Project title

Approximating the solution of problems in physics and engineering by means of discrete geometric calculus

Aims and background

The project aims to develop theory, techniques and tools for the approximate solution of problems in physics and engineering, including equations describing electromagnetism, acoustics and fluid flow. Relevant problems include those which are usually modelled using linear or non-linear differential equations on a manifold. A simple example is the use of Maxwell's equations to model electromagnetic phenomena within a region.

The theory, techniques and tools to be developed encompass a relatively new field of study which may be called "Discrete Geometric Calculus". This field combines the theory and techniques of compatible discretization with those of geometric calculus. The theory and techniques to be used to develop Discrete Geometric Calculus include the study of the symmetries of differential equations, approximation theory, algebraic topology, and Grassmann and Clifford algebras.

Related previous work falls into three categories: (1) compatible discretization; (2) Clifford analysis and geometric calculus; and (3) discrete Clifford analysis. This work is briefly described below.

Compatible discretization. Many physical quantities can be formulated in terms of a variational principle, that is, in terms of a trajectory in a suitably defined abstract space which makes some functional of the motion stationary, usually at a maximum or a minimum. The prototypical example of such a principle is Hamilton's Principle of Stationary Action [43, Section 1.8] [16, Section 10.2]. Noether's Theorem [36] [43, Chapter 3] [16, Section 20.1] states that certain symmetries in the equations describing a variational principle give rise to quantities which are conserved by the motion. Simply put, symmetries are equivalent to conservation laws. Noether's Theorem has also been generalized to cover some non-conservative systems [43, Section 3.12].

The idea of compatible (or *mimetic*) discretization [2, 4] is to create a discrete description of a physical phenomenon which preserves many or all of the same conservation laws which are obeyed by the continuous description given by a differential equation. Thus if a method using compatible discretization can calculate a conserved quantity accurately, the accuracy is maintained by the incorporation of the conservation law into the discretization.

Some of the tools of compatible discretization include (1) the continuous description of the physical phenomenon using equations involving differential forms on manifolds; (2) the analysis of the symmetries of the equations; and (3) discretization by dividing the manifold into cells, chains and complexes, with corresponding differential forms.

A recent survey article by Arnold, Falk and Winther describes finite element exterior calculus [2]. Related work includes the work of Bochev and Hyman on a discrete cochain approach to mimetic discretization [4], the work of Mansfield and Quispel on variational complexes for the finite element method [34], and the work of Harrison on chainlets, extending the domain of integration from smooth manifolds to soap bubbles and fractals [19, 20]. Recent applications of compatible discretization methods to Maxwell's equations include Tonti's finite formulation of the electromagnetic field [42], Kangas, Tarhasaari and Kettunen's use of Whitney's finite element theory [23] and Stern, Tong, Desbrun and Marsden's combination of compatible discretization with variational integration, using a Lagrangian action principle [41].

Clifford analysis and geometric calculus. Clifford algebras are used to describe the motion and spatial relationship between objects in Euclidean or Minkowski space. In general, they can be constructed on any vector space with a quadratic form [31, Chapter 14], including tangent spaces on orientable manifolds with a metric. Clifford algebras as hypercomplex algebras generalize the complex numbers.

The theory of exterior calculus uses exterior differential forms, based on Grassmann's exterior algebra. Grassmann and Clifford algebras are intimately related. Essentially, given a metric, a Clifford algebra can be defined on the same vector space as a Grassmann algebra using the same basis elements but a different multiplication rule [31, Chapter 14]. Geometric algebra provides a "unified language" for physics and engineering [26], based on multivectors, which supports Grassmann's exterior product, and left and right contractions as well as the Clifford product. For example, reflections, rotations and "boosts" in Minkowski space can all be described using Clifford products of vectors [9, Sections 4.2, 5.3].

Clifford algebras are a natural setting for the Dirac (vector derivative) operator [38, 10]. A well-developed theory, Clifford analysis, studies the Dirac operator and its kernel in various contexts, including smooth manifolds [8]. Geometric calculus encompasses both Clifford analysis and the use of exterior derivatives and differential forms on orientable "spin" manifolds with arbitrary metric signatures [9, Chapter 6].

Clifford analysis, in the sense of hypercomplex analysis, has traditionally proceeded by finding structures, functions and relationships in the Clifford algebra setting analogous to those found in complex analysis. To date, this has been remarkably successful, resulting in generalizations of the Cauchy-Riemann operator, the Cauchy integral theorem and holomorphic function theory [31, Chapter 20] [18]. Generalized series expansions, generating functions, kernels, and special functions including orthogonal polynomials have also been studied [8] [18, Chapter IV] [33]. This study has been accompanied by the study of the Clifford formulation and solution of a number of equations, including Maxwell's equations [6, 25] and the Navier Stokes equations [24].

Discrete Clifford analysis. Multivectors provide a natural data structure for simplices and other cells, chains, complexes, and multiforms [38, 39, 32]. (A multiform is a linear combination of differential forms of different grades.) The Dirac operator can be defined as a limit of a directed integral over the boundary of a simplex [38, Section 5].

Theoretical frameworks for discrete versions of Clifford analysis and geometric calculus have recently been developed. The PhD thesis of Nelson Faustino [13] provides one such framework. The thesis combines the ideas of finite element exterior algebra with various types of discrete Dirac operators, including operators on lattices [12, 15]. Similar frameworks for the Dirac-Kahler operator date to the 1980s [3, 21]. Researchers at the Clifford research group at Ghent University in Belgium have also recently published a paper aimed at further development of the theory of discrete Clifford analysis [5].

The systematic study of the discrete counterparts to the operators, spaces and domains encountered in Clifford analysis also includes work by Gürlebeck and Sprössig on finite differences [17, Chapter 5].

Discrete Geometric Calculus Discrete Geometric Calculus combines the approaches of compatible discretization and geometric calculus at a fundamental level. First, the equations are formulated in terms of multivector-valued quantities and Dirac and related operators. Second, the equations are examined for symmetries. Third, a compatible discretization is created, including the discretization of Dirac operators on simplicial complexes.

Ideally, this combination of approaches retains the advantages of both approaches: the numerical stability of compatible discretization along with the economy of expression of geometric calculus.

Significance and innovation

The approximate solution of equations arising in physics and engineering is important to more than just their immediate application to the practical problems of understanding, building and managing electrodynamic, fluid and other physical systems. A better understanding of the solution of these types of equations gives us a deeper understanding of the physical world and may suggest new equations and new science.

The theory, techniques and tools to be developed during the project would include

1. New and improved algorithms for the approximate solution of the Helmholtz, Maxwell, shallow water, Navier-Stokes and similar equations;
2. New theory which ideally explains why the new algorithms are faster and more accurate than existing algorithms, or in the worst case, explains why the existing algorithms are the best possible;
3. Improvements to the available open source software packages for calculation with Clifford algebras, and the solution of differential equations, including implementations of the new algorithms, and sufficient documentation to make the new algorithms practical and immediately usable.

The research therefore has the potential to

- Improve the current understanding of the connections between, exterior algebras and Clifford algebras in the solution of differential equations; and
- Result in better toolkits for calculations with Clifford algebras and for the approximate solution of certain problems in physics and engineering.

The availability of an immediately usable, practical toolkit increases the value of this project, because this is likely to result in the development of novel applications by the users of the toolkit. For example, the creation of the EQSP Matlab Toolbox by the APD candidate resulted in papers on the analysis of spatial variations in temperature on the surface of the earth [11]; improvements in the efficiency of the operational forecast system of the European Centre for Medium Range Weather Forecasting [35]; an approximate optimal strategy for unemployment insurance [22]; an approximate optimum mask for optical lithography [1]; and the sampling of spatial conformations of an RNA molecule [7].

The research approach combines a number of key innovations:

1. Clifford algebras and exterior algebras are to be used as an integral part of the basic theoretical and numerical framework;
2. The numerical algorithms are to be implemented in the form of open source software packages, which are intended to be universally available and continuously improved.

The research is relevant to Research Priority 3: Frontier Technologies for Building and Transforming Australian Industries. It addresses Breakthrough Science in two ways: (1) by seeking to increase our understanding of the mathematics underlying the approximate solution of some of the problems encountered in physics and engineering, and (2) by seeking to increase our ability to solve these problems. It addresses Frontier Technologies by providing open source software tools as well as techniques for computation and problem solving in physics and engineering.

Approach and methodology

The proposal is for a program of research which would include three main themes:

1. Constructive approximation:

   The study of multidimensional differential operators, and associated function spaces and bases, including kernels and polynomial bases.

2. Compatible discretization:

   The study of discretization in relation to Clifford algebras, and the relationships between geometric calculus and discrete and continuous exterior calculus, leading to the further development of Discrete Geometric Calculus.

3. Approximation of solutions to equations:

   The study of approximations to the solution of differential equations, by means of Discrete Geometric Calculus.

The program would consist of three main threads, distinguished by the types of outcomes and deliverables expected:

1. Techniques

   New and improved algorithms for the approximate solution of various equations.

2. Theory

   (a) Theory which ideally explains why the new algorithms are faster and more accurate than existing algorithms, or in the worst case, explains why the existing algorithms are the best possible;

   (b) Theory which improves our understanding of the relationships between geometric calculus, discrete exterior calculus and compatible discretization.

3. Tools

   Improvements to the available open source software packages for calculation with Clifford algebras, and the solution of differential equations, including implementations of the new algorithms, with sufficient documentation to make the new algorithms practical and immediately usable.

The subprojects within the threads and the methodologies which would be employed are elaborated in more detail below.

Techniques. The subprojects within this thread would focus on algorithms to be developed or improved.

The algorithms would address the approximate solution of the following equations:

1. Linear equations:

   Helmholtz, Maxwell, and others;

2. Nonlinear equations:

   Shallow water, Navier-Stokes and others.

For the most part, the methodology employed to develop and improve approximation algorithms would be theory-driven numerical experimentation. This consists of a number of stages:

1. Review existing literature and existing theory, algorithms and code;
2. Devise new or improved algorithms;
3. Implement the algorithms as computer programs;
4. Test the algorithms and compare the results with existing algorithms;
5. Characterise the scope of the algorithms in terms of domain, stability and rate of convergence;
6. Publish the theory and description of the algorithm, as well as the code implementing the algorithm.

These stages are then repeated. More specifically, for Discrete Geometric Calculus, the general scheme for creating algorithms for a particular physical phenomenon, would be to:

1. Formulate the Lagrangian and corresponding Euler-Lagrange equations in terms of multivector-valued quantities and Dirac and related operators and differential forms.
2. Examine the equations for symmetries, especially conformal and spin group symmetries.
3. Create a discretization, which respects as many symmetries as possible, including the discretization of Dirac operators on simplicial complexes.
4. Theoretically examine consistency, numerical stability and rate of convergence.
5. Implement the scheme and examine its performance in practice.

The numerical experimentation and the publishing of code would take maximum advantage of an existing open source library for Clifford algebra calculations, developed by the APD candidate. This is the GluCat C++ library [27]. The implementation in GluCat of a fast algorithm for the real representation of Clifford algebras, as well as the accompanying paper [28] is an example of the results of the theory-driven numerical experimentation method.

Theory. Besides the theory directly related to the approximation algorithms listed above, the theory thread would consist of a number of subprojects which would address some key questions within each theme:

1. Constructive approximation:

   How do various spaces, kernels, basis functions generalize in the setting of Discrete Geometric Calculus?

2. Compatible discretization:

   Elaborate the geometric calculus equivalents of discrete exterior calculus and finite element exterior calculus.

3. Approximation of solutions to linear equations:

   In compatible finite element formulations of Maxwell's equations, the electric and magnetic fields are separated and are carried on dual meshes [42] or on different faces of a single spacetime mesh [41]. In Clifford algebra formulations of Maxwell's equations, the electric and magnetic fields are united into a single Clifford valued electromagnetic field [31, Chapter 8] [6]. What, then is the most suitable finite element Clifford algebra formulation of Maxwell's equations?

4. Approximation of solutions to nonlinear equations:

   What is the best way to discretize equations which describe waves travelling at multiple different velocities, and which may include shocks?

   What are the relationships between integrable systems, compatible discretization, and geometric calculus?

Tools. The subprojects in the tools thread would concentrate mainly on enhancement of tools for the solution of differential equations by means of Discrete Geometric Calculus, in particular interfaces to the GluCat C++ library. Enhancements would concentrate on improved algorithms and improved usability:

1. GluCat interfaces to Python, Sage, FEniCS and other Finite Element packages, CLAWPACK and other Finite Volume packages.

   Sage [40] is an open source software package for experimentation in algebra and geometry. It is supported by U.S. National Science Foundation grant DMS 0713225. Creation of a Sage interface would also have the effect of creating a more comprehensive test suite and user documentation. The Sage interface would be implemented using Cython. A prototype Cython interface already exists.

   FEniCS [14, 30] is a suite of open source software for the Finite Element Method, including Finite Element Exterior Calculus, written in Python and C++.

   CLAWPACK [29] "is a collection of Fortran subroutines for solving hyperbolic systems of conservation laws" using Finite Volume techniques.

   Interfaces from GluCat to existing Finite Element and Finite Volume packages would not only reduce the work required to implement new algorithms, it would also potentially create a wider use community.

2. GluCat and scripting language implementations of new and enhanced algorithms.

3. More complete end user documentation, including a users manual.

Timeline. Following is a timeline which indicates the years in which the bulk of the work for each subproject would be expected to be completed.

2011–2012

- Theory: Constructive approximation; Compatible discretization; Approximation of solutions to linear equations.
- Techniques: Helmholtz, Maxwell and other linear equations.
- Tools: GluCat interfaces to Sage, FEniCS and other Finite Element packages.

2013–2014

- Theory: Approximation of solutions to nonlinear equations.
- Techniques: Shallow water, Navier Stokes and other nonlinear equations.
- Tools: GluCat interfaces to CLAWPACK and other Finite Volume packages. GluCat user documentation, including user manual.

National benefit

The benefits of the results of successful completion of this project would potentially include

- the further development of capability and expertise in Australia in this field, with strengthened ties to overseas researchers;
- the availability of an immediately usable, practical toolkit for the approximate solution of a number of problems in physics and engineering;
- immediate applications of this toolkit to the practical problems of understanding, building and managing communications networks, signal processing systems, electrodynamic, fluid and other physical systems; and
- a deeper understanding of the physical world and possibly new equations and new science.

The research is relevant to Research Priority 3: Frontier Technologies for Building and Transforming Australian Industries. Its potential contributions to Breakthrough Science would be: (1) an increase in our understanding of the mathematics underlying the approximate solution of some of the problems encountered in physics and engineering, and (2) an increase in our ability to solve these problems. Its potential contributions to Frontier Technologies would be techniques and open source software tools for computation and problem solving in physics and engineering.

Communication of results

The theory, techniques and tools developed by the project would be disseminated through

- Talks given at local and international conferences;
- Publication in peer-reviewed journals in preference to conference proceedings, along with the posting of a publicly available preprint on the World Wide Web; and
- Posting of the implementation of algorithms as open source software, available via the World Wide Web, including improvements to the GluCat C++ library [27].

Role of personnel

Both investigators will collaborate on all aspects of the project, but there will be some specialization.

The APD candidate would be project leader and sole Chief Investigator. His primary roles would be the implementation and analysis of algorithms, and the creation of interfaces and further improvements to the GluCat software. His background and achievements make him most suitable for this role. This includes his work in approximation theory; his work on discretization, notably on the unit sphere; his work on numerical analysis in Clifford algebras; his experience in the development, testing and public release of open source mathematical and scientific software, including his authoring and maintenance of the GluCat software library; and his experience in project leadership and time management, gained through a career in the ICT industry.

Rolf Sören Krausshar would be the Partner Investigator. His primary role would be in investigating the relationships between the theories of Discrete Geometric Calculus and Clifford analysis with respect to the equations to be studied, and their symmetries. He has a deep background in Clifford analysis and has most recently published papers on the application of Clifford analysis to Maxwell's equations [25], the Navier-Stokes equations [24] and other equations, and has collaborated with many of the most well-known researchers in both Clifford analysis and discrete Clifford analysis.

There will also be scope for informal collaboration with Australian and overseas researchers as the project progresses.

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