Agency Name: National Science Foundation

**Application** Agency Tracking Number: **2111351**

Project Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

**Program**

Program Title:

COMPUTATIONAL MATHEMATICS

Program Code: 1271

Funding Opportunity Number: PD 16-1271

Division/Area of Science: Division Of Mathematical Sciences

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**Application Status History**

| [**Status**](https://www.research.gov/gapps-web/gapps/viewDetail?agencyId=NSF&d-49653-o=2&d-49653-p=1&applicationId=2111351&grantsGovId=&d-49653-s=0) | [**Status Date**](https://www.research.gov/gapps-web/gapps/viewDetail?agencyId=NSF&d-49653-o=2&d-49653-p=1&applicationId=2111351&grantsGovId=&d-49653-s=1) |
| --- | --- |
| Declined | 05/29/2021 |

**Cognizant Program Officer Comments**

PROPOSAL ID: 2111350 (Lead) and 2111351 (Non-Lead)   
PI: Hickernell, Fred J. (Lead) and Hyman, James M. (Non-Lead)   
INSTITUTION: (Lead) and Tulane University (Non-Lead)   
TITLE: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery   
PROGRAM OFFICER: Malgorzata Peszynska   
  
Dear Drs Hickernell and Hyman,   
  
During the FY2021 competition, the Computational Mathematics program received a number of outstanding proposals. The quality of the submissions was very high, and we are simply unable to fund all deserving proposals.   
  
I regret to inform you that the National Science Foundation is unable to support your proposal referenced above. The elements of the review analysis on which the recommendation for this award is based is enclosed at the end of this letter. The reviews and panel summary are available through Fastlane. 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 you will find the reviews of assistance in the preparation of future proposals. Please do not hesitate to contact me for more information regarding this decision.   
  
Malgorzata Peszynska   
Program Director   
Computational Mathematics Program   
Division of Mathematical Sciences   
National Science Foundation   
mpeszyns@nsf.gov   
  
ELEMENTS OF REVIEW ANALYSIS   
  
REVIEW PROCESS: The proposal was reviewed by one of several panels organized by the Computational Mathematics Management Team which met in Spring 2021 virtually by zoom. Each of these panels was comprised of experts in various aspects of computational mathematics. The panel was asked to review the proposals on the basis of the two main NSF review criteria: (1) Intellectual Merit and (2) Broader Impact. Each proposal was reviewed by at least three reviewers. A panelist was appointed by the Managing Program Officer as a scribe to write a summary of the panel's discussion of the proposal. In addition to being reviewed by the Computational Mathematics panels, some proposals were also submitted to other NSF programs for co-review, and some were sent for further review.   
  
The set of proposals receiving no review rating higher than Good was presented to the panel at the start of deliberations. Panelists were given the opportunity to identify proposals in this set that merited further discussion; the remainder were not discussed further and did not receive panel summaries, and were placed in the category "Not Discussed by Panel". For each proposal discussed in detail, the panel was asked to place the proposal into one of the following two categories: (I) Competitive, (II) Not Competitive. The panel was also asked to rank (if possible) proposals within the first category "Competitive".   
  
PROJECT OVERVIEW: The project will develop methodology for sampling large scale model inputs aiming to reduce the uncertainty in model outputs which are some quantities of interest depending on the inputs through results of some computationally expensive simulations. Towards this goal, surrogate models will be constructed via multivariate approximations, moving least-squares, quasi-interpolation in reproducing-kernel Hilbert spaces, kriging based on data, and Bayesian inference and bootstrapping. Error bounds will be developed; in the end, only few simulations will be needed. The results and methods to be developed would be applicable to challenging large-scale problems such as in climate science and spread of STDs. Collaborations with, e.g., lab scientists, from Los Alamos and Goddard Institute for Space Studies as well as with public health scientists are planned.   
  
Graduate and undergraduate students will be involved, and software to be developed will be made available in public domain. Outreach to K-12 and various organizational efforts are outlined.   
  
PRIOR NSF SUPPORT: PI Hickernell outlines results from NSF-DMS-1522687, and PI Hyman from DMS-1563531. Several publications are listed, and various research and mentoring activities are described.   
  
PANEL AND REVIEW RATINGS: The project received reviews with ratings [G, G, G, and G].   
  
The proposal was placed in "Not Discussed in Panel" (NDP) category by unanimous consent of the panelists. No panel summary was produced.   
  
INTELLECTUAL MERIT: The reviews included comments on both strengths and weaknesses of the project, and I agree with the assessment expressed in the reviews. The PIs are considered well qualified, and the problems considered are important. The connection to the applications is compelling. However, the reviewers express concerns on the lack of details on various critical components of research proposed. Along these lines, some reviews consider the approaches proposed "standard". Overall there are concerns on the potential impact of theoretical developments, especially in view of that there exists already related work on methodologies with similar goals.   
  
BROADER IMPACTS: These were considered strong by all reviewers. One in particular says "The PI's will develop publicly available code for adaptive sampling, and have made substantial software contributions in the past. The research will strengthen collaborative efforts between academia and the national labs. Students will be involved in the research and mentored".   
  
POST-PANEL REVIEW: Following the panel meeting, I considered the panel reviews, deliberations, rankings, and recommendations which evaluated proposal's intellectual merit and broader impacts in relation to other proposals reviewed in this panel, the need to maintain appropriate balance among subfields, the total amount of funds available to the program, and general Foundation policies.   
  
SUMMARY AND RECOMMENDATION: The project has various strengths and weaknesses. Overall these render this proposal less compelling than those which were placed in the first category "Competitive". I recommend, regretfully, declination of the proposal.   
  
RECOMMENDATION: Decline   
  
Malgorzata Peszynska   
Program Officer   
Computational Mathematics Program

**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.*

**Proposal Review** [**Summary of All Reviews**](https://www.research.gov/gapps-web/gapps/viewApplicationReview?action=viewApplicationReview)

| **Review** | **Release Date** |
| --- | --- |
| [Proposal Review #4](https://www.research.gov/gapps-web/gapps/viewApplicationReview?action=viewApplicationReview&reviewGrantAppReview=3) | 03/29/2021 |
| [Proposal Review #3](https://www.research.gov/gapps-web/gapps/viewApplicationReview?action=viewApplicationReview&reviewGrantAppReview=2) | 03/29/2021 |
| [Proposal Review #2](https://www.research.gov/gapps-web/gapps/viewApplicationReview?action=viewApplicationReview&reviewGrantAppReview=1) | 03/29/2021 |
| [Proposal Review #1](https://www.research.gov/gapps-web/gapps/viewApplicationReview?action=viewApplicationReview&reviewGrantAppReview=0) | 03/29/2021 |

**Context Statement**

Computational Mathematics Program   
  
Proposal Review Context, 2021   
  
Proposals handled by the Computational Mathematics Program are evaluated using mail and panel reviews. The number and type of reviews used for each project depend on the complexity of the proposal and the areas of expertise required. A recommendation for declination or award is not considered until three or more substantive reviews are received. When reading reviews, please keep in mind that reviewers address their comments chiefly to the NSF, not necessarily to the investigators. Some reviews may contain irrelevant, insubstantial, or erroneous statements that were not used for making the recommendation.   
  
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 (issues related to problem formulation and approach, relevant work in other areas of mathematics, perspectives on the importance of a particular problem within a subarea of computational mathematics or in a broader context, or relevance to applications or other disciplines). Reviewers' comments are considered in the context of other reviews they have provided. Thus, the average rating is not the determining factor; rather, a clear and detailed picture of each proposal's strengths and likely impact is used for deriving a recommendation.   
  
Decisions about particular proposals are often difficult and may be reached by using factors other than reviewer comments and ratings. For renewal proposals, program directors often have additional information not available to reviewers, for example, progress reports. Appropriate balance among subfields, the balance between new investigators and those previously supported, contribution to particular initiatives or to interdisciplinary efforts, effect on education and human resource development, the availability of other funding, the total amount of funds available to the program for new and renewal proposals, and NSF policies are other important factors used for arriving at a decision.   
  
The hallmark of a successful proposal is one or more salient strengths. Usually this is reflected in high ratings, although not all reviewers give bold but risky proposals the highest marks. It has long been impossible to fund all the meritorious proposals. Proposals recommended for award, are distinguished from other high-quality proposals, by having a strong potential for impact in the field or more broadly in science. Taken collectively, funded proposals represent a balance across the dynamic and essential areas of the discipline. This means that factors other than a simple rank ordering of proposals are used for making recommendations for declination or award.   
  
This year the computational mathematics program expects to review over 300 competing proposals, many of them of an interdisciplinary or group nature, and to fund less than one third of them. As always, this will include a substantial number of awards that do not provide sufficient salary support for the investigators.

# Proposal Review 1 : 2111351

Agency Name: National Science Foundation

Agency Tracking Number: **2111351**

Organization: NSF Program:

COMPUTATIONAL MATHEMATICS

PI/PD: Hyman, James

Application Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

Rating: 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 project focuses on developing adaptive sampling strategies for high dimensional problems.   
  
Strength: The proposed approach utilizes a combination of "trend model" ST and "variation model" SV. ST will be constructed by moving least squares (MLS) with discrepancy points. SV will be constructed by adaptive approach to sequentially add sampling points. The criterion is a greedy algorithm to maximum "gain" by the new point. The PIs plan to apply the algorithms to real-world problems of large scale.   
  
Weakness: The approach is rather standard, as it has been explored by others. For example, the sequential sampling strategy based on maximum variance for SV, which uses Gaussian process, is a standard strategy for GP. The alternative approaches reviewed in Section 2.4 are quite limited. Adaptive sampling theories, for example, Leja sequence and others, are overlooked.   
  
In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.   
  
Many aspects of broader impacts are proposed and discussed. Most of them are, however, rather vague and routine, without clearly defined goal or plan. The proposed software development is worth noting.   
  
Please evaluate the strengths and   
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if   
applicable

# Proposal Review 2 : 2111351

Agency Name: National Science Foundation

Agency Tracking Number: **2111351**

Organization: NSF Program: COMPUTATIONAL MATHEMATICS

PI/PD: Hyman, James

Application Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

Rating: 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.   
  
Adaptive sampling for computer model surrogates, the central theme of the proposed work, is a very well-studied topic.   
  
Strengths:   
The most compelling aspect of the proposed work is developing sequential design approaches that are applicable to (relatively large) input dimensions by exploiting low dimensional structures using something like active subspaces.   
  
The PIs are well-qualified to carry out the proposed work.   
  
Weakness:   
Beyond the extension to target input spaces, the proposed work seems very standard.   
  
In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.   
  
The methodology is widely application to domain sciences. The PIs plan to apply their methodology to aid in studying the impact of volcanic ash on the North Atlantic Oscillation and in studying stochastic models of STIs.   
  
The PIs are planning research experiences for both undergrads and high school students.   
  
Please evaluate the strengths and   
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if   
applicable   
  
Summary Statement   
The PIs propose adaptive sampling for computer models with (moderately) high dimension input spaces. The proposed methodology looks for and exploits low-dimensional structures to efficiently determine good estimates of range parameters.

# Proposal Review 3 : 2111351

Agency Name:

National Science Foundation

Agency Tracking Number:

**2111351**

Organization:

NSF Program:

COMPUTATIONAL MATHEMATICS

PI/PD: Hyman, James

Application Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

Rating: 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.   
  
Strengths:   
1) The proposal addresses an important problem of building a surrogate   
model for a high-dimensional input data with limited samples (because   
each sample is expensive to obtain)   
2) The proposal touches upon all the issues: modeling with uncentainty,   
adaptive sampling acquisition functions, hyperparameter tuning,   
data-driven error bounds.   
3) The PIs have identified two realistic simulations to be used to test   
their methods.   
4) The lead PI was funded previously by NSF (2015-2018). The team has produced   
many publications, which laid the foundational work.   
  
Weaknesses:   
1) The design of the acquisition functions is a critical component   
of the model construction phase, which affects the model accuracy.   
The proposal only briefly mentions this, without much detail.   
2) In the variation models, the PIs intend to develop different kernels.   
But the details are missing, and the benefits of different kernels   
are not well articulated.   
  
  
In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.   
  
Strengths:   
1) The proposal involves many junior scholars, including   
a junior faculty, two undergraduate students, and one   
graduate students, as well as high school summer students.   
2) The PIs have plans to make software avaialble, give tutorials,   
in addition to publishing papers.   
  
Please evaluate the strengths and   
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if   
applicable

Summary Statement   
The PIs propose a combined surrogate model, incorporating a trend model   
obtained from a deterministic least square fitting and a variational   
(statistical) model from Gaussian process. Even though the proposal   
touches upon all the issues in building the surrogate models, the   
details of two critical components are missing, that is, the design   
of the acquisition functions and the choice and benefits of   
different kernels.

# Proposal Review 4 : 2111351

Agency Name:

National Science Foundation

Agency Tracking Number:

**2111351**

Organization:

NSF Program:

COMPUTATIONAL MATHEMATICS

PI/PD: Hyman, James

Application Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

Rating: 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.   
  
This proposal explores adaptive sampling procedures. After an initial exploration phase, samples are iteratively added in a way which reduces minimizes model uncertainty.   
  
STRENGTHS   
-The sampling procedure is adaptive not just in terms of the data/parameter vectors x, but also in terms of the function to be learned.   
-The applications are compelling and seem closely tied to the proposed research.   
-The PI’s have thought about developing a sampling procedure which avoids the curse of dimensionality in several ways.   
  
WEAKNESSES   
-What in the theoretical framework ensures that the function class C is chosen to be large enough? Although the PIs note this is an area to be investigated, the class introduced in (13) seems artificial, almost like they assume C to be the function class where the method works, and then say the method works on C. I may be misunderstanding something in the framework, but this was a concern. I am thus not sure the research will make a significant theoretical contribution.   
-The proposal didn’t have a clear assessment plan, i.e. it was unclear how progress would be evaluated.   
  
  
In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.   
  
STRENGTHS   
-The PI’s will develop publicly available code for adaptive sampling, and have made substantial software contributions in the past.   
-The research will strengthen collaborative efforts between academia and the national labs.   
-Students will be involved in the research and mentored.   
  
WEAKNESSES   
-I didn’t observe any weaknesses in terms of broader impacts.   
  
  
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 good proposal which develops adaptive sampling methods and has strong broader impacts. However the rationale for the theoretical framework was unclear to me, so I would not give the proposal high priority for funding.