Proposal Review 3 : 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:	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 proposal focuses on the development and analysis of methodologies for the study of self-assembly of amphiphilic particles into bilayer membranes.

Intellectual Merit:
STRENGTHS:

This is an ambitious proposal, and builds on earlier work by the PIs, in which they developed the so-called Hydrophobic-Attraction potential (HAP). This potential is obtained by solving a linearized Poisson-Boltzmann equation, which leads to a Helmholtz-type equation.

The model presented lies in between molecular dynamics and continuum mechanics. In the proposed approach, a collection of rigid amphiphilic particles is considered. The particles interact with each other via the screened electrostatic potential described by the HAP coupled to hydrodynamic interactions. This approach also eliminates the need for a predefined surface, and has been shown to produce self-assembly and spontaneous segregation of bilayers. Using their approach, it is proposed to to study elastic and hydrodynamic properties of bilayer membranes, even in the presence of electrical charges and external fields.

WEAKNESSES:

The model presented appears to be phenomenological, so I would have liked to see some description of how the model will be validated, and possibly improved if necessary. If parameters are fitted to experiments, it would be interesting to see how predictive this approach is.

In terms of methodology, I would have liked to understand better the connection between the HAP and the Debye-H\"uckel theory, or Poisson-Boltzmann, and why the linearized model is preferred in this context.

It is proposed to analyze the model presented in connection to continuum models for membranes, such as the one introduced by Hamm and Kozlov (HK). There is a strong connection between the HK model and the Willmore Functional in differential geometry that is not mentioned in the proposal, and for which there is a rich literature. There is also a mention the Γ-convergence in the context of numerical approximation, which is not new, but has several drawbacks: The order of convergence is rather weak, and the convergence is usually only up to subsequences. I would have liked to see a more clear statement in the proposal as to what the concrete objective is in this respect.

The statement after equation (10) seems confusing: The proposal states that equation (10) does not require knowledge of ∇u on particle boundary i, but ∇u_i and ∇u_j appear in the definition of σ_{ij}.

The section on fluctuation hydrodynamics needs more details.

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

STRENGTHS:

The educational aspects of the proposal are strong: It is proposed to work with undergraduates for 8 weeks during the summer, and include outreach to High-Schools. These would interact with graduate students and postdocs.

WEAKNESSES:
None.

Results from prior NSF Results:
Two of the PIs have had earlier NSF-funded research, and were very productive. In addition, several graduate and undergraduate students were mentored.

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

Summary Statement

The topic described in the proposal is very interesting, and fairly well developed. The numerical approaches, although not particularly novel, seem appropriate for the proposed model. The rigorous derivation of continuum models for membranes is very attractive, but the proposal lacks details regarding how this would be done. The educational component is strong.

I rank this proposal in the middle third of those reviewed.

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