UNIVERSITY OF MARY WASHINGTON

Faculty Research Grant Proposal
Cover Sheet
DUE: November 6, 2017

Name:	James Collins	**Funding Period:**	July 1, 2018- June 30, 2019
Department:	Mathematics	**IRB Required** ☐	
Project Title:	A Posteriori Error Estimation for the Spectral Deferred Correction Method		

Abstract (250 words maximum)

Many physical phenomena are modeled by mathematical equations. These equations are often very complicated and their solutions must be approximated using a computational method. These approximations necessarily include error, and an important area of mathematics is to estimate the error in these approximations. These error estimates can be used to determine the accuracy of an approximation, as well as determine the most efficient method for improving the solution. In recent years, a computational method called the Spectral Deferred Correction (SDC) method has been introduced. In this project, I propose to derive and test formulas for determining the error associated with an approximation obtained from the SDC method. After deriving these formulas, my goal is to use them to develop an algorithm for improving an approximate solution in the most efficient way.

Budget Request: ☒ Summer Stipend Only ☐ Summer Stipend with expenses ☐ Project Expenses Only ☐ Fall Course Release ☐ Spring Course Release

Simultaneous Applications ☐ Internal Grant ☐ External Grant

Previous FRG Awards: ☐ 2014-15 ☐ 2015-16 ☐ 2016-17 if the funding period has ended.

☒ By checking here I indicate that I understand that my application will not be considered if the office of the dean cannot verify the receipt of a final report for a previously funded faculty development research grant.

☒ By checking here I indicate that I have followed the guidelines (http://cas.umw.edu/dean/guidelines-for-faculty-research-grant-applications/) and that my application consists of the following eight elements: project description, project significance, timeline and logistics, results, documentation, budget, simultaneous applications, and supporting materials.

SIGNATURES:

Applicant:	[signature]	Date:	11/1/17
Department Chair:	[signature]	Date:	11-1-17

Project Proposal:
A Posteriori Error Estimation for the Spectral Deferred Correction Method

October 21, 2017

1 Project Description

Many phenomena (physical, biological, financial, etc.) can be modeled by mathematical equations. These models can then be used to test theories about the phenomena to predict future results or to design optimal structures. Mathematical modeling is ubiquitous in society today; it can be observed in weather models or the design of a plane wing or car engine. However, these equations are incredibly complex, and exact solutions are often impossible or very expensive to obtain. Therefore, computational methods have been developed to find approximate solutions to these equations.

However, a problem exists with an approximate solution because there is error inherent in the solution, i.e. some difference between the theoretical exact solution and the computable approximate solution. This error could be small and of no significance, or large and result in the model being unreliable. One of my research areas is to develop methods and formulas for estimating the error in an approximation, that is, in determining how "wrong" an approximation is and what can be done to improve it. In particular, I specialize in the area of **goal-oriented a posteriori error estimation** along the lines of [1, 9, 10]. In this type of error estimation, focus is on a particular goal or what is called a **quantity of interest** in the approximation. I perform additional computations to determine the difference between the exact and approximate solutions in this particular quantity of interest. For example, if we are modeling the speed of the air as it flows over an airplane, we may be interested in very accurately approximating that speed near the tip of the wing. In this case, one could estimate the error only near the tip of the wing, and ignore the error over the plane body. This method of estimation allows us to focus exactly on the specific data under consideration and not waste time and effort on data related to the entire plane.

In this project, I propose to develop error estimation formulas that apply specifically to approximations obtained from the **spectral deferred correction (SDC) method** [8, 11]. This method has been developed in recent years as a way to solve certain equations which have proved difficult using standard methods. The SDC method can produce approximations of high accuracy with less computation than other methods employed. Currently, there exists no goal oriented error estimation for approximations obtained from this method, and I intend to derive formulas for that estimate.

In addition, the SDC is generally implemented in **serial**, meaning that all computations are done on a single computer. However, recent work has been conducted to implement the SDC method in **parallel** [2] which allows the work to be distributed among multiple computers simultaneously. This is accomplished by breaking up the equation into multiple smaller parts. Referring to the plane example again, this process is similar to breaking the plane into multiple patches and solving the equation on each patch separately and simultaneously, then taking each solution and gluing them together. This gluing process introduces additional error to the approximation. Another goal of this project is to account for this additional error in the error estimation formulas.

This research will be conducted in collaboration with Dr. Jehanzeb Chaudhry at the University of New Mexico. He also specializes in error estimation, and, in particular, has worked with error estimation for parallel methods [4]. In this collaboration, I will seek to understand the serial SDC method; how it functions and developing the best way to represent the error of approximations obtained from this method. I will also implement the SDC method which is needed for us to test the error estimation formulas. Dr. Chaudhry will be focussing on the parallel implementation of the SDC method, implementing the method in parallel and deriving error estimation formulas for the parallel version of the method. Deriving the error estimation formulas is the most difficult portion of this project, and we will be collaborating heavily on this segment of research in order to check each other's work and to obtain the best results.

Dr. Chaudhry and I were both postdoctoral fellows under Dr. Estep at

Colorado State University. I have collaborated with Dr. Chaudhry previously on a different project which resulted in a published article in a peer-reviewed journal [3]. This previous project demonstrated that we are able to work well together and produce publishable results. We have complimentary skills in the field of error estimation, in that I have experience with serial methods and he has experience with parallel methods. Therefore, we are ideally suited to collaborate on this project.

2 Project Significance

This project is significant for many reasons. First, the SDC method does not currently have a goal-oriented error estimation formula. This research would develop such a formula and give modelers using this method a better understanding of the error in their approximations. Error estimation is also used to determine the most efficient means of improving an approximate solution. This formula would also allow modelers to improve their solutions based on which part of the model they want to focus their attention.

In this work, we will also be developing error estimation for parallel methods, which is an important class of methods. Computers are close to reaching their maximum individual speeds, and the current best practice for accelerating computations is to distribute the work across many computers, i.e. parallel methods. Developing error estimation tools for this class of methods is crucial to advancing the field of error estimation as these methods are increasingly applied in practice.

Finally, this work is important for my professional development as it continues the line of work I have done previously with error estimation. I have published multiple articles on error estimation of other computational methods [3, 5, 6, 7]. This research would allow me to learn about another method, but more importantly, to learn about a parallel method. My work thus far has involved serial methods, and I would like to expand my knowledge about parallel methods. Collaborating with Dr. Chaudhry is an ideal way for me to expand my research in this direction. In addition to expanding my research field, I will also be able to share the experience I gain from this project with my students either in a course on computational methods or in an independent research project.

3 Timeline and Logistics

Due to my success with previous research in error estimation formulas, I have every confidence that this work will also be a success. The timeline for this project will be as follows:

Summer 2018: I will continue researching the serial SDC method while Dr. Chaudhry considers the parallel version. In collaboration with Dr. Chaudhry, I will develop formulas for estimating the error in this method both in serial and parallel. Then, I will write a computer program to test those formulas in serial while Dr. Chaudhry writes a program to test the formulas in parallel.

Fall 2018: I will begin to write an article with Dr. Chaudhry on the results we obtained during the summer.

Spring 2019: I will present my research at the Joint Mathematics Meetings in January. The article will be completed and submitted during the spring semester.

4 Results

For each error estimation formula I have researched previously, I have written an article that has been accepted to a peer-reviewed mathematics journal [3, 5, 6, 7]. Once this work is completed, I intend to submit at least one, possibly two articles to a peer-reviewed journal for publication. One article will involve the error estimation formulas we derive for the parallel method. If our research on the serial method yields sufficient results for an article, we will also submit one focussed solely on the serial method. In addition, I will present the result of this research during a presentation at the Joint Mathematics Meeting. This is the largest meeting of mathematicians in the world and will thus be an excellent forum for disseminating these results.

5 Documentation

References

[1] M. Ainsworth and J. T. Oden, *A posteriori error estimation in finite element analysis*, Comput. Methods Appl. Mech. Engrg., 142 (1997), pp. 1–88.

[2] M. Bolten, D. Moser, and R. Speck, *A multigrid perspective on the parallel full approximation scheme in space and time*, Numerical Linear Algebra with Applications, (2016).

[3] J. H. Chaudhry, J. B. Collins, and J. N. Shadid, *A posteriori error estimation for multi-stage Runge-Kutta IMEX schemes*, Appl. Numer. Math., 117 (2017), pp. 36–49.

[4] J. H. Chaudhry, D. Estep, S. Tavener, V. Carey, and J. Sandelin, *A posteriori error analysis of two-stage computation methods with application to efficient discretization and the parareal algorithm*, SIAM Journal on Numerical Analysis, 54 (2016), pp. 2974–3002.

[5] J. B. Collins, D. Estep, and S. Tavener, *A posteriori error estimation for the Lax-Wendroff finite difference scheme*, J. Comput. Appl. Math., 263 (2014), pp. 299–311.

[6] J. B. Collins, D. Estep, and S. Tavener, *A posteriori error analysis for finite element methods with projection operators as applied to explicit time integration techniques*, BIT, 55 (2015), pp. 1017–1042.

[7] J. B. Collins, D. Estep, and S. Tavener, *A posteriori error estimation for a cut cell finite volume method with uncertain interface location*, Int. J. Uncertain. Quantif., 5 (2015), pp. 415–432.

[8] A. Dutt, L. Greengard, and V. Rokhlin, *Spectral deferred correction methods for ordinary differential equations*, BIT Numerical Mathematics, 40 (2000), pp. 241–266.

[9] D. Estep, *A posteriori error bounds and global error control for approximation of ordinary differential equations*, SIAM J. Numer. Anal., 32 (1995), pp. 1–48.

[10] M. B. Giles and E. Süli, *Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality*, Acta Numer., 11 (2002), pp. 145–236.

[11] M. L. Minion et al., *Semi-implicit spectral deferred correction methods for ordinary differential equations*, Communications in Mathematical Sciences, 1 (2003), pp. 471–500.

6 Budget

I am asking for $4000 for a summer stipend.

7 Simultaneous Applications

I am not applying for any other funding for this project.

8 Previous Awards

I have not obtained any previous university awards as I started at the university in Fall 2017.

9 Supporting Materials

A letter from Dr. Chaudhry stating his willingness to collaborate with me on this project.