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# Proposal: 2109048

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## Agency

Agency Name: National Science Foundation

## Application

Agency Tracking Number: 2109048

Project Title: Collaborative Research: Mathematical modeling and simulation of self-assembling amphiphilic particles in solvent

Requested Amount: \$268,867

Received Date: 11/16/2020

PI/PD: Bryan Quaife

Authorized Representative: Dale Meeks

Submitting Institution: Florida State University

SAM Legal Business Name: FLORIDA STATE UNIVERSITY

## Program

Program Title: APPLIED MATHEMATICS

Program Code: 1266

Funding Opportunity Number: PD 16-1266

Division/Area of Science: Division Of Mathematical Sciences

Program Contact Name: Tiziana Giorgi

Program Contact Phone: (703) 292-8090

Program Contact Email: [tgorgi@nsf.gov](mailto:tgorgi@nsf.gov)

## Application Status History

Status	Status Date
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Status	Status Date
Declined	05/17/2021

## Cognizant Program Officer Comments

Dear Professor Quaife,

I regret to inform you that the collaborative proposal DMS – 2109048 (Collaborative Research: Mathematical Modeling and Simulation of Self-Assembling Amphiphilic Particles in Solvent) was not recommended for funding. This recommendation follows the process described in the Context Statement available to you on FastLane; the reviews and the panel summary for this proposal are available there as well.

The comments included below are excerpts from the review analysis prepared in support of the recommendation.

Please understand that reviewers address their comments chiefly to NSF, not to Principal Investigators. Reviews containing irrelevant, non-substantive, or erroneous statements are not used in evaluating the merits of a proposal.

I hope that a careful reading of the comments of the reviewers and panel, and the excerpts below will provide useful feedback when preparing future submissions.

All the best,

Tiziana Giorgi  
Program Director  
Applied Mathematics Program, MPS/DMS

**REVIEW PROCEDURE:** This proposal was evaluated by one of the FY21 panels managed by the Applied Mathematics program. The panel comprised researchers with expertise relevant to the main thrusts of the projects under consideration and was asked to evaluate proposals with respect to the two main NSF review criteria (Intellectual Merit and Broader Impacts), and additional solicitation specific criteria, when applicable.

Each proposal reviewed by the panel received three written reviews. Based on the review preferences expressed by the panelists prior to the panel meeting, at least two panelists not conflicted were assigned as reviewers. Additional ad hoc reviews were solicited for the projects that did not receive three reviews from members of the panel. The ad hoc reviews were independent of the panel, and the panel had no access to them. For each project, the assigned reviewers were asked to provide written reviews, as well as a letter rating of Excellent (E), Very Good (V), Good (G), Fair (F), Poor (P), or a combination of these, prior to the start of the panel deliberations. During the panel meeting, each project was discussed in turn by the assigned reviewers, followed by a discussion involving the panel. For each of the projects, a panelist, who was not a reviewer for the project and not conflicted with it, was assigned as a scribe to prepare a written summary of the panel's discussion. Following the discussion of its intellectual merit, broader impacts, additional solicitation specific criteria (if applicable), and the results from prior NSF support (if applicable), the panel was asked to place each proposal into one of three categories: (i) Highly Competitive, (ii) Competitive, and (iii) Not Competitive.

## REVIEW ANALYSIS

**INTELLECTUAL MERIT:** The panel noted that the PIs have a strong track record pertinent to the field of the proposal and have already established a collaboration related to the proposed approach, obtaining some results in two dimensions. There was an expectation that these activities would continue, strengthen their successful path, and lead to advances in the proposed research. Reviewers commented that the proposal line of research is interesting, the topics are in a challenging and actively studied field of applied mathematics related to biology, and the questions addressed are relevant to the study of the self-assembly process of amphiphilic particles into bilayer membranes. The panel agreed that the proposed approach contained several interesting aspects. Among them, the removal of the need to identify a pre-definite surface in its formulation, its simplicity accompanied by preliminary numerical results that suggests its ability to capture self-assembly and spontaneous segregation of bilayers, and its numerical approximation which wouldn't require the use of the computationally costly molecular dynamics methods but would allow for the capturing of features that a standard continuum theory can't handle.

During the panel discussion, because of the phenomenological character of the proposed model, concerns were raised about the mechanisms that would be adopted to validate it and to improve it, if for example the fit of simulations with experimental data would prove to be inaccurate, providing further information on these mechanisms would have made for a more compelling case. Another aspect that panelists agreed would have benefited by the addition of details pertained to the use of Gamma-convergence as tool for numerical approximations, this is not a new idea but there are known drawbacks to it that could have been addressed, and to the connected stated goal of developing tools to explain functionals, such as the quoted elastic energy used in the Hamm and Kozlov theory of membrane continuum mechanics, from first principle in terms of HAP. The new challenges, and possible ways of overcoming them, expected in this rigorous derivation would have made possible a better assessment of the feasibility of this part of the proposed research. The section on incorporating fluctuating hydrodynamics was also highlighted as lacking sufficient details.

**BROADER IMPACTS:** The panel found the educational component of the Broader Impacts strong, and praised the PIs plans of outreach to local high schools and including undergraduate students in the research. Reviewers considered to be particularly noteworthy the intention of integrating educational activities at all levels, from involvement of high school students to postdoc mentoring. The proposal also indicated the plan to prioritize funding so to increase the impact on the community of the activities, including targeting students from underrepresented groups and students whose socio-economic background would be an obstacle to participating in out-of-state research experiences. The addition of details on specific research projects suitable for undergraduate and graduate students, and on possible recruiting strategies to achieve the stated goals would have further strengthened the broader impacts component.

**SUMMARY and RECOMMENDATION:** This is a collaborative proposal from a group of well-established researchers that addresses interesting and challenging problems related to the modeling and numerical analysis of self-assembly biological processes, and includes strong educational broader impacts. The panel underlined several strengths in the Intellectual Merit, notably a high significance for potential applications in biology. However, some shortcomings were also identified, such as a somewhat insufficient discussion on how the model will be validated, on aspects of the numerical approach adopted, and on details in the fluctuating hydrodynamics section. Comparing with some other proposals in this very strong competition, the panel found the proposal less persuasive and placed it in the lower half of the Competitive category. Given its ranking, and due to program budget constraints, this proposal was not in reach of the program funds available for this fiscal year.

#### Review Information

*Please note: The Sponsored Projects Office (or equivalent) at the submitting organization is NOT given the capability to read the below review information.*

### Panel Summary

Panel Summary	Release Date
<a href="#">Panel Summary #1</a>	05/09/2021

### Proposal Review [Summary of All Reviews](#)

Review	Release Date
<a href="#">Proposal Review #3</a>	05/09/2021
<a href="#">Proposal Review #2</a>	05/09/2021
<a href="#">Proposal Review #1</a>	05/09/2021

### Context Statement

Division of Mathematical Sciences

Applied Mathematics Program

#### Proposal Review Context --- 2021

Proposals handled by the Applied Mathematics Program are usually assessed by some combination of mail and panel review. The number of reviewers depends on the complexity of the proposal and the areas of expertise required. A recommendation for declination or award is not considered until two substantive reviews, and usually three or more reviews, are received. Verbatim copies of all reviews used in the decision are provided. When reading them, please keep in mind that reviewers address their comments chiefly to the NSF, not necessarily to the investigators. Some reviews may contain irrelevant, unsubstantive, or erroneous statements that were not used in evaluating the merits of the proposal.

While reviewers' ratings are considered, the content of their reviews is more important in assessing the merits of each proposal. Different reviewers may offer insights into different aspects of a proposal (problem formulation and approach, relevant work in other areas of mathematics, perspectives on the importance of a particular problem within the subarea of applied mathematics or in a broader context, as well as broader impact such as consequences for education, human resources development, public outreach, applications, other disciplines, or other technological, industrial, or societal issues). Reviewers' comments and ratings are considered in the context of other reviews they have provided. Thus average rating is not the determining factor in a recommendation; rather, a clear picture of each proposal's strengths and likely impact is sought.

Decisions about particular proposals are often difficult, and factors other than reviewer comments and ratings enter into them. For renewal applicants, often the program has additional information not available to reviewers, such as progress reports. Appropriate balance among subfields, the balance between new investigators and those previously supported, contribution to initiatives or to interdisciplinary efforts, effects on education and human resources development, the availability of other funding, the total amount of funds available to the program for new and renewal proposals, and Foundation policies are other important decision factors.

The hallmark of a successful proposal is one or more salient strengths. Usually this is reflected in high ratings, although not all reviewers give provocative but risky proposals the highest marks. It is not possible to fund all the meritorious proposals. Proposals recommended for award, as distinguished from other proposals of fundable quality, have a strong potential for impact in the field or in science more broadly. Taken collectively, the

funded proposals present a balance across the dynamic and essential areas of the discipline. This means that recommendations for award go beyond a simple ordering of proposals.

This year Applied Mathematics expects to receive over 350 competing proposals, many of them of an interdisciplinary or group nature, and to fund about a fourth of them. As always, this will include a substantial number of awards that do not provide salary for the investigators.

**CONFERENCE REQUESTS:** Conference proposals submitted to the program under solicitation NSF 16-550 with budget requests of up to \$50,000 are evaluated in accordance with NSF policy, which allows the program to forego the use of outside reviewers in assessment of proposals for such conferences and workshops. Among the criteria used to evaluate the intellectual merit and broader impacts of conference proposals are the following:

- \* Timeliness of the event with respect to developments in the area(s) of the conference
- \* Quality of the invited speakers and the scientific program
- \* Diversity and breadth of participation by individuals and institutions
- \* Involvement of participants from underrepresented groups and of students and junior investigators
- \* Overall impact of the conference on the US mathematical community

Conference proposals with budget requests between \$50,000 and \$100,000 are evaluated using the criteria just cited but following procedures that entail either more substantial internal NSF review, or external review. Conference proposals whose budget requests exceed \$100,000 require external review, just as research proposals do.

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