Part E - Proposal Description

E1 Proposal title

Solving problems in physics and engineering involving differential and integral equations by means of multivariate approximation theory and Clifford algebras.

E2 Aims and background

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 equipped with a quadratic form [17, Chapter 14]. Clifford algebras as hypercomplex algebras generalize the complex numbers.

The aim of the project is to develop the theory, techniques and tools needed for the application of both multivariate approximation theory and Clifford algebras to the numerical solution of certain problems encountered in physics and in engineering.

Some relevant problems include those which are usually modelled using differential or integral equations on a manifold. A typical example is the use of Maxwell's equations to model electromagnetic phenomena within a region of space. Related examples include the motion of rigid bodies and the flow of fluids.

Other relevant problems include problems in signal processing, coding theory and quantum computing. An example in signal processing is the use of multidimensional transforms and filters to reconstruct images and multidimensional signals.

Related previous work falls into three categories:

- Approximation of matrix functions;
- Compatible discretization using discrete exterior calculus;
- Applications of hypercomplex operator, function spaces and special functions to partial differential equations.

Approximation of matrix functions

Recent work in this area is summarized and exemplified by Higham's book on function of matrices [11]. Many matrix approximation algorithms are based on Taylor expansion and Padé approximation, for example, the matrix logarithm of Cheng, Higham, Kenney and Laub [4].

One of the goals of the project is to further develop efficient algorithms for the approximation of functions in Clifford algebras. Matrix approximation algorithms are relevant to functions on Clifford algebras because the elements of a Clifford algebra can be represented as real or complex matrices [17, Chapter 14] [20, 16].

Compatible discretization using discrete exterior calculus

A recent survey article by Arnold, Falk and Winther describes finite element exterior calculus [1]. The idea is to use discretizations which are compatible with the differential equation to be solved. Related work includes the work of Mansfield and Quispel on variational complexes for the finite element method [19], and the work of Harrison on chainlets, extending the domain of integration from smooth manifolds to soap bubbles and fractals [8, 9]. Recent applications of compatible discretization methods to Maxwell's equations include Tonti's finite formulation of the electromagnetic field [23], Kangas, Tarhasaari and Kettunen's use of Whitney's finite element theory [12] and Stern, Tong, Desbrun and Marsden's combination of compatible discretization with variational integration, using a Lagrangian action principle [22].

One of the goals of the project is the further development of the extension of compatible discretization methods from exterior calculus to calculus based on Clifford algebras. 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 quadratic form, 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 [17, Chapter 14].

Given this correspondence, theories of finite element Clifford calculus and discrete Clifford calculus should be expected. Harrison states, "A forthcoming extension of the theory to Clifford algebras, however, is clearly deeply important." [9, p. 29].

Hypercomplex operators, function spaces and special functions

One of the goals of the project is the further development of numerical methods for the approximate solution of differential and integral equations using calculus based on Clifford algebras.

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 [17, Chapter 20] [7]. Generalized series expansions, generating functions, kernels, and special functions including orthogonal polynomials have also been studied [5] [7, Chapter IV] [18]. This study has been accompanied by the study of the Clifford formulation and solution of a number of equations, including Maxwell's equations [14] and the Navier Stokes equations [13].

Recent study on the Clifford numerical solution of Maxwell's equations includes work by Chantaveerod, Seagar and Angkaew on the formulation of Maxwell's equations as a boundary integral problem and its approximate numerical solution using quadrature in a Clifford algebra [2].

The systematic study of the discrete counterparts to the operators, spaces and domains encountered in Clifford analysis includes work by Gürlebeck and Sprössig on finite differences [6, Chapter 5].

E3 Significance and innovation

The approximation of functions and the approximate solution of equations arising in physics and engineering is important to more than just their immediate applications to the practical problems of understanding, building and managing communications networks, signal processing systems, 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 course of the project would include

1. New and improved algorithms for the approximation of Clifford, matrix and vector functions;
2. New and improved algorithms for the approximate solution of the Maxwell, Helmholtz, Navier-Stokes, and shallow water equations;
3. New and improved signal processing and related engineering algorithms;
4. 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;
5. Improvements to the available open source software packages for calculation with Clifford algebras, including implementations of the new algorithms, and sufficient documentation to make the new algorithms practical and immediately usable.

Thus, if the research succeeds as anticipated, it would

- Improve the current understanding of the connections between matrix algebra, exterior algebra and Clifford algebra in approximation theory and in the solution of differential and integral equations; and
- Result in a better toolkit both 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 often results in the development of novel applications by the users of the toolkit. Examples of this phenomenon are given in section B10.4 of this proposal.

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.

E4 Approach and methodology

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

1. Approximation of functions:

   The approximation of functions in Clifford algebras, including Padé approximation.

2. Constructive approximation:

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

3. Compatible discretization:

   The study of discretization in relation to Clifford analysis, and the relationships between Clifford analysis and discrete and continuous exterior calculus.

4. Approximation of solutions to equations:

   The study of Clifford approximations to the solution of differential and integral equations.

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

1. Techniques

   (a) New and improved algorithms for the approximation of Clifford, matrix and vector functions;

   (b) New and improved algorithms for the approximate solution of various equations;

   (c) New and improved signal processing and related engineering algorithms.

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 (1) between Clifford analysis and the approximation of matrix functions, (2) between Clifford analysis and constructive approximation, and (3) between Clifford analysis, discrete exterior calculus and compatible discretization.

3. Tools

   Improvements to the available open source software packages for calculation with Clifford algebras, including implementations of the new algorithms, and 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 consist of algorithms to be developed or improved. These would be:

1. Approximation of Clifford, matrix and vector functions:

   The square root, logarithm, exponential and related transcendental functions;

2. Approximate solution of the following equations:

   Maxwell, Helmholtz, Navier-Stokes, and shallow water equations;

3. Signal processing and related engineering algorithms:

   Discrete Clifford wavelet transforms and discrete Clifford Fourier transforms.

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. New algorithms may suggest principles which can be used in other contexts, for example the methods used for the matrix sign function in connection with functions of matrices [11, Chapter 5].

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 sole CI. This is the GluCat C++ library [15]. To date, GluCat already implements Clifford variants of some algorithms for the approximation of matrix functions, such as the matrix square root and logarithm of Cheng, Higham, Kenney and Laub [4]. The implementation in GluCat of a fast algorithm for the real representation of Clifford algebras, as well as the accompanying paper [16] is an example of the results of the theory-driven numerical experimentation method.

The development and improvement of algorithms for the approximation of functions of matrices also relies on numerical experimentation [4, 11] and "the principal vehicle for transmitting the results of this research to the community at large is software" [3, 10]. The research which led to Higham's book on functions of matrices was supported in part by U.K. Engineering and Physical Sciences Research Council grants GR/L94314 and GR/R22612/01 [3, 10, 11].

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. Approximation of functions:

   - How are the matrix forms of transcendental functions related to the transcendental functions encountered in Clifford analysis?
   - Can Clifford analysis suggest new algorithms for special cases of matrix functions?

   The approximation of functions in Clifford algebras, including Padé approximation.

2. Constructive approximation:

   - How do various spaces, kernels, basis functions generalize in the Clifford setting?
   - How can function approximation and quadrature of high dimensionality (eg. more than 100 dimensions) be dealt with?
   - In the Clifford setting, does it help if different dimensions are weighted according to smoothness?

3. Compatible discretization:

   - What are the Clifford algebra equivalents of discrete exterior calculus and finite element exterior calculus?

- How do Clifford algebras and the Dirac operator fit into Harrison's chainlet theory [8, 9]? Is there more than one "natural" way to incorporate Clifford algebras into chainlets?

4. Approximation of solutions to equations:

   In compatible finite element formulations of Maxwell's equations, the electric and magnetic fields are separated and are carried on dual meshes [23] or on different faces of a single spacetime mesh [22]. In Clifford algebra formulations of Maxwell's equations, the electric and magnetic fields are united into a single Clifford valued electromagnetic field [17, Chapter 8] [2]. What, then is the most suitable finite element Clifford algebra formulation of Maxwell's equations?

Tools

The subprojects in the tools thread would concentrate mainly on the enhancement of the GluCat C++ library, especially in relation to improved algorithms and improved usability. This would consist of the following subprojects:

1. Multiprecision floating point arithmetic within GluCat;

   This would allow a more precise study of the convergence behaviour of algorithms by allowing the effect of rounding error to be studied independently of other sources of error.

2. GluCat interfaces for Sage, Python, Octave, Matlab, Ruby etc.

   Sage is an open source software package for experimentation in algebra and geometry. It is supported by U.S. National Science Foundation grant DMS 0713225 [21]. Comments from the Sage community during the implementation of the Sage interface are likely to make GluCat much more usable to that community. 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. This would make it easy to create a GluCat interface to Python. A prototype Python interface already exists, based on work done by Paul Leopardi during the Sage Days 10 meeting.

   More interfaces to scripting languages would potentially create a wider use community, and would also make it easier to interface GluCat into existing software for finite elements, signal processing etc. It would also make it possible to publish the code for some of the new algorithms in scripting languages rather than C++.

3. GluCat and scripting language implementations of new and enhanced algorithms;

   This is part of stage 6 of the methodology used in the techniques thread.

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

   One of the current impediments to the wider use of GluCat is the relative lack of user documentation.

Timeline Following is a timeline which indicates the year in which the bulk of the work for each subproject would be expected to be completed. No time ordering is implied within each year.

2010

- Techniques: Approximation of Clifford, matrix and vector functions.
- Theory: Approximation of functions.
- Tools: Multiprecision floating point arithmetic within GluCat.

2011

- Techniques: Maxwell and Helmholtz equations.
- Theory: Approximation of solutions to equations.
- Tools: Sage and Python interfaces to GluCat.

2012

- Techniques: Shallow water and Navier Stokes equations.
- Theory: Compatible discretization.
- Tools: GluCat user documentation, including user manual.

2013

- Techniques: Signal processing and related engineering algorithms.
- Theory: Constructive approximation.
- Tools: Octave, Matlab and Ruby interfaces to GluCat.

E5 National benefit

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

- 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.

E6 Communication of results

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

- Talks given at local and international conferences, notably ICNAAM, the International Conference of Numerical Analysis and Applied Mathematics;
- Publication in peer-reviewed journals in preference to conference proceedings, along with the posting of a publically 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 [15].

E7 Role of personnel

The APD candidate would be sole Chief Investigator. His background and achievements as listed in Section B10 make him most suitable for this project. There may be scope for informal collaboration with local and overseas researchers as the project progresses.

E8 References

[1] D. N. Arnold, R. S. Falk and R. Winther, *Finite element exterior calculus, homological techniques, and applications.* Acta Numerica, 15, 2006, pp. 1-155. `doi:10.1017/S0962492906210018`

[2] A. Chantaveerod, A. D. Seagar, and T. Angkaew, *Calculation of Electromagnetic Field with Integral Equation Based on Clifford Algebra.* PIERS Proceedings, 62 - 71, August 27-30, Prague, Czech Republic, 2007.

[3] S. H. Cheng, N. Higham, T. L. Freeman, J. R. Gurd, *Final report on EPSRC grant GR/L94314: Parallel computation of matrix functions.* January 2002.

[4] S. H. Cheng, N. Higham, C. S. Kenney and A. J. Laub, *Approximating the logarithm of a matrix to specified accuracy.* SIAM. J. Matrix Anal. and Appl. 22:4, 2001, pp. 1112-1125. `doi:10.1137/S0895479899364015`

[5] R. Delanghe, *Clifford Analysis: History and Perspective.* Computational Methods And Function Theory, 1:1, 2001, pp. 107-154.

[6] K. Gürlebeck and W. Sprössig, *Quaternionic and Clifford calculus for physicists and engineers.* Wiley, New York, 1997.

[7] K. Gürlebeck, K. Habetha, and W. Sprössig, *Holomorphic functions in the plane and n-dimensional space.* Birkhäuser, Basel, 2008.

[8] J. Harrison, *Geometric Hodge star operator with applications to the theorems of Gauss and Green.* Mathematical Proceedings of the Cambridge Philosophical Society, 140:1, 2006, pp. 135-155. `doi:10.1017/S0305004105008716`

[9] J. Harrison, *Differential complexes and exterior calculus.* Arxiv preprint math-ph/0601015, 2006.

[10] N. J. Higham, *Final report on EPSRC grant GR/R22612/01: Numerical analysis of matrix functions.* April 2004.

[11] N. J. Higham, *Functions of matrices.* SIAM, Philadelphia, 2008.

[12] J. Kangas, T. Tarhasaari and L. Kettunen, *Reading Whitney and finite elements with hindsight.* IEEE Transactions on Magnetics, 43:4, April 2007, pp.1157-1160. doi:10.1109/TMAG.2007.892276

[13] R. S. Kraußhar and D. Constales, *On the Navier-Stokes equation with free convection in three dimensional unbounded triangular channels.* Mathematical Methods in the Applied Sciences, 31:6, 2008, pp. 735-751.

[14] R. S. Kraußhar, I. Cação and D. Constales, *Explicit representations of the regular solutions of the time-harmonic Maxwell equations combined with the radial symmetric Euler operator.* Mathematical Methods in the Applied Sciences, 32:1, 2009, pp. 1-11.

[15] **Paul Leopardi**, *GluCat: Generic library of universal Clifford algebra templates*, 2001-2007. http://glucat.sourceforge.net

[16] **Paul Leopardi**, *A generalized FFT for Clifford algebras.* Bulletin of the Belgian Mathematical Society - Simon Stevin, Volume 11, Number 5, 2005, pp. 663-688.

[17] P. Lounesto, *Clifford algebras and spinors.* Cambridge University Press, 1997.

[18] H. R. Malonek, G. Tomaz, *Bernoulli polynomials and Pascal matrices in the context of Clifford analysis.* Discrete Applied Mathematics, in press, corrected proof online, 9 July 2008. doi:10.1016/j.dam.2008.06.009

[19] E. L. Mansfield and G. R. W. Quispel, *Towards a variational complex for the finite element method.* Group theory and numerical analysis, CRM Proc. Lecture Notes, 39, Amer. Math. Soc., Providence, RI, 2005, pp. 207–232.

[20] I. R. Porteous, *Clifford algebras and the classical groups.* Cambridge University Press, 1995.

[21] W. Stein and D. Joyner, *SAGE: system for algebra and geometry experimentation.* ACM SIGSAM Bull. 39:2, June 2005, pp. 61-64. doi:10.1145/1101884.1101889

[22] A. Stern, Y. Tong, M. Desbrun, and J. E. Marsden, *Variational integrators for Maxwell's equations with sources.* PIERS Proceedings, July 2-6, Cambridge, USA 2008, pp. 443-447. doi:10.2529/PIERS071019000855

[23] E. Tonti, *Finite formulation of the electromagnetic field.* Progress In Electromagnetics Research, PIER 32, 2001, pp. 144.