Research Statement
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Summary of Research

The overarching theme of my research is the analysis, implementation, and use of numerical methods to solve multiple types of problems involving differential equations. I have multiple different areas to my research, with the two major ones being **a posteriori error estimation** through adjoint-based methods and **numerical algebraic geometric** algorithms. I have also recently begun research involving **symmetric spaces** of Weyl groups.

Working on such a wide variety of numerical methods and problems gives me a large base of knowledge and skills with which to expand my current research, or establish new research directions. I enjoy working on new problems and always seek to find collaborators and research areas where my mathematical expertise can be useful. Both areas of a posteriori error estimation and numerical algebraic geometry are widely funded and provide ample projects for student research.

Student Research

I am currently directing both **undergraduate** and **graduate** student research, as well as leading multiple **capstone** projects. Many of these projects are extensions of my own research, however one is a project the student wished to investigate further, and I am directing his efforts. As my current research projects progress, they will generate further student projects. For instance, my collaboration with the members on the numerical algebraic geometry team will lead to many small projects that will be accessible to students . In the future, I look forward to collaborating with other mathematicians and especially with researchers from other disciplines to find additional interesting problems for students to consider. I also intend to pursue funding to allow my students to travel to conferences to present their research results and connect with the mathematical community for the first time. For specific ideas, see the **Student Research Projects** sections below where I have listed some possible research projects associated with my current research directions.

Research Directions

A Posteriori Error Estimation

A posteriori error estimation is a method by which an approximate solution is used to estimate the error in that approximation. Often, the computation of the error in an approximation is as important to scientists as the approximation itself. Adjoint based error estimation uses the solution of the adjoint or dual problem to estimate a linear functional of the error. These methods are used to drive **adaptivity** codes, which find the most effective use of computational power to reduce the error in an approximation.

Error Estimation for Finite Difference and Finite Volume Methods

A large portion of my research in this area involves deriving reliable and accurate error representation formulas for discretization methods that have not previously been considered for adjoint-based error estimation. These include: **explicit time integrators**, such as Runge-Kutta and Adams-Bashforth schemes; methods for solving **conservation laws** such as Lax-Wendroff; **Implicit-Explicit (IMEX)** schemes; methods for solving **interface problems** with discontinuous coefficients; and methods for **fully nonlinear second order elliptic** partial differential equations. Each of these problems and numerical methods are distinct, and developing accurate and informative error estimation for each requires a new and innovative approach.

Representation of a General Class of Numerical Methods in a Finite Element Framework

Error estimation that involves the adjoint operator provides a way to quantify the effects of stability on the accuracy of a quantity of interest. However, while such analysis is natural for finite element methods, this approach is not easily extended to finite difference and finite volume methods. My work extends such error estimation techniques to *nodal* schemes by representing finite difference schemes as finite element methods. These finite element methods are said to be **nodally equivalent** to their corresponding finite difference scheme. Nodal equivalence is a concept I developed to describe two numerical methods whose approximations agree at the nodes of a discretization. An approximation obtained from a nodally equivalent finite element method is identical to its corresponding finite difference approximation, but is amenable to adjoint-based error estimation.

In my work developing nodally equivalent finite element methods, equivalency requires two approximation steps. First, the differential operator must be approximated, leading to a modified differential equation, for instance,

$$\underbrace{\dot{y} = f(t, y)}_{Original} \quad \rightarrow \quad \underbrace{\dot{\tilde{y}} = f(t, P\tilde{y})}_{Modified},$$

where P is some approximation operator, generally piecewise defined on the discretization subintervals. This modified equation is solved with a typical finite element method, where a particular (often atypical) quadrature must be used to approximate the integrals. Both of these approximations are specific to the method being analyzed.

In my work, I derive equivalent finite element methods for multiple types of numerical schemes, each of which requires a unique approach. When considering **explicit multi-stage time integrators** [3], I use a Taylor series approximation to derive the modified equation. The corresponding quadratures are defined from the method's Butcher table. For **explicit multi-step time integrators**, a polynomial extrapolation operator is used and the integration in the finite element method is done exactly. My work also looks at the Lax-Wendroff method for solving hyperbolic PDEs [2] in which both a temporal and spatial approximation are performed to obtain equivalency. Finally, for **Implicit-Explicit (IMEX)** schemes, a separate approximation is performed for the explicit and implicit parts.

Student Research Projects: Students can develop nodally equivalent finite element methods for other finite difference schemes such as Lax-Friedrichs or an upwind scheme. With their new equivalent scheme, they can derive corresponding error representation formulas and analyze them. This project will give them experience with the finite element method and introduce them to error estimation.

Derivation of Error Representation Formulas

Once a nodally equivalent finite element method is obtained, typical adjoint-based error analysis can be performed for that method. Since the finite difference schemes being considered are often low-order, numerical error can be significant in practical applications. Therefore, it is crucial that we are able to accurately quantify the error in a particular quantity of interest. Also, due to the computational complexity of the code within which these methods lie, adaptive refinement based solely on the quantity of interest is critical to keeping the methods tractable.

In deriving the error representation formula for finite difference methods, I find additional terms which represent the particular finite difference method being used. For instance, the general form of an error representation formula for an explicit time stepping scheme for a quantity of interest $\mathcal{Q}$ is written as:

$$\mathcal{Q}(e) = \text{Discretization Error} + \text{Explicit Error} + \text{Quadrature Error}.$$

Decomposing the error in this way gives useful information for adaptivity. Using this decomposition, I develop an adaptive quadrature scheme in which a higher order quadrature is used adaptively based on the error decomposition. This is similar to p-adaptivity for the finite element method, but can be applied to explicit finite difference methods.

Student Research Projects: Students can take my current work with adaptivity using quadrature and develop it further, considering other explicit methods and analyzing specific differential equations to determine when this type of adaptivity is most effective. In addition to applied work, there is theoretical work for exceptional students which involves analyzing the new finite difference methods obtained from using various quadratures.

Use of Adjoint for the Modified Equation to Quantify Numerical Stability

In addition to being used to obtain an equivalent finite element method, this work discovers that the modified equation can also be used to estimate numerical stability for a particular quantity of interest. For a general equation, the solution of the corresponding adjoint equation quantifies the stability of a particular quantity of interest to perturbations in the residual. I discover that an adjoint to the *modified* equation for a certain method quantifies the *numerical* stability of that method, for a quantity of interest. For certain methods, I derive the adjoint equations to the highly nonlinear modified equation and examine the adjoint solution for situations that are known to be numerically unstable. By examining the adjoint solution, I determine that the error in the quantity of interest becomes unstable for some discretizations, and remains stable for finer discretizations. This method is used to determine a posteriori if a method is numerically stable for a particular quantity of interest.

Student Research Projects: Student can examine specific cases using the adjoint to determine numerical stability of methods corresponding to a quantity of interest. This can be purely computational, and can involve theoretical proofs as well. Through this they will learn about well known numerical methods and numerical stability analysis for finite difference methods.

Numerical Algebraic Geometry

I began to be involved in this area of research because I was a founding member of the development team for Bertini 2.0, a redesign of Bertini which implements homotopy continuation methods for solving polynomial systems of equations [1]. My work with this project has been to redesign and implement this software package from the ground up. The second version of Bertini is being ported to C++ and in doing so many of the core components are being improved. My work in this project uses Git for source control. Also, I utilize Boost in many parts of the development, including Qi to write a polynomial parser for the project. As my work on this projects gives me expert experience with the software, I will be called upon in the future by various groups to assist with modules and application runs, which will lead to publications.

I have also been working with the original designers of Bertini to use the software to solve fully nonlinear second order elliptic PDEs. One method for solving such PDEs involves a simplistic homotopy to determine a good initial condition for Newton's method [5]. I am using the more involved homotopy implemented in Bertini to improve both efficiency and accuracy of the current method.

Student Research Projects: Coding for the Bertini 2.0 software package is an excellent area for students interested in computation and computer science, as there are many areas of this code that need to be optimized and a great deal of coding to be done. Both my collaborators and I will write modules for Bertini 2.0, and these will be an excellent source of projects for students. The development of Bertini 2.0 can also be a source of projects for students interested in algebraic geometry.

Extended Symmetric Spaces of Weyl Groups

In summer of 2016, I attended the Research Experience for Undergraduate Faculty (REUF) at the American Institute for Mathematics (AIM). This program introduces faculty to a new research area that can be easily continued and applied to undergraduate research projects. My project examined the extended symmetric space of a group G, defined by

$$R_\theta = \{g \in G|\ \theta(g) = g^{-1}\},$$

for an automorphism θ. My group examined this set and determined how it was related to the involution graph of G, a graph that is determined by particular generators of G and the automorphism θ. We determined how this relationship changed based on the generators chosen and the automorphism θ. Thus far we have examined the case where $G = S_n$, the symmetric group. We determined that the set of vertices of the involution graph is equal to R_θ for all inner automorphisms. We have also examined when the involution graph is a poset under a certain relation.

Currently, my group and I are considering these questions for different finite groups, such as other classes of Weyl groups. We will also consider outer automorphisms, particularly the outer automorphism of S_6.

Student Research Projects: Many student projects can be developed from this research area. Permutations are easy for students to understand, and there are many questions that students can research by examining the original work and changing small portions. For instance, different groups G can be considered, or different classes of automorphisms can be considered. The involution graph also requires a considerable amount of effort to create, but a computer program could generate it very quickly. A group of students could work on writing such a program to generate the involution graphs for any group or automorphism.

Other members from the REUF group will also be starting undergraduate research projects based on this area. This will give the opportunity for students to collaborate with other students from across the country.

Uncertainty Quantification for Interface Problems with the Ghost Fluid Method

Interface problems are partial differential equations involving a domain divided by a surface Γ of codimension one, called an interface. In addition, some or all of the data for the PDE are discontinuous across the interface. In this work, we consider an elliptic problem where the diffusivity coefficient $\alpha(\mathbf{x})$ is discontinuous across Γ.

Experimentally, the location of the interface is determined by a small number of uncertain measurements. This research considers the situation where a deterministic elliptic interface problem exists, however, the location of the interface is uncertain and dependent on measurement data. A Monte Carlo approach is used which assumes a statistical model for the independent errors of the measurements and constructs N realizations of the interfaces, generating N "sample" problems. The Ghost Fluid method is used as this allows the use of a single grid for each sample interface. A posteriori error estimates are derived in [4] for the Ghost Fluid method. In this work [6], I derive an error representation formula for each sample problem using a perturbation of the error for a "nominal" problem. This perturbation error formula allows the error to be computed for each sample problem using a single adjoint solution. For small variance in the measurements, it is shown that the error can be approximated without computing the solution of each sample problem. This allows statistical results about the problem to be obtained independent of the number of samples. I also show that the error can be written as:

$$\mathcal{Q}(e) = \text{Discretization Error} + \text{Sample Error}$$

where the sample component describes the effect of the uncertainty in the measurements on the total error. This decomposition informs the type of adaptivity to be implemented, either a refinement of the mesh or an increase in the number of sample measurements.

Student Research Projects: I intend to extend this research to consider time-dependent problems and more general numerical methods. Through this work I will develop collaborations with researchers that model interface problems such as fluid flow through heterogeneous porous media and fluid-structure interaction. I will obtain modeling projects for students from these collaborations.

Error Estimation for Fully Nonlinear Second Order Elliptic Problems

Fully nonlinear second order elliptic equations are partial differential equations of the form,

$$F(D^2u, Du, u, x) = 0$$

for some nonlinear function F. A typical example is the Monge-Ampére equation, $F = \det(D^2u) - f$, which arises from applications such as mass transportation, meteorology and geostrophic fluid dynamics [5]. My research focuses on developing adjoint-based a posteriori error estimation for fully nonlinear second order elliptic equations. There are multiple finite element methods for solving these problems. Currently this work considers a C^0 finite element method using a variation of Nitsche's technique [7]. Error estimation for these problems is important as methods for solving fully nonlinear problems are computationally expensive, and accurate error estimation is necessary for computation saving methods such as adaptive mesh refinement.

Funding

I recognize the importance of applying for and receiving grants to fund my research and the research of students that work with me. I have already applied and received funding to attend multiple workshops, and I have received an internal grant for travel to present my research at a conference. The REUF conference was entirely funded. As I continue my research I plan to submit proposals both individually and with collaborators to agencies such as the National Science Foundation's Division of Mathematical Sciences. My research in a posteriori error estimation has many real-world applications and was actively funded throughout my postdoctoral fellowship, therefore there are multiple agencies who are willing to fund this area of research. The Bertini research group is currently funded and has paid for my travel to multiple conferences. I intend to apply for funding to continue the symmetric space research with my fellow collaborators from REUF through American Institute for Mathematics. I plan to seek out collaborations to discover new research avenues which lead to funding and continue working with past collaborators to advance my current research. This funding will be used to present my work at conferences, pay students during the summer or semester, and allow students to attend conference to discover the mathematics community.

Future Research

I plan to continue developing lines of research I have started, as well as look into new areas to expand my research base and increase opportunities for funding and student projects. Here are some of the areas I intend to pursue in future research.

- Expand my work on interface problems with my postdoc advisor Simon Tavener. We will look at more complex methods, such as the Immersed Interface Method, and Nitsche based finite element methods. In addition we will consider the application of these methods to time-dependent problems and fluid-structure interaction applications.
- Use numerical algebraic geometry, and in particular the software package Bertini, to solve fully nonlinear second order elliptic PDEs with the vanishing moment method. This method perturbs the fully nonlinear equation with a fourth order term and then reduces the higher order term to zero. This procedure is similar to the homotopy continuation methods used in numerical algebraic geometry. I intend to use Bertini to develop a more accurate way of implementing the vanishing moment method.
- Develop software modules for Bertini 2.0 to customize it to solve discretized differential equation problems.
- Continue the work on extended symmetric spaces with my REUF team. Expand the research to consider outer automorphisms of general Weyl groups.
- Examine further the equivalency between finite difference and finite element methods. I would like to attempt to determine if convergence rates for finite difference methods can be proved using this equivalency.
- Examine further the adaptive quadrature scheme I developed. I would like to examine other methods and other problems and formalize the adaptive scheme to be used for explicit methods.

- Examine further the quantification of numerical stability using the adjoint to the modified equation. I would like to rigorously prove that the adjoint quantifies numerical stability and use that result to show when certain nonlinear problems are stable and unstable.
- Derive a posteriori error estimation formulas for fully nonlinear second order elliptic PDEs solved using the vanishing moment method. Such error representation formulas would have a component that represents the error due to the fourth order perturbation term, I intend to develop an adaptive method for improved accuracy using this component.

Summary

My main research fields of a posteriori error estimation, numerical algebraic geometry, and symmetric spaces have many possibilities for research still to be done. I intend to continue working with current collaborators to explore these opportunities and develop new and innovative research. However, I am also excited to develop new collaborations with mathematicians I meet at conferences, through my current collaborators, or through organizations such as Project NExT, of which I am a fellow. Through these collaborations I will branch into new research areas and intend to have a broad base of research. This will give me many opportunities both for publication and grants, and will expand the number of student research projects I generate. I look forward to funding my research through internal and external grants, and presenting my research through publications and mathematical conferences.

References

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