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Proposal: 2053714

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Agency

Agency Name: National Science Foundation

Application

Agency Tracking Number: **2053714**

Project Title: Collaborative Research: Quasi-Monte Carlo Community Software

Requested Amount: \$395,338

Received Date: 09/15/2020

PI/PD: Fred Hickernell

Authorized Representative: Toni Allen

Submitting Institution: Illinois Institute of Technology

Program

Program Title: CDS&E-MSS

Program Code: 8069

Funding Opportunity Number: PD 20-8069

Division/Area of Science: Division Of Mathematical Sciences

Program Contact Name: Yong Zeng

Program Contact Phone: (703) 292-7902

Program Contact Email: yzeng@nsf.gov

Application Status History

Status

Status Date

Declined

03/14/2021

Cognizant Program Officer Comments

Proposal ID: DMS 2053714

PI: Fred J Hickernell

Institution: Illinois Institute of Technology

Title: Collaborative Research: Quasi-Monte Carlo Community Software

Collaborative Proposal Information

Proposal ID: DMS 2053715

PI: Simon Mak

Institution: Duke University

Dear Professors Hickernell and Mak,

I regret to inform you that the National Science Foundation is unable to support the proposal referenced above.

During the FY21 competition, the CDS&E-MSS program received a number of outstanding proposals representing many different areas of CDS&E-MSS from both junior as well as established senior researchers. The quality of the submissions was very high, and we are simply unable to fund all deserving proposals.

Your proposal was reviewed by a CDS&E-MSS panel, whose members represent a broad range of expertise within the mathematical, statistical and computational sciences. 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 members of the panel. During the panel meeting, all proposals were discussed and a panel summary of the discussion was prepared as part of the review process. Following the discussion, the panel was asked to place proposals into one of the following three categories: (I) Highly Recommended for Funding, (II) Recommended for Funding if Possible, and (III) Not Recommended for Funding.

Your proposal received reviews with ratings: E/V, V, F and F. respectively. Based on the reviews and the panel deliberations, your proposal was placed in the lower half of Recommended for Funding if Possible category.

My recommendation is based on the following analysis of the reviews and panel summary:

Project Overview:

The PI propose to grow QMCPy, a Quasi-Monte Carlo (QMC) Python software library in three directions: (1) implement in a broader offering of low discrepancy sequence generators, (2) implement a broader array of algorithms, and (3) develop and implement a broader spectrum of use cases for QMC.

Intellectual Merit:

While the reviewers and panel noted that industry collaborators are mentioned and viewed it as a strength, the panel had divergent opinions on the proposal. Some panelists felt that the proposal, framed as a software development project for easy access to quasi Monte Carlo methods, presents new statistical methodology as well, not just software. Other panelists felt that there is just potential for the software development to spur statistical methodology development. One reviewer, who rated the proposal high, acknowledged that "The technical and mathematical developments are sprinkled in with some good ideas, but not fleshed out," and that "This proposal deals directly with software development, but the theory and mathematical results are not described." Another reviewers who also rated high commented that "It would have been helpful to include a page or so with a worked example on a real application, to provide some evidence that this is useful for real problems." And another reviewer remarked that "It is not clear that the project will produce substantial methodological innovations. It is not clear if the project will have an impact outside the community dedicated to QMC." One more reviewer wrote that "Details on the actual tasks, their challenges, innovations, etc would have made the proposal competitive."

Broader Impacts:

Beside potential impacts in Bayesian inference, financial risk, uncertainty quantification, and machine learning where QMC employs, the PIs describe plans for open-source software development, educating and mentoring cross-disciplinary computational researchers including both undergraduate and graduate students, outreaching and mentoring under-represented minorities, women, and students from colleges where research experiences are rare.

Outlying Review:

One reviewer felt that the development of a QMC package for python is important and impactful, and rated the proposal as E/V. However, the reviewer pointed out several weaknesses of the proposal, including “questions about scope, organization and deployment for this particular project.” The reviewer also agreed with the panel summary, ranking and placement.

Summary: The reviewers found strengths and several weaknesses in this proposal. While some panelists felt that the proposal also presents new statistical methodology, other panelists and reviewers felt differently. The panel and the reviewers raised several concerns including the insufficient description on the actual tasks, the challenges, and the innovations as well as the vagueness of the impact outside the community dedicated to QMC. These concerns made the proposal less compelling than other proposals in the competition and ranked higher.

Recommendation: In the current highly competitive funding situation, those concerns put the proposal at a disadvantage compared with other highly rated proposals. Taking into account the comments of the reviewers, the goals of the program, and the available budget, unfortunately this proposal is not as competitive as several other proposals submitted to the CDS&E-MSS competition this year and ranked higher.

The Management Team of the CDS&E-MSS Program recommended that this proposal be declined.

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.

Sincerely,

Yong Zeng
Program Officer
CDS&E-MSS Program
Division of Mathematical Sciences
National Science Foundation

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
Panel Summary #1	03/11/2021

Proposal Review [Summary of All Reviews](#)

Review	Release Date
Proposal Review #4	03/11/2021
Proposal Review #3	03/11/2021
Proposal Review #2	03/11/2021
Proposal Review #1	03/11/2021

Context Statement

Virtually all proposals submitted to the DMS CDS&E-MSS Program requesting support with Fiscal Year 2021 funds were reviewed in two virtual panels through Zoom run by the program. The panels, composed of researchers with inter-disciplinary expertise in a variety of mathematical, statistical, and computational sciences, were asked to review the proposals based on the two main NSF review criteria of Intellectual Merit and Broader Impacts, as described in the solicitation.

For each proposal, three or more independent reviews were obtained. Each proposal under panel review was considered, one at a time, as a candidate for detailed discussion of the proposal's intellectual merit and broader impacts. All conflicted panelists and NSF staff members left the Zoom virtual panel room prior to discussion and did not participate in any way in the review and decision process. Following the discussion, the proposal was placed into either one of three categories: (1) Highly Competitive, (2) Competitive, and (3) Not Competitive; or one of the three: (1) Highly Recommended for Funding, (2) Recommended for Funding if Possible, and (3) Not Recommended for Funding. The proposals reviewed also received a Panel Summary reflecting the panel's discussion and recommendation.

With a few proposals, Program Directors sought further ad-hoc mail reviews after the panel. These additional reviews were deemed necessary to arrive at a funding decision. The number of ad-hoc reviewers depended on the complexity of the proposal and the areas of expertise required.

Verbatim copies of all reviews and the panel summary are provided to the PIs. The PIs are advised that reviewers address their comments to the NSF, not to the principal investigators. Reviewers may make remarks without giving detailed references or specific suggestions for improvement. Any lined-out statements in a review were judged irrelevant, non-substantive, or erroneous, and were not used by the NSF in making decisions.

While reviewer ratings are taken into account in a recommendation, the content of their reviews is more important in assessing the merits of individual proposals. Different reviewers may offer insights into different aspects of a proposal (e.g., problem formulation, qualification of the PIs, relevant work in other areas, perspectives on the problem's importance, assessment of its importance to the discipline, and relevance to applications or other disciplines when the research has an interdisciplinary thrust). Thus, ratings are not the sole determining factor in a recommendation; rather, an assessment of each proposal's strengths and likely impact is sought.

Decisions about individual proposals are often difficult, and factors beyond reviewer comments and ratings influence end recommendations. For renewal applicants, additional information not available to reviewers, such as progress reports, may be important. Other factors Program Managers consider include: NSF policies and emphases, balance among subfields, balance between new and repeat investigators, contribution to Federal initiatives or interdisciplinary efforts, effect on education and human resource development, the availability of external funding, and the total funding available to the program. Sometimes, revised versions of proposals declined one year are awarded in subsequent years; conversely, research that has been supported for multiple funding cycles can be declined as new, more promising, proposals enter the competition.

The hallmark of a successful proposal is one or more salient strengths. Due to budgetary constraints, it is not possible to fund all meritorious proposals. Proposals recommended for an award, as distinguished from other proposals "of fundable quality," have a strong potential to impact the field or general science. Taken collectively, the funded proposals strike a balance across the dynamic and essential areas of the discipline. This means that recommendations for awards go beyond a simple panel ordering of proposals.

The Program Directors for CDS&E-MSS in FY2021 are

Malgorzata Peszynska, mpeszyns@nsf.gov

Andrew Pollington, adpollin@nsf.gov

Yong Zeng, yzeng@nsf.gov

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Proposal Panel 1 : 2053714

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Agency Name: National Science Foundation

Agency Tracking Number: **2053714**

Panel Summary

Panel Summary

Brief Summary of Project

The PIs plan to grow QMCPy, a Quasi-Monte Carlo Python software library, from its nascent form to be a library more widely embraced by the scientific community. Quasi-Monte Carlo methods potentially yield significant improvements in computational efficiency over the usual independent identically distributed sampling for a wide range of important problems.

Intellectual Merit

Strengths:

This proposal, framed as a software development project for easy access to quasi Monte Carlo methods, presents new statistical methodology as well, not just software. Other panelists felt there is just potential for the software development to spur statistical methodology development. Industry collaborators are mentioned in the proposal.

Weaknesses:

The importance and relevance of the contribution is not clearly spelled out. The potential impact of the proposal should have been explained better.

Broader Impacts

Strengths:

Software development can reach a broad community of users. Graduate student mentoring is mentioned.

Weaknesses:

None noted.

Results from Prior NSF support:

The PIs have been very productive under previous NSF support.

Data Management plan:

Adequate.

Post-doctoral Mentoring Plan
N/A

RECOMMENDATION

This is a proposal for software development, which is always important and necessary for the scientific community, but the specific relevance and importance of this proposal should have been explained more clearly.

The panel placed this proposal in the category: Recommended for Funding if Possible

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

PANEL RECOMMENDATION: Recommended for Funding If Possible

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Proposal Review 1 : 2053714

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Agency Name:	National Science Foundation
Agency Tracking Number:	2053714
Organization:	
NSF Program:	CDS&E-MSS
PI/PD:	Hickernell, Fred
Application Title:	Collaborative Research: Quasi-Monte Carlo Community Software
Rating:	Fair

Review

Summary

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

Brief Summary of the project:

The aim of the project is to develop a library of quasi Monte Carlo (QMC) Python software that is adopted by the QMC community as a platform and repository of software. The effort seeks to integrate the contributions of different research groups into a cutting edge package available to other researchers and practitioners. The proposal includes two PIs from two different institutions and one senior personnel.

Intellectual Merit

Strengths

The proposal seeks to provide a software platform for the implementation of

QMC methods. QMC is surging as a potential alternative to more traditional Monte Carlo methods that provide high efficiency and fast convergence rates for the estimation of functionals of a multivariate probability distribution. By making available a common environment for QMC, the project aims at creating a focal point for the community, fostering links between research groups, and between researchers and practitioners. This will enhance the growth of QMC.

Weaknesses

The narrative of the proposal is very focused on engineering a software to enable fitting models that use QMC. The narrative highlights the need for implementation of QMC approaches, rather than development of new QMC methodologies. In fact, the aims of the project are described in Section 3 with a list of subsections that describe different components that will be part of the proposed platform. Each subsection concludes with a sentence indicating the algorithm that will be implemented. QMC is not a very mainstream part of computational statistics research, and, unfortunately, the narrative fails to convey its advantages and potential. But most importantly, the project puts the emphasis in the software development, rather than in the development and study of QMC methods and the exploration of their theoretical properties. The narrative vaguely indicates that the availability of a platform and the ability of the community to tackle interesting applications will spur the needs for better methods and theory.

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

Broader Impacts

Strengths

The proposal has a strong potential to impact the development of QMC methods by providing a focus point for the QMC community.

Weaknesses

The narrative does not make a strong case to illustrate the potential of the proposed platform to have a broad impact in the area of computational statistics. Beyond the fact that the existence of a good platform for QMC will facilitate the use of such methods, there are no solid examples of the power of the methods that the project aims to implement.

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

Summary Statement

The project proposes the implementation of methods that correspond to some of the goals of CDSE. It is not clear that the project will produce substantial methodological innovations. It is not clear if the project will have an impact outside the community dedicated to QMC.

This proposal ranks at the bottom 33% of the ones I reviewed.

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Proposal Review 2 : 2053714

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Agency Name: National Science Foundation

Agency Tracking Number: **2053714**

Organization:

NSF Program: CDS&E-MSS

PI/PD: Hickernell, Fred

Application Title: Collaborative Research: Quasi-Monte Carlo Community Software

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.

The proposal seems to focus on constructing and updating a specific package and the tools it would need. Given the importance of sampling to a host of applied scientific settings, this has good potential and there are a range of potential applications discussed in the proposal. A major concern is that there is no explanation of how this software will be integrated with existing software packages. Namely, is the idea simply to recreate existing methods or something else? As an example, to improve posterior sampling would be great, but how will this interface with popular modeling frameworks like Stan? AS another example, `ray tracing` seems thrown in as an aside.

As a software development proposal, it is lacking key details on internal testing, how the API will be handled, and what use cases will be used during development. There is not a userbase discussion or any version control philosophy outlined. Licensing appears to currently be Apache, which does not mesh well with BSD or MIT. There are more detailed argument against the deployment, for example the idea that `Python code does not execute particularly quickly.` I am skeptical of this argument, as when you use something like `\verb|numpy|` or `\verb|cupy|` then you can take advantage of this. Writing your backend in C might seem faster, but does this mean a user will have provide a compatible likelihood for example? Moreover, is C the actual package, will python be only used as front end? If so, why not write front ends for several packages like R?

The technical and mathematical developments are sprinkled in with some good ideas, but not fleshed out. The organization is a little odd in terms of a development project. Funding students on project like this can be risky because it requires significant development and less core research. Also, Art

Owen is mentioned quite often but appears to be only an unfunded collaborator.

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

The project would be hugely impactful if deployed correctly, but there are many questions about the development process. There is a lack of discussion of unit/regression tests that would help give users confidence in the method's function. The API should be designed with a userbase in mind to have broad impact, but the proposal does not outline the userbase.

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

This proposal deals directly with software development, but the theory and mathematical results are not described.

Summary Statement

Development of a QMC package for python is important, but there are questions about scope, organization and deployment for this particular project.

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Proposal Review 3 : 2053714

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Agency Name:	National Science Foundation
Agency Tracking Number:	2053714
Organization:	
NSF Program:	CDS&E-MSS
PI/PD:	Hickernell, Fred
Application Title:	Collaborative Research: Quasi-Monte Carlo Community Software
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.

This proposal is to build on a new software project called QMCPy, which implements quasi monte carlo sampling for numerical evaluation of expected values of functions of random variables. The proposed work will implement new features into the software project and engage the community of researchers in QMC sampling to grow the project.

The idea to build software that people can actually use is worth pursuing. The authors list several use cases for QMC sampling, and show the benefits of the method on some toy examples.

It would have been helpful to include a page or so with a worked example on a real application, to provide some evidence that this is useful for real problems.

The authors list some challenges for parallel implementation, but then go on to say they will do it, without any indication of how they will solve the aforementioned challenges.

Overall, I think this is a project that has a high chance of success and a good chance of having a real impact for researchers.

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

The authors list potential impacts within the community of bayesian software projects. They also predict that the work will lead to new theoretical developments in QMC sampling. Their claim that their work will "showcase the right way" to do QMC sampling, and that they will set an example of good software development for students, and that they will publish their work in journals, present at conferences, and offer tutorials on the software.

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

Summary Statement

This proposal has a high chance of success and impact on fields that need easy access to QMC methodology.

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Proposal Review 4 : 2053714

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Agency Name: National Science Foundation

Agency Tracking Number: **2053714**

Organization:

NSF Program: CDS&E-MSS

PI/PD: Hickernell, Fred

Application Title: Collaborative Research: Quasi-Monte Carlo Community Software

Rating: Fair

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 plans to grow the existing software package QMCpy, a quasi Monte-Carlo python software library. Several existing approaches and applications will be implemented. If successful, QMCpy is potentially useful for the QMC community and beyond.

Strengths:

- + QMCpy is already in place and the PIs have worked on various aspects of QMC.
- + Most latest developments in QMC community will be implemented/added to QMCpy and will be made available to broader communities
- + QMCpy seems to have strong supports from academia (Stanford and Warwick) and industry (SigOpt) through collaborative letters.

Weaknesses:

- The proposal focuses on implementing available methods. Most, if not all places, tasks are simply with one sentence "we will implement...". Challenges, and hence innovations must be made, etc to carry out the implementations are not discussed. The proposal would be much stronger if these aspects have been detailed/identified and approach to overcome.

- Other more descriptive tasks, such as in Section 3.1: "implement some numerical optimization algorithms for constructing low discrepancy designs" lack details, which makes the actual work uncertain. Other examples are "we will implement LD sequences taking advantage of multiple cores of the same CPU. We will also explore the possibility of GPU implementations", and "We will strengthen QMCPy's rudimentary MLQMC, including extending the theory and implementation of the single level stopping criteria developed by PI FH, SCTC, and their collaborators [45, 47, 49, 56, 59] to the multilevel case."

As a consequence, it is not clear what the actual tasks will be taken and how to assess their success.

- The proposal would have been stronger had the PIs provided the history of downloads, the number of users, etc of the current QMCPy package.

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

Strengths:

+ The PIs are known in the communities and the PIs have made effort to reach out the user communities via tutorial, talks, etc.

Weaknesses:

- Since this is a software proposal, details on deliverables, delivery mechanism and community usage metrics should have been discussed in details.
- Sustainability, especially beyond the life of the project, is not discussed.

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

Summary Statement

The idea of collecting on the implementations of well-established algorithms and latest algorithms in one community software is important for the appropriate communities. The PIs are qualified to achieve such a task. Details on the actual tasks, their challenges, innovations, etc would have made the proposal competitive.

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