Proposal Panel 1 : 2109048

Back to Proposal

Agency Name: National Science Foundation

Agency Tracking Number: **2109048**

Panel Summary

Panel Summary

This proposal concerns the development, analysis, and numerical simulation of methodologies for describing the amphiphilic self-assembly of membrane bilayers. The proposed model establishes a platform for efficiently simulating collective dynamics of particles at large scales. The goals of the proposal include quantifying collective properties of amphiphilic ensembles, studying the connection to continuum elastic theories, efficient, high-order numerical algorithms for large-scale simulations, and incorporating external fields through electric charge.

INTELLECTUAL MERIT:
Strengths:
• The proposal builds on strong earlier work by the PIs.
• The PIs have developed a mesoscale model – between molecular dynamics and continuum mechanics – which allows for much more reasonable computation than more expensive molecular dynamics approaches which are more common. This may have powerful applications in many areas of biology.
• The PIs present some very promising preliminary numerical results which give evidence that their model gives rise to spontaneous self-assembly of bilayers. Their methods also eliminate the need for a pre-defined surface.
• The use of Janus particles as a prototype model for attractive-repulsive interactions is very clever and allows for comparison to other systems.
• The proposed model is very useful and not overly complicated, and the creation of the model itself is valuable. The focus is on applications and plans for very involved numerical calculations — not necessarily the mathematical analysis of the model.

Weaknesses:
• Since the model is phenomenological, it is difficult to connect the parameters to specific systems, so how predictive should this model be? If it is not predictive, how can it be improved to better agree with experiments? The discussion of how experimental feedback will be used to improve the model could be more detailed – a better description of how the model can be validated and improved is needed.
• The use of Gamma-convergence for numerical convergence presents some drawbacks: the convergence is only up to subsequences, and the convergence might be in a weak sense.
• There is some confusion regarding equation (10) and some claims made about independence of gradients, since the gradient of u appears in the equation.
• The discussion of fluctuating hydrodynamics would benefit from more details.

BROADER IMPACTS:
Strengths: The educational aspects of this proposal are strong and include an 8-week summer undergraduate research program as well as outreach to local high schools. The proposal involves interaction between undergraduate/high school students with graduate students and postdocs.

Weaknesses: The specific problems that undergraduate and graduate students would be working on are not identified.

Results of Prior NSF Support:

Prior NSF support is mentioned for two of the PIs. The PIs have been very productive with prior NSF support and their mentoring of undergraduate and graduate students has been very strong.

Postdoctoral mentoring plan:
The postdoc plan is very good, especially the plans to involve postdocs in outreach activities.

Data Management Plan:
The data management plan is adequate.

Recommendation:
The model proposed here is simple but useful and will have important applications in biology. The significance of potential applications was deemed to be very high, but there were some concerns about comparisons of the model to experiments and also concerns about the analysis proposed.

The panel placed the proposal in the "Competitive" category.

The summary was read by/to the panel and the panel concurred that the summary accurately reflects the panel discussion.

PANEL RECOMMENDATION: Competitive