapse

which the Darcy fluid flows is interpolated from the position of the point-particles using a fast Gauss transform. In this way, the fluid and the particles are coupled. Initial results are promising (see Figure 3) and current work is on scaling this algorithm to handle numbers of particles necessary to obtain continuum-like behavior (on the order of 10,000).
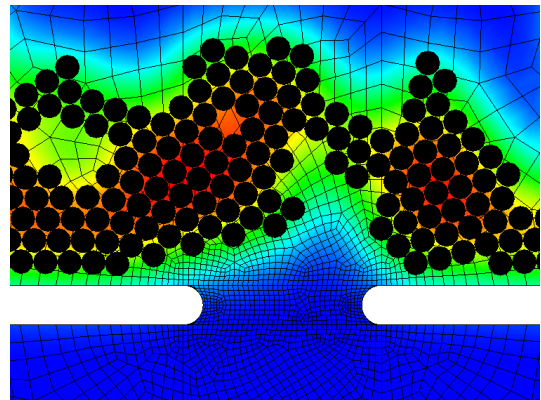
Development of open-source Finite Element library

The Julia programming language is relatively new, but is already making an impact for its ability to solve the "two-language problem", where programming is typically needs to be done first in an interpreted language that is easy to code in and modify, but then once the algorithm and model is set, one needs to re-write everything in a compiled language such as Fortran or C++ for speed and memory efficiency. The fact that Julia solves this issue, by both being easy to write, but also can be as fast as Fortran if done correctly, makes it an ideal programming language for a researcher, such as myself, who is actively writing code to solve problems that have not yet been well-defined.

I started writing my own Finite element library first as a educational experience – I didn't exactly understand the method, and the best way to learn is to write everything yourself. Then, as my package grew, I realized that it did a lot of things better (at least in my opinion), than the existing finite element library in Julia, at least with regards to solving fluids-focused problems. This fact, coupled with my growing interest in open-source software, encouraged me to put my code on the popular open-source repository Github under the name "eFEMpart".[4]

As I see it, there are several advantages, both to myself and to the larger scientific community, for publishing my package as open-source. First, the fact that anyone can look at the base code makes transparency easier and, if any bugs are found, fixing them is easy. Second, the fact that my code is open-source and easily installable makes it ideal for collaboration. Third, and this is specific to my package in particular, my front-end is written with modelers, not developers, in mind. This means that someone who is inexperienced with Julia but knows what PDE they want to solve can do so in about 50 lines using the eFEMpart package. This is immensely helpful even to researchers who do not do numerical computing – for example, prototyping their domain and PDE solutions for particular parameter sets can guide intuition about what the best analytic or asymptotic approach for a problem can be.

References

[1] P. S. Eastham, M. N. J. Moore, N. G. Cogan, Q. Wang, and O. Steinbock. Multiphase modeling of precipitation-induced membrane formation. *arXiv e-prints*, page arXiv:1906.04216, Jun 2019.

[2] Kourosh Shoele and Patrick S Eastham. Effects of nonuniform viscosity on ciliary locomotion. *Physical Review Fluids*, 3(4):043101, 2018.

[3] Patrick S. Eastham and Kourosh Shoele. Axisymmetric Squirmers in Stokes Fluid with Nonuniform Viscosity. *arXiv e-prints*, page arXiv:1904.01946, Apr 2019.

[4] Patrick S Eastham. eFEMpart. https://github.com/pseastham/eFEMpart, 2019.