Research Statement

I am an applied mathematician with research interests in numerical and computational methods for partial differential equations (PDEs). I design and develop numerical methods to simulate and analyze PDEs, with an eye towards improving their accuracy and efficiency, as well as expanding their applicability across a wider range of complex systems. I particularly focus on problems involving complex geometries, for example in fluid-structure interaction problems that may also be coupled with concentration dynamics. My general objective is to develop accurate and robust numerical methods that can be readily adapted for use in applications of interest to collaborators in other disciplines. Such applications include aquatic locomotion, flows through complex domains, and mixing analysis for animal or industrial applications. In the following research statement, I summarize my research accomplishments and outline my future plans. The first and second sections discuss numerical methods that we developed for solving fluid-structure interactions and reaction-diffusion problems. The third section discusses a 3-D computational technique that I used to analyze a fluid-structure interaction *after* running numerical simulations. The last section briefly touches on another class of numerical methods for fluid dynamics that I have recently started working with in a new project.

1. Immersed Boundary Double Layer (IBDL) method

Main result: *We developed a reformulation of the Immersed Boundary method for flows with rigid objects to capture the better conditioning of a double layer integral equation [1, 2].*

Background: Over the past several decades, the Immersed Boundary (IB) method, developed by Charles Peskin [3], has become a valuable tool in simulating fluid-structure interactions. By making use of a regular Cartesian grid that is independent of the structure geometry, the IB framework yields a robust numerical scheme that can efficiently handle the boundary conditions of immersed deformable structures. It does this by using two coordinate systems illustrated in Figure 1: a Lagrangian system that moves with the structure and a fixed Eulerian system on which the fluid equations are solved. The IB method uses discrete delta functions to link these systems together by mapping forces from the structure to the grid. The physical boundary is then essentially eliminated and replaced by forces in the fluid on the regular Cartesian mesh; therefore, very efficient solvers can then be used on the PDE. Because of the convenience and robustness of the IB framework, its use has been extended to many problem types outside of deformable structures.

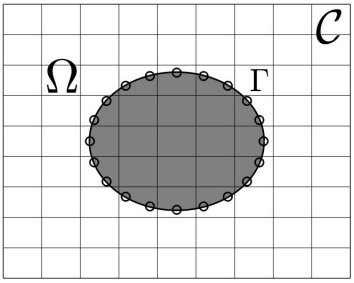

Figure 1: Diagram showing the two Immersed Boundary coordinate systems for an immersed structure, Γ, embedded in a 2-D domain.

One area of development for the IB method that my research focuses on is that of applying the framework to problems that have prescribed boundary values. While the IB force for deformable structures is found using a constitutive law, such as elasticity, in the case of rigid bodies, we must find or interpret these forces differently. One method would be to consider the structure to be tethered to a location, for example by stiff springs, and the boundary force is interpreted as the restoring force of these springs [4]. Such penalty methods are straightforward to use, but the resulting numerically stiff equations necessitate very small time steps. Additionally, the fact that the boundary conditions are enforced only approximately can result in fluid penetration into the solid object. A different approach is to enforce the boundary constraint *exactly* by viewing the force as an unknown Lagrange multiplier [5]. In this *IB constraint method*, the boundary condition is used to solve for the unknown force distribution. One can solve this system with an iterative method, but the associated operator is poorly conditioned, resulting in the need for many iterations, the number of which increases as our grid is refined. As is demonstrated for the Helmholtz equation in the first and third columns of Table 1, these iteration counts are even worse in 3-D. This is prohibitive for a time-dependent fluid-structure interaction problem, for which this solve would be done at each time step.

Iteration Counts				
	2-D		3-D	
Δx	Original IB	IBDL	Original IB	IBDL
2^{-3}	26	4	2172	7
2^{-4}	216	5	6687	7
2^{-5}	611	5	9969	7
2^{-6}	1101	4	–	7

Table 1: Number of iterations of `minres` and `gmres` needed to solve the Helmholtz equation where the circular structure boundary has prescribed boundary values given by $\sin 2\theta$.

My contribution: In my Ph.D. work with Robert Guy, we developed an Immersed Boundary method for boundary value problems that has bet-

ter conditioning. We first identified a connection between the IB constraint method and boundary integral methods, which rely on reformulating a boundary value problem as an integral equation with an unknown density on the boundary. One main advantage of these methods, which we sought to exploit, is that there are well-conditioned integral representations available. For example, the equation resulting from Dirichlet boundary conditions for a double layer integral representation has much better conditioning than the equation from the single layer representation [6].

We developed a numerical method with two goals in mind: (1) to utilize the simple, robust Immersed Boundary framework on flows with rigid objects in order to avoid the disadvantages of other methods, including expensive re-meshing or the need for analytical Green's functions, and (2) to improve the conditioning of the system for a faster Krylov solve. We were first able to demonstrate that the IB constraint method corresponds to a regularized single layer integral equation. We then utilized this relationship between the two communities of methods in order to develop a new ***Immersed Boundary Double Layer (IBDL) method***, which is able to achieve the same order of accuracy as the original IB constraint method with only a small number of iterations. The number of iterations also remains constant as we refine our grid. This method therefore can be utilized in moving and 3-D problems without the need for stiff parameters or preconditioners. Table 1 shows the drastic difference between the two methods in the number of iterations of a Krylov method required to solve the Helmholtz equation.

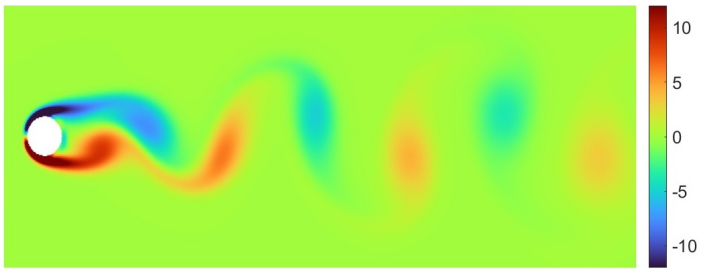

Figure 2: Vorticity plots for Navier-Stokes flow past a cylinder for $Re = 100$, using the IBDL method.

Scalar elliptic PDEs: We first derived, implemented, and analyzed the IBDL method for 2-D and 3-D Helmholtz and Poisson problems [1]. While the original IB constraint method used a regularized delta force distribution to enforce the known boundary values, the IBDL method instead utilizes a regularized *dipole* force distribution. This scalar version of the IBDL method has led to further advances in using the IB framework for PDEs that were previously unapproachable by the IB framework, as will be further discussed in the second section of this research statement.

We have also explored other advantages to the better conditioning of our method, including the ability to freely decrease the space between our immersed boundary markers to maintain the impermeability of an object. When this space is decreased in the original constraint method, the conditioning is further worsened. Additionally, as a result of the good conditioning of our system, the strength of the dipole distribution also converges as the mesh is refined. This is in stark contrast to the potential strength in the original IB method, which develops high frequency oscillations as the grid is refined.

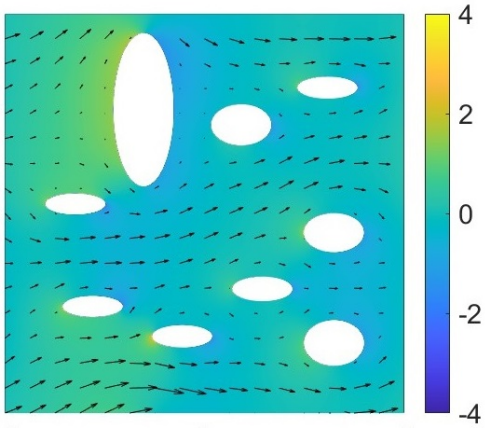

Figure 3: IBDL solution plot for Stokes flow past a periodic array of 9 arbitrarily placed ellipses.

Fluid Equations: We have also derived and implemented the IBDL method for the Stokes, Brinkman, and Navier-Stokes equations, simulating fluid flows with rigid bodies or complex domains. This work is presented in the Ph.D. Dissertation [2] and will be in a forthcoming paper. Guided by the decomposition of the stresslet into its constitutive parts, the IBDL method in this context involves a distribution of dipoles and a distribution of point sources. Figure 2 shows the vortex shedding in flow past a cylinder for Reynolds number 100. As in the scalar PDE case, the efficiency is greatly improved. This improvement is even more dramatic for more complex domains. In Figure 3, we can see the velocity and pressure for flow past 9 arbitrary elliptical obstacles. In this 2-D problem, the original IB method can require more than 1200 times the number of iterations.

Future research

This method has great potential for further explorations and improvements. All of the forthcoming project descriptions were submitted in a grant proposal to the NSF Computational Mathematics program.

A few immediate numerical analysis projects are outlined below. In addition to these projects, two other important aspects of my research plans are to **(1) apply the IBDL method to applications of interest**, such as particle suspensions and aquatic locomotion, and **(2) implement the IBDL method into the open-source `IBAMR` software package**, which allows for adaptive mesh refinement and parallelization [7, 8], in order to make the method available to scientists and mathematicians at large.

Project 1: Our reformulated Immersed Boundary method results in a solution that is discontinuous across the boundary. This necessarily leads to large errors in the region within a couple meshwidths of the boundary. This width is determined by the support of the discrete delta function, as well as the underlying PDE discretization. We were able to evaluate points near the boundary to adequate accuracy using simple linear interpolation. For a future project, I seek to **eliminate the need for this interpolation step** either by utilizing the convergence of the potential strength or by combining this method with an immersed interface-type method.

Project 2: I then seek to utilize the IBDL method to obtain **higher order accuracy**. The main disadvantage of the IB method is the that we typically only achieve first order accuracy with these fluid-structure interaction problems. The Immersed Boundary Smooth Extension (IBSE) method [9] was developed to achieve higher order accuracy, but the subsequent system suffers from worse conditioning, resulting in the need for an expensive precomputation step. I believe that I can use our more efficient double layer implementation in conjunction with an IBSE-like method to achieve high order accuracy without this computational cost.

Project 3: I also plan to undergo a **detailed analysis into finite difference grid structures for the IBDL method applied to fluid problems**. Two common structures are collocated and staggered grids, the latter of which stores scalar and vector components on different cell locations. A staggered grid is preferred for other IB methods since in this scheme, the discrete divergence of the gradient corresponds to the discrete Laplacian. The IBDL method involves the spreading of a *tensor* to the grid, and it is threfore not obvious how to adapt this formulation to a staggered mesh. We therefore currently use a collocated mesh and approximate the so-called wide Laplacian with the standard five-point Laplacian. This does achieve our designed convergence, but I plan to further analyze the collocated discrete system and how the system may be affected by the presence of two different discrete Green's functions. Additionally, I will explore different options for instead using a staggered grid.

2. Immersed boundary method for Neumann and Robin boundary conditions and reaction-diffusion problems

Main Result: *We developed an Immersed Boundary scheme for enforcing Neumann and Robin boundary conditions and utilized this scheme for reaction-diffusion problems in deforming domains.*

Ongoing and future research

In a new work with Lewis, Guy, and Khatri, we again utilized the connection we made between IB methods and boundary integral equations to formulate a new IB scheme for Neumann boundary conditions that corresponds to a single layer integral equation. This is noteworthy because the original IB method does not achieve convergence in the solution derivatives near the boundary. Therefore, it appeared to be unfeasible to enforce a boundary condition on the derivative. However, using our connection to integral equations, we saw that we could obtain derivatives exactly *on* the boundary by accounting for the size of the jump given by the potential strength. We can therefore enforce both Neumann and Robin boundary conditions.

When simulating a time-dependent reaction-diffusion problem, we can use an implicit-explicit time discretization scheme. By treating the nonlinearities explicitly in time and the diffusive terms implicitly, we arrive at an elliptic problem to solve at each time step. Since we are now able to enforce Neumann and Robin boundary conditions on these elliptic problems, this opens up the door to utilizing the IB method in interesting reaction, advection, and diffusion problems.

In [10], Lewis et al. study the amoeboid locomotion seen in experiments by developing a model of a motile cell balancing forces on the liquid cytosol, the porous elastic cytoskeleton, and the adhesive interactions with the substrate. In order to drive the deformation of the cell, they prescribe an active contractile stress within the cytoskeleton. This results in back-to-front directed waves that determine the migration of the cell. An illustration is shown in in Figure 4. Instead of prescribing this force, our goal now is to capture the spontaneous emergence of the wave-like patterns of contraction via the coupling of the mechanics and chemistry. With our new developments, the Immersed Boundary method is particularly well-suited to this type of problem, as the chemical and fluid dynamics are occurring within the moving and deforming domain of the cell.

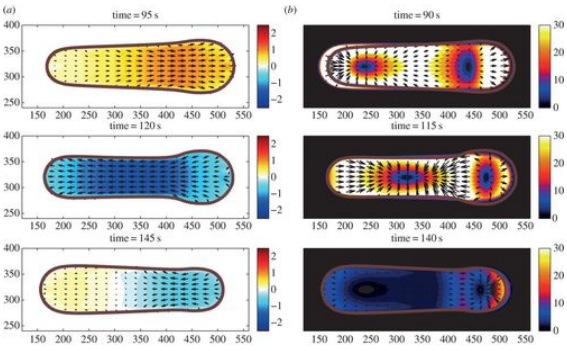

Figure 4: Intracellular flow (left) and traction stresses (right) in a model cell. Figure obtained from [10].

Through this and the previous project, we have discovered another numerical analysis question worth investigation, namely which characteristics of discrete delta functions are vital for convergence in certain applications of the IBDL method. Smoothness, moment conditions, and several other characteristics have been examined in other IB schemes, and conducting a thorough analysis of this issue in our new method is needed.

3. Pulsation in Soft Corals

Main Result: *I implemented 3-D Poincaré map techniques to analyze mixing in pulsing corals.*

Figure 5: Pulsing Xeniidae corals [11].

Ongoing and future research

Soft corals of the family Xeniidae, pictured in Figure 5, have a pulsing behavior unique to sessile marine organisms. Experiments and recent numerical results suggest that the energetically expensive pulsing behavior of the corals facilitates the oxygen-limited photosynthesis of the symbiotic algae by decreasing the oxygen buildup around the tentacles [12–16]. Analyzing and quantifying the mixing of the fluid caused by the pulsing action can provide insight into the effects of climate change on the species and in the development of industrial or engineering pulsing mechanisms for facilitating mixing.

Mixing Analysis: In the new work by Santiago et al. [17], the 3-D coral motion is modeled by both active tension mimicking muscle contraction and passive elastic forces. Simulations of the flow induced by the pulsing corals are then run using the Immersed Boundary Finite Element (IBFE) method, which is a hybrid finite element and IB method [15, 18, 19] that is part of the `IBAMR` software package [7, 8]. An illustration of the finite element coral mesh is shown in Figure 6.

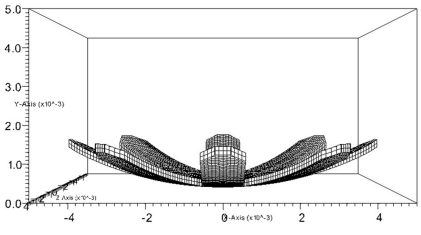

Figure 6: Finite element coral mesh.

In order to illustrate manifolds that separate regions of flow, a common method is finite time Lyapunov exponents (FTLEs). In this method, we use our obtained velocity fields to form a discrete version of a flow map. By using the gradient of the flow map, we can calculate FTLEs in order to measure the separation that occurs between nearby particles. By calculating FTLEs for forward and backward time, and plotting them as a color map, we are able to see Lagrangian coherent structures (LCS) that are the analogue for stable and unstable manifolds in these time-dependent flows. The color map in Figure 7 illustrates the FTLEs on a 2-D plane through the middle of the coral, showing one tentacle in black.The yellow curves indicate Lagrangian coherent structures.

However, once our simulations reach steady state, the Eulerian velocity fields are periodic in time. This periodicity of our system allows us to instead analyze these flow regions by using a section of a Poincaré map, or a heteroclinic tangle. A Poincaré map takes a fluid particle from one location and maps it to its final location after one period. To form a heteroclinic tangle, we advect points seeded along the eigenvectors of the gradient of the Poincaré map for a period forward and backward in time. The resulting heteroclinic tangle gives *capture*

and escape lobes which illustrate the amount of fluid that gets brought into the interior of the coral within one pulse. The manifolds match up well with the structures seen in an FTLE illustration. However, since these tangles create a discrete version of the manifolds themselves, we can use this method to more easily *quantify* the amount of mixing by finding the volume of the lobes. These heteroclinic tangles were formed on a 2-D coral model by Santiago in [16]. I am now extending the Poincaré map technique to 3-D. The coral motion has proven to be an excellent candidate for this analysis because the tangle creates a very well-defined three-dimensional capture lobe at the biologically relevant frequency-based Reynolds number of about 47. We will utilize this method to quantify mixing for varying Reynolds numbers and other kinematic parameters. This work then has implications in industrial mixing quantification.

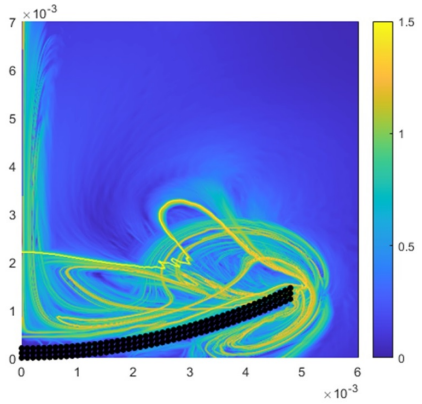

Figure 7: A color map showing the size of the finite time Lyapunov exponents.

Chemical Concentration:

Aim: To develop a 3-D numerical method coupling chemical concentration to the pulsing coral fluid model using the IBFE method.

Another method we will use to analyze the mixing will be to couple the fluid-structure interaction with the advection and diffusion of the oxygen concentration, where the moving coral tentacles are a source of the oxygen. The mappings between Eulerian and Lagrangian coordinate systems undergone by the Immersed Boundary method provide a simple framework for providing a source term for the chemical concentration that is located on the moving Lagrangian mesh of the coral. The desorption rate of the oxygen from the tentacles to the fluid can be modeled to decrease as the concentration near the tentacles increases, emulating the decreasing ability of the algae to photosynthesize in the presence of high levels of oxygen. Just as in the fluid dynamics problem, the mapping between coordinate systems is then used in both directions for the additional chemical dynamics. This coupling of the Immersed Boundary method with the concentration PDE has recently been implemented in 2-D [16].

Since the 3-D simulations utilize the more complex IBFE method and the `IBAMR` software package, extending this to 3-D is a non-trivial undertaking. I will develop and implement this method. The inclusion of this method into this software library will enable researchers to immediately apply the method to current open problems involving chemical concentrations in addition to fluid-structure interactions.

4. Other ongoing research: The method of regularized stokeslets

I recently attended a collaborative workshop at The Institute for Computational and Experimental Research in Mathematics (ICERM) at Brown University. In this workshop, called Empowering a Diverse Computational Mathematics Research Community, our group of 7 researchers was led by Ricardo Cortez and Shilpa Khatri. We began a project utilizing the method of regularized Stokeslets, developed by Ricardo Cortez [20]. In this project, we are working to extend the work of [21] to incorporate source doublets into the method to model permeable membranes by effectively introducing sources and sinks on either side of the membrane. The parts of this project that I have been involved in are extending this to 3-D, analyzing the order of error, and exploring the possibility of utilizing these source doublets to improve volume conservation for the method of regularized Stokeslets.

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