Proposal Review 2 : 2109048

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Agency Name:	National Science Foundation
Agency Tracking Number:	**2109048**
Organization:	
NSF Program:	APPLIED MATHEMATICS
PI/PD:	Quaife, Bryan
Application Title:	Collaborative Research: Mathematical modeling and simulation of self-assembling amphiphilic particles in solvent
Rating:	Multiple Rating: (Excellent/Very Good)

Review

Summary

In the context of the five review elements, please
evaluate the strengths and weaknesses of the proposal with respect to intellectual merit.

Topic: Collaborative Research: Mathematical modeling and simulation of self-assembling amphiphilic particles in solvent
This proposal is in the area of biophysics. It aims to mathematically model, simulate and analyze membrane biophysics through the study of collective dynamics of amphiphilic self-assembly.
Self-assembly is a ubiquitous process in biology and is a major source of nonspecific interactions in soft matter. In the case of membranes, lipids self-assemble into bilayer and micelle morphologies.
To design better membrane models than existing continuum or molecular dynamics models, the proposal aims to quantify the collective physical properties and processes of amphiphiles. The proposed mathematics establishes a platform for simulating the collective dynamics at large scales in a manner that allows for direct comparison with pre-existing theory and experiment.
Intellectual Merit
Strengths
The purpose of this research is to reach interesting physical phenomena and model bilayer membranes with less computational cost than molecular dynamics, and account for more general features that continuum theory misses, such as the dynamics brought about by inclusions or topological changes.
The main ingredient is defining a nonlocal interaction through the solution of an elliptic boundary value problem. This has the phenomenological

characteristics of long-range hydrophobic attraction.
This minimal model gives rise to rich phenomena for Janus particle aggregates and correctly predicts the elastic properties of bilayer.
The technical research tasks include: 1) quantifying collective properties of amphiphilic ensembles, 2) mathematical analysis of continuum elastic energies, 3) high-order numerical algorithms for large-scale simulations, and 4) incorporating external fields through electric charge.
The proposal extends the results using three-dimensional boundary integral formulations. The development of three- dimensional models describing colloidal systems could be transformative in biomedicine and material science.
The simulations use a new, yet intuitive, approach that can account for important and complex systems that are out of reach in computational material science. These complex systems include fusion and fission of amphiphilic bilayer membranes and optimal shape design in meta-materials.
The research draws from expertise in scientific computing, physics of fluids, and incorporates techniques from geometric analysis.
Weaknesses

In the context of the five review elements, please
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.

Broader Impact
Strengths
The proposal requests funding to support one undergraduate researcher per year. The NSF funded undergraduate (along with peers) will work part-time for 8 weeks, collaborate directly with the senior personnel, have tutorials in topics such as numerical quadrature and integral equations, and train in mathematical writing and presentation. Undergraduates will train with graduate students and postdocs.
The PIs will prioritize funding students from underrepresented groups as well as individuals whose socio-economic background might otherwise prevent them from participating in mathematical research.
Weaknesses

Please evaluate the strengths and
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if
applicable

Prior NSF Support
NSF-DMS-1222550, Mathematical and experimental study of lipid bilayer shape and dynamics mediated by surfactants and proteins, $212,603, 9/15/2012 - 08/31/2016 (with no-cost extension), PI. Intellectual merit: The focus of this grant is modeling the interaction between a pure lipid bilayer membrane with surfactant, cholesterol and protein.Broader impacts: One PhD student (Szu-Pei Fu) was funded to work with YNY, and work has resulted in seven papers [65, 151–153, 157, 219, 220]. YNY has been actively involved with promotion of underrepresented students at NJIT. The other PhD student (Herve Nganguia) is African. YNY has taught a broad spectrum of courses in fluid mechanics and applied math modeling.
Bryan Quaife: NSF DMS-2012560, Erosion, Transport, and Dispersion in Granular and Porous Media, $249,636, 08/01/2020–07/31/2023, PI.
Intellectual Merit: The goal of this research is to develop high-order numerical methods to simulate hydrological processes including erosion.
Broader impacts: A second-year PhD student (Jake Cherry) has been assigned to this project. Since the funding just began, results have not yet been published or presented.
Postdoc Mentoring Plan: One postdoc at Fordham and Florida state. Standard.
Data Management Good on page 78/85
Collaborative proposal value: Project management: The success of the proposed research requires complementary expertise and collaborative efforts in physics, applied mathematics, algorithms, and computing. Ryham has been working on mathematical modeling with a strong analytical background. Young has been working on many areas of computational fluid dynamics and applications to math biology for many years. Quaife has been working on integral equation methods, fast algorithms, and their applications to fluid dynamics for many years. Their recent collaborative work on the HAP model in two dimensions has provided a solid foundation for the proposed research. Collaboration plan: The management responsibility of this collaborative research will reside with the lead PI (Ryham) for this endeavor. The PIs, their postdocs, and students will meet frequently on Zoom and in person when possible. Once the pandemic is under control, PI RR and PI YNY will conduct biweekly meetings in person, with PI BQ Zoom in from Florida. The PIs will share software packages, paper sources, and references on a common Git repository. The resulting software packages will be posted on the Github software repository.

Summary Statement

Innovation in Mathematical Content: V
Significance of Potential Applications: E
Rating: V/E