Bryce Palmer - Research Statement

Introduction: Externally actuated micro/nanorobots have generated considerable excitement over the last decade due to their potential to carry out controllable microbiological tasks.[7] Specifically, microrobotic swarms, containing tens of thousands to millions of individual robots the size of bacteria, have the capacity to perform diagnostics and directed drug transport within deep tissues and microvasculars hitherto inaccessible by conventional means.[7] Unlike individual microrobots, swarms leverage the coupled interactions between constituents to form large-scale collective motions that far exceed the speed, strength, and functionality of a single microrobot. Because these swarms are externally actuated by magnetic or optic fields, actuation schemes can be programmed to control a swarm's collective motions and morphology. Specific examples include clustering, swirling, dispersion, or ribbon formation, which together allow for high environmental adaptivity.[4] Unfortunately, experimentation alone is insufficient to properly design microrobotic swarms for real-world applications; instead, efficient computational tools are needed to augment experiments by enabling rapid investigation into the effect of design parameters. However, modeling swarming microrobots is inherently challenging—owing to the theoretical and computational complexity of resolving the many-body hydrodynamic effects and short-ranged collisions. No state-of-the-art method is currently capable of accurately simulating real-world microrobotic swarms. This issue is further exacerbated by the general lack of fundamental understanding of how to best generate and control a swarm's collective motions for specific tasks, especially within confined microfluidic environments. **I aim to overcome these challenges by (1) creating the first high-fidelity, scalable computational framework able to simulate dense suspensions of complex-shaped, microrobots and (2) numerically investigating how key parameters, like robot shape, actuation scheme, and geometric confinement affect a swarm's collective motions.**

Intellectual Merit: Accurate simulation of microrobotic swarms within real-world microfluidic environments is essential if these systems are to be designed for practical biological applications. Previous work toward modeling these systems has primarily focused on dilute suspensions, where the long-range hydrodynamic interactions dominate the system dynamics, allowing the effect of near-body dynamics to be approximated by representing complex-shaped particles in terms of simple geometries like spheres, ellipsoids, or rods. However, as the number of particles per unit volume increases, near-body interactions become increasingly important causing these approximations to break down. Within dense suspensions, even seemingly insignificant modifications to robot shape, like using spherical robots vs cubic robots, will result in drastically different close-to-contact dynamics, which directly impacts internal pattern formations. Therefore, for dense microrobotic swarms, it is imperative that the near-body dynamics between complex-shaped particles be accurately captured to correctly predict/control their collective motions.

Task 1 - Isogeometric analysis: To address these issues, I propose to develop a high fidelity model capable of accurately resolving the hydrodynamic interactions between complex-shaped microrobots. Guided by this goal, I have been working in direct collaboration with Prof. B. Shanker (an electromagnets expert) and Prof. H. M. Aktulga (a high-performance computing expert) to develop an isogeometric boundary integral model, which I am implementing within Python. The fundamental principal of isogeometric analysis is to utilize smooth basis functions to represent particle geometries and the physics on their surfaces, thereby providing higher order description of fields and enabling accurate resolution of near-body dynamics. Towards this end, I reformulated an existing boundary integral solver[3] based on the assumption that microrobots are typically genus-zero shapes, allowing me to pull back surface quantities to the unit sphere and then discretize in terms of spherical and vector spherical harmonic basis functions. I then solve the governing boundary integrals through Galerkin's method. One of the challenges when solving hydrodynamic boundary integrals is the evaluation of the nearly-singular integrals that arise when solving particle to self and particle to nearby particle interaction. To address this difficulty, I derived a singularity-free method for evaluating particle self-interaction through established techniques of singularity subtraction/isolation. My next step is to integrate adaptive quadrature techniques to handle the interaction between close-to-contact particles. Once complete, I will resolve the effect of no-slip confinements by added additional constraints to my linear system based on well-established methods.[6] My first milestone will be to benchmark this model against analytical solutions for the flow between spherical particles both with and without confinement.

Task 2 - High performance software development: High fidelity simulation of microrobot swarms is computationally intensive and requires fast, scalable numerical methods to make modeling real-world systems feasible. The key bottleneck is the rapid computation of pairwise hydrodynamic interactions between N particles, which scales as $\mathcal{O}(N^2)$. To overcome this issue, I will integrate my hydrodynamic solver into the parallel computing framework developed by Prof. Shanker. This FORTRAN-based framework centers around the Accelerated Cartesian Expansions (ACE) algorithm, which reduces the computational complexity of evaluating the pairwise interactions from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$.[1] To accomplish this task, I will first convert my current Python implementation into FORTRAN. I will then develop suitable data structures for the efficient computation and communication of spherical harmonic coefficients and create custom MPI communication schemes for the tonsorial kernels that arise in our calculations. These implementation details are vital for ensuring that our framework remains computationally tractable and will be validated based on scalability. **The NSF GRFP will supplement our computational resources by providing access to XSEDE, enabling me to fully harness the capabilities of this high-performance framework.**

Task 3 - Dense microrobotic swarms under rigid confinement: The simulation of dense microrobotic swarms requires simultaneously resolving the hydrodynamic interactions and short-ranged collisions between particles. Unfortunately, traditional collision resolution algorithms become numerically unstable when applied to dense assemblies. To overcome this limitation, my collaborator Dr. W. Yan (a computational biologist) developed a collision resolution algorithm using geometrically constrained optimization.[5] Through this collaboration, I will expand Dr. Yan's existing open-source code-base to include fast methods for evaluating the distance functions and surface-normals between colliding non-convex particles based on advances within the computer graphics community.[2] I will then couple this code-base with the framework developed in Task 2. Once complete, I intend to leverage the speed and flexibility of this computational tool to analyze how key parameters like robot shape, robot actuation type, and confinement geometry affect a swarm's collective motions and pattern formations. By systematically performing simulations within this expansive parameter-space, I intend to provide experimentalists with a comprehensive picture of how to best design their microrobotic swarms. To quantify the effects these parameters have on a swarm's collective motions, I will utilize my existing post-processing toolkit, which I have applied to active matter systems for extracting their large-scale topological structures and ensemble averaged statistics. Based on these results, **I will iteratively design loading schemes and robot shapes to streamline the transport and capturing of large-scale cargo within simulated microvascular-like environments**.

Broader Impacts: Controllable microrobotic swarms have the potential to profoundly improve public health by facilitating novel treatment methods like the transport of chemotherapy drugs directly to cancer sites.[7] My work's efficient computational framework will augment existing experimental techniques by enabling researchers to virtually prototype their swarm designs within realistic environments. To facilitate the use of this framework by others, I will open-source and thoroughly document all software I develop. In doing so, I hope to have a far-reaching impact on the fields of soft condensed matter, robotics, and microfabrication, which could benefit significantly from a model for dense particulate suspensions. Furthermore, I will disseminate this research to non-engineers by participating in the Alliances for Graduate Education and the Professoriate's Chalk Talks, which seek to distill complex scientific works for general audiences.

References: [1] Baczewski, A. D., et al. 2010, Journal of Computational Physics, 229 [2] Bender, J., et al. 2014, Comput. Graph. Forum, 33, 246–270 [3] Corona, E., et al. 2017, Journal of Computational Physics, 332, 504 [4] Xie, H., et al. 2019, Science Robotics, 4, eaav8006 [5] Yan, W., et al. 2019, The Journal of Chemical Physics, 150, 064109 [6] Zhao, H., et al. 2010, Journal of Computational Physics, 229, 3726 [7] Zhou, H., et al. 2021, Chemical Reviews, 121, 4999