Proposal Review 2 : 2206369

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Agency Name:	National Science Foundation
Agency Tracking Number:	**2206369**
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.

Overview

This is a collaborative proposal between Ryham (lead-PI), Quaife (FSU), Young (NJIT) on mathematical modeling of self-assembling amphiphilic particles in a solvent. The idea is to develop a continuum model that can capture the self-organization of so-called Janus particles. These are spherical particles, with biphasic (hydrophilic, hydrophobic) coating on each hemisphere, and have been used as models of amphiphilic colloids. Two of the PIs developed a Hydrophobic Attraction Potential (HAP) model and the model was used by all three PIs to simulate the self-assembly of vesicle-like structures. The HAP model introduces an order parameter that minimizes a Ginsberg-Landau type energy functional and generates forces via a variational derivative of the energy. The essence of the model is simulating the motion of spherical, rigid particles in a viscous fluid subject to forces from externally applied flows, electric fields, hydrodynamic interactions and hydrophobic attractions. The proposal consists of three Aims. In Aim 1, the HAP model will be extended to incorporate a double-well potential where the order parameter has the interpretation of the mean number of nearest neighbors per water molecule. The result is a stationary Allen-Cahn equation in the solvent. The effects on self-assembly will be investigate and compared to experiments. In Aim 2, novel numerical methods are proposed for solving the equations using integral equation methods, efficient preconditioners and adaptive time stepping. In Aim 3, the approach will be extended to include electric fields (cations/anions) and the use of an externally applied fields to control the self-assembly process will be explored. The project will provide interdisciplinary training for 2 undergrad students

(Fordham), a graduate student at FSU, and potentially high school students.

Intellectual Merit

Strengths:

The use of the HAP is a strength. The HAP is a very simple, but very effective method, for modeling hydrophobic attraction. The model will certainly be more efficient than molecular dynamics, and will be solved in 2D and 3D, but there are significant numerical challenges that need to be overcome. The use of a piecewise quadratic approximation of the HAP potential is also a strength as it enables a fast solution of the Allen-Cahn HAP equation. Accurately tracking a large number of particles subject to hydrodynamic, hydrophobic and electrostatic forces is very challenging. The use of integral equation methods for doing this is a strength because these methods can be made very accurate, there exist fast methods for the evaluation of the integrals and for solving the resulting integral equations. The use of adaptive, spectral deferred correction time stepping method to aid in the temporal resolution of near contact regions is a strength.

Weaknesses:

Another challenge in simulating the near contact of the spherical particles is the accurate evaluation of the integral equations. While a number of methods have been developed for evaluating such nearly singular integrals, this is not discussed. Another weakness is that the proposal does not address the scaling of the algorithm as the number of particles increases. This is particularly important in 3D.

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

Strengths:
The proposed work will provide interdisciplinary training for undergraduate students, a graduate student and very likely some high school students, mostly through existing programs. The proposed work has the potential to impact a broad class of problems in soft matter with applications ranging from the design of new materials to drug delivery systems.

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

Summary Statement

This is a strong, well-written proposal on a challenging and important problem in soft materials. The team has complementary strengths and is very well suited for this project. The research team has been working together on preliminary aspects of the proposed research. This preliminary work is of very high quality and provides a compelling case for the approach. The proposal would have been strengthened if further discussion had been included as to how the near-contact interactions will be handled, and how the algorithms scale with the number of particles. The intellectual merit of the results from prior NSF support (Quaife, Young) is difficult to assess since only the goals of the NSF grants are listed, but not the results (e.g., new theories, simulation methods, papers, etc). The broader impacts listed include interdisciplinary training of graduate students, which is strong. The Data Management plan is appropriate. Overall, this proposal ranked at the top of the middle third of proposals I reviewed.