Proposal Review 1 : 2109048

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:	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.

The purpose of this research is to study complex physical phenomena with less computational cost than molecular dynamics, and account for some general features that the continuum theory omits. The main ingredient of the proposed method is to define a nonlocal interaction through the solution of an elliptic boundary value problem that has the phenomenological features of a long-range hydrophobic attraction. It turns out that this minimal model gives rise to rich phenomena for Janus particle aggregates, and it correctly predicts elastic properties of bilayer membranes. The research tasks include quantifying collective properties of amphiphilic ensembles, mathematical analysis of continuum elastic energies, design of efficient, higher order numerical algorithms for large-scale simulations, and incorporating external fields through electric charge. Lastly, the proposal extends the results to higher dimension by using three-dimensional boundary integral formulations. A strong aspect of the proposed approach is in being computationally more efficient than the Monte Carlo and molecular dynamics methods, commonly used in modeling repulsive interactions in complex systems. Although the PI makes a good case that such an approach is likely to work in modeling amphiphilic self-assembly, it is not obvious how it can be extended to other soft matter systems such as genome packing. Overall, the research draws from expertise in scientific computing, physics of fluids, and mathematics. The mathematical component incorporates leading techniques from geometric analysis and gives deep insight into fundamental problems in material science. The proposal is very rich in intellectural merits.
The PIs' prior research activity is very strong.

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

This project aims to advance the mathematical modeling of collective dynamics of amphiphilic particles. 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 metamaterials. The development of three-dimensional models describing colloidal systems could be transformative in biomedicine and material science. The project offers undergraduates in a socially impactful manner the opportunity to do research and train with graduate and postdoctoral personnel. It incorporates research in the classroom, and with its combination of mathematical modeling, analysis, and scientific computing, the project highlights the importance of mathematics and computation to all areas of science and engineering. The propsal is also very strong in its broader impacts, with the PI having very good track record in mentoring at different levels. A possible weakness is that it may lack of a diversity focus.

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

Summary Statement

This proposal specifically aims to advance mathematical modeling and analysis in 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. From this point of view, the proposal addresses a broad class of important open problems in biology and is possibly relevant to materials sciences as well.
The intellectual merit of the proposal is very strong, the problems are very challenging, and the PIs look very well equipped to solve them. The broader impacts, specially in mentoring several tiers of students and young researchers is also impressive, although it may not be particularly strong in diversity. The research has the potential to impact the biology of membranes as well the modeling of self-assembly in soft matter physics. Overall, it is a very strong proposal. This panelist rates it as 'very good'.