Project title

High performance computation in Grassmann and Clifford algebras, with applications to number theory and partial differential equations.

Project

In 1996, well after completing my undergraduate degree in computer science and mathematics, I was astonished to learn about *geometric algebras* and their many uses in physics. Why, I thought, are these algebras not better known?

The overall aim of my project is to improve our ability to calculate using geometric algebras, specifically the Grassmann and Clifford algebras, and related algebraic systems. In these systems, the "numbers" embody the idea of *direction* as well as quantity, that is they answer the question "which way?" as well as "how much?" Simple examples of such systems are the real numbers, the complex numbers and vector spaces. Because of these examples, and for other reasons, the elements of geometric algebras are often called *hypercomplex numbers*, *multivectors* or sometimes, *polyvectors.*

While geometric algebras have long had an important use as theoretical tools, their use in practical calculation has lagged behind that of complex numbers and linear algebra. For example, Matlab, which is based on linear algebra, has been a commercial success for most of the last 20 years. In contrast, computer libraries and packages for numerical and symbolic calculation in Grassmann and Clifford algebras, such as CLICAL [63], CLIFFORD [33], CLUCalc [64], and Gaigen [54, 49], remain relatively obscure. The possible exception to this obscurity is the use of quaternions in software for simulation, animation and computer games [66]. One of the main aims of this project is to help change this situation, to make calculation with geometric algebras at least as well known and well accepted as calculation with complex numbers and linear algebras. There is a very long way to go, but the small steps of this project may help make this happen.

Background

Real numbers include the idea of direction on a single one dimensional "number line." Complex numbers can be used to encode directions and rotations in the usual two dimensional plane of Euclidean geometry. Finite dimensional vectors can be included in the higher dimensional directed number systems of geometric algebra, such as Grassmann and Clifford algebras [57].

Such directed number systems have been very important in the history of mathematics in the nineteenth and twentieth centuries. This is especially true in the area of differential geometry, where one of the main objects of study, the *differential form* is the main example of a directed number system. The geometric algebra of differential forms is Grassmann's *exterior algebra* [56].

The *Clifford algebras* [65, 62] are also important in the study of geometry. They are used in the study of movement and transformations, such as reflections, rotations and translations. These algebras therefore have applications in computer vision, animation and robotics, as well as applications in physics [61, 48].

In physics, Dirac's theory of the electron is based on an application of a Clifford algebra. As theoretical tools in the higher calculus, Clifford algebras and a differential operator called the *Dirac operator* are very important [35, 50]. (The Dirac operator is essentially a type of directed derivative, which is in a sense more fundamental than the more familiar *gradient*, *divergence* and *curl* operators used in three dimensional calculus [57, 46].) These tools have been used in research leading to award-winning results such as the Atiyah-Singer index theorem [35] (M. Atiyah and Singer, Abel prize 2004) and the solution of the Kato square root problem [36] (A. McIntosh, Moyal medal 2002).

Subprojects

Mathematical research is risky, in the sense that it is often very difficult to tell how long it will take to solve a problem, if it can be solved at all, how original and significant the solution will be, or where the process of looking for solutions will lead. It is also often difficult to predict the significance of results in terms of possible applications. To increase project diversity and reduce risk, rather than just addressing one problem, this project is split into three semi-independent parts: (1) a core project in numerical analysis of geometric algebras, (2) applications to high precision computation of automorphic forms in Clifford algebras, and (3) applications to the numerical solution of partial differential equations.

(1) Core project. For the core project in numerical analysis of geometric algebras, the key issues are that (a) an element of a geometric algebra over the real numbers often cannot be represented exactly on a computer, because this would take an infinite number of bits of storage; and (b) exact calculations may be impossible, because they would need an infinite number of steps. Thus computers usually perform *approximate* calculations instead. These involve a tradeoff between the number of operations performed and the accuracy which can be obtained. The core project aims to better understand this tradeoff in for Grassmann and Clifford algebras, in order to devise and implement algorithms which perform the smallest number of operations to achieve a required level of accuracy.

I will pursue the core project mostly by applying existing techniques and theoretical results. This is possible mainly because the representation theory of Clifford algebras allows results in numerical linear algebra to be used. Since I am the author of *GluCat,* a C++ template library for calculations in Clifford and Grassmann algebras [8, 25, 26], it will be one of the main focus points for my research. I will use GluCat as a vehicle for developing and testing algorithms, as a tool for numerical experimentation, and as a means to publish results.

The core project is split into subprojects addressing the following related problems:

1. Accuracy and stability of numerical algorithms.

   This problem has to do with each of the various algorithms used to perform basic calculations, such as multiplication, division, and transformations between different representations of directed numbers. Approximate calculations do not only need to be accurate, they need to be *backward stable:* the results need to be the same as those obtained from an exact calculation with only slightly different input. The subproject for this problem is to ensure that the accuracy and stability of the algorithms used for approximate calculation with directed numbers is known and guaranteed.

   The theory of the effects of rounding error on numerical algorithms goes back at least to Wilkinson. My work will focus on applying the theory as described by N. Higham. Higham's book [58] describes his own work as well as the work of many others, including that of R. Brent on matrix multiplication. The work will consist of performing error analysis on the algorithms actually used in my GluCat library, and in other geometric algebra packages, testing the analysis by performing numerical experiments, and possibly adjusting the algorithms so that they are more stable.

2. Arbitrary precision calculations.

   Up until now, most computer calculations performed on directed numbers have either been symbolic or have been limited in precision by the usual IEEE floating point arithmetic standards. This subproject aims to build on the previous one so that calculations can be performed on directed numbers to an arbitrary precision, and with a guaranteed accuracy.

   A number of computer libraries exist for arbitrary precision floating point calculation, including MPFR [55]. My work will apply not only the existing computer code, but the principles underlying the code, to arbitrary precision calculation in geometric algebras. This will build on the work of the previous subproject. Some of the work will involve building interfaces from GluCat to MPFR, so that the existing algorithms can be performed with arbitrary precision arithmetic. I will use numerical experiments test these interfaces, and make necessary adjustments. I then use this enhanced version of GluCat to test the algorithms treated in the previous subproject, to ensure that rounding errors behave as expected.

   The next step will be to devise algorithms which have guaranteed accuracy. Detailed work on this project will involve collaboration with the authors of MPFR, notably P. Zimmermann, so that I can better understand the principles behind it, and how to apply these principles in the case of directed numbers. I have already visited Zimmermann at LORIA in Nancy, for a very brief preliminary discussion.

   I will also need to track any progress the case of arbitrary precision numerical linear algebra, in particular the use of MPFR and related libraries with linear algebra packages and libraries.

3. Improved approximation of common functions.

   A number of functions, based on power series expansions, are common to complex numbers, square matrices, and directed numbers. These include the exponential function, trigonometric functions, and their inverses. The square root function is at least as important as these. This subproject aims to improve the approximate calculation of these functions so that they also can be performed to an arbitrary precision, with a guaranteed accuracy.

Because of the representation theory of Clifford algebras, all of the work on functions of matrices is also applicable to functions in Clifford algebras. N. Higham's book on the subject [59] describes much of this work, by himself, and many others.

My approach for this subproject will be to continue to apply the algorithms, principles and theory described in Higham's book and related references. GluCat already contains simple implementations of some of these algorithms, including the Denman-Beavers square root algorithm, and the inverse scaling and squaring method of Cheng, Higham, Kenney and Laub, for the matrix logarithm [43].

This work will build on that of the previous two subprojects. The use of arbitrary precision calculation will allow me to distinguish between rounding errors and truncation errors when evaluating the results of numerical experiments. Experience with the principles underlying MPFR will help me to devise algorithms with guaranteed accuracy.

Success of the core project would:

- Improve our ability to calculate with geometric algebras.

  We would have better tools for efficient approximate calculation with geometric algebras, with guaranteed accuracy.

- Lead to greater acceptance and use of geometric algebras as tools for practical calculation.

  The first version of Matlab was one of the results of a long period of research into numerical linear algebra, and it took a long time for Matlab to achieve widespread commercial success, but its success made numerical linear algebra much more well known and more widely used. Success in this project could eventually contribute to similar results for numerical calculation with geometric algebras.

(2) Applications to the Explicit Calculation of Automorphic Forms. An interesting and valuable application of the arbitrary precision computation with Clifford algebras is the explicit calculation of values associated with genwralized automorphic forms. Since 1998, R. S. Krausshar and his collaborators have been developing a theory of automorphic forms over real and complex Clifford algebras [60].

The classical automorphic forms over the complex numbers are complex functions f such that $f(g(z)) = h(z)f(z)$, where g is an element of a finite group acting over the complex numbers and h is an analytic function. Such automorphic forms have wide application.

In number theory, the special case of modular forms is essential to Wiles' proof of Fermat's Last Theorem (Wolfskehl Prize, 1997). Two questions involving automorphic forms, and the closely related concepts of L-series and zeta functions are included in the list of Millenium Prizes of the Clay Mathematics Institute. These are the Riemann Hypothesis and the Birch and Swinnerton-Dyer Conjecture. In physics, modular forms are used in String Theory and Conformal Field Theory.

Quite a bit of work has already been done on algorithms for explicit computation of quantities associated to modular forms, including work by W. Stein and collaborators [70], which has been incorporated into the Sage computer algebra system [69]. J. Bruinier and F. Strömberg's work on Maass forms includes extensive numerical computation to high precision using Sage [42]. J. and P. Borwein and D. Bailey have also made use of arbitrary precision calculations involving Eisenstein series and modular forms [40]. In contrast, not much work has been done on explicit calculation with the generalized analytic automorphic forms treated by Krausshar, though these have application to the solution of partial differential equations in certain special cases [44].

My approach will be to: (1) closely examine the definitions and theorems involving Krausshar's analytic automorphic forms; (2) examine the existing algorithms of Stein, Bruinier, Borwein, their collaborators and others, to see if and how they can be modified for use with Krausshar's forms; (3) closely collaborate with Krausshar, Bruinier, and others at Darmstadt, to develop new algorithms; and (4) determine the convergence properties of modified algorithms and any new algorithms.

The arbitrary precision calculations used by this subproject will ultimately depend on the facilities provided by the core project, but much of the work can begin before these facilities are available.

Success in this subproject would:

- Provide an important example of the use of arbitrary precision calculation with Clifford algebras.

- Contribute to a greater understanding of automorphic forms, their application and their generalization to Clifford algebras.

(3) Applications to the Solution of Partial Differential Equations. The main problem addressed by this subproject is in the foundations of methods such as the Finite Element Method.

The Finite Element Method is a method for solving certain types of differential and integral equations over a region of space. It breaks the region up into small pieces, each one of which supports a small number of basic functions, and uses linear algebra to find a combination of these basic functions which is a close approximation to the solution of the original problem.

In the theory of the Finite Element Method, there are fundamental objects called *chains* and *cochains*. Roughly speaking, these are discrete objects which correspond in some continuous limit to domains of integration and to differential forms, respectively. Concepts of chains and cochains are important in the foundations of a number of branches of higher calculus, including differential geometry and algebraic topology (H. Cartan, Wolf Prize 1980; H. Whitney, Wolf Prize, 1982).

These concepts and their relationships with the Finite Element Method have recently been examined more carefully. This has resulted in new refinements of these methods, one of which is called Finite Element Exterior Calculus [34], and a new area of study called compatible discretization. Finite Element Exterior Calculus is based on Grassmann's exterior algebras. The idea of compatible (or *mimetic*) discretization [38] 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. A feature of many formulations of compatible discretization, such as that of Desbrun et al. [47] is the use of discrete differential forms and exterior calculus, often using both primal and dual cell complexes ("meshes").

D. White, J. Koning and R. Rieben [71] recently formulated, implemented and tested a high order finite element compatible discretization method for Maxwell's electromagnetic equations using only the primal mesh. From all accounts this method has been successful. More recently, M. Costabel and A. McIntosh have produced regularity results for certain integral operators [45] which can be used to explain the convergence of compatible discretization methods for Maxwell eigenvalue problems [39].

Clifford analysis is essentially the study of the Dirac differential operator. The geometric calculus of Hestenes, Sobczyk and others, places Clifford analysis into the wider context of geometric algebras. It has been known for quite some time how Clifford analysis, in the form of geometric calculus, relates both to differential forms and to cell complexes [67, 48, 68]. Theoretical frameworks for discrete versions of Clifford analysis and geometric calculus have recently been developed, notably the work of N. Faustino [51, 52] and of the Clifford research group at Ghent University in Belgium [41], but these have been mainly oriented towards finite difference rather than finite element methods.

The aim of the subproject in this theme area is to create a theory of Finite Element Geometric Calculus, based on a combination of exterior algebras and Clifford algebras. Besides filling what looks to be a gap in the fundamental theory, such methods may be useful in solving equations which involve the Dirac operator.

A seemingly straightforward method of proceeding would be to discretize equations involving the Dirac operator by using Hodge decomposition followed by the use of the existing techniques of Finite Element Exterior Calculus. While this may work well for Maxwell's equations, which can be expressed in terms of a Dirac operator, the method may encounter obstacles in higher dimensions, similar to those mentioned by Boffi et al [39].

My work on this subproject has already begun. I am writing a paper on the prospects for Finite Element Geometric Calculus to be presented at the International Conference on Clifford Algebras and their Applications to Mathematical Physics, in July, and a related paper for presentation to ICIAM, also in July.

The subproject will proceed by examining and combining existing methods which are known to work, especially those of Finite Element Exterior Calculus. Informal and possibly formal collaboration with A. McIntosh and R. S. Krausshar will help me to establish the correctness of the theory and associated estimates. I will also investigate whether explicit calculation with Grassmann and Clifford algebras is useful in implementation, by interfacing the GluCat library and PyCliCal with Finite Element Exterior Calculus libraries such as FEniCS [53] and PyDEC [37].

Success in this subproject would:

- Improve our understanding of the relationship between continuous problems involving Dirac operators and discrete versions of these problems.
- Lead to improved methods of solution for these problems, or at least lead to a better understanding of how well these methods work in practice.

Institutional support

ANU has an active world-class research environment in Pure Mathematics, as evidenced by its scoring 5 in the recent ARC ERA exercise. Nine of the academic staff of the MSI have published research which mentions Clifford algebras or Dirac operators, (P. Bouwknegt, C. Burden, A. Carey, M. Eastwood, A. Hassell, A. Isaev, A. McIntosh, A. Rennie, B. Wang). In addition, Computational Mathematics and High Performance Computing are key developing areas for ANU in the near future. More detail on this is given in the Strategic Statement.

There are essentially three types of facilities needed for this project, computing, information and collaboration. Available computing facilities include workstations, the Orac research cluster, and a teaching cluster which is currently being purchased. Large-scale computation would be conducted via the National Computation Infrastructure (NCI) through the ANU Supercomputer Time Allocation Scheme and the separate NCI Merit Allocation Scheme. Information facilities include the ANU Library, ANU Library access to electronic sources, interlibrary loans and Article Reach. Collaboration would include collaboration within the Computational Mathematics group (especially R. Brent, M. Hegland, S. Roberts, L. Stals), within MSI (especially M. Eastwood, A. McIntosh, A. Neeman, A. Rennie, B. Wang), and external collaboration. External collaboration is described in more detail in Project section above, and in the Budget Justification.

In addition to facilities, ANU will contribute $ 17, 750 per annum in salary and oncosts, to cover the gap between the ARC DECRA salary contribution and my appointment at level A8 with loading to B2.

I will promote and spread my research outcomes through a number of channels, including local and external collaboration, presentations at national and international academic conferences, and journal articles. Besides these traditional means, the project aims to disseminate the resulting implementations of algorithms as open source software. The vehicles to be used for this software will vary, but will most likely include the GluCat library, PyCliCal and the Sage computer algebra system. I also aim to use the algorithms and software to teach courses at the Honours level at ANU. The inclusion of a PhD student in the project will also provide more ways to disseminate results.

References

[33] R. Ablamowicz *Computations with Clifford and Grassmann Algebras.* Advances in Applied Clifford Algebras 19:3-4, 2009, pp. 499-545.

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

[35] M. F. Atiyah and I. M. Singer, *The index of elliptic operators on compact manifolds.* Bull. Amer. Math. Soc. 69 1963, pp. 422-433.

[36] P. Auscher, S. Hofmann, M. Lacey, J. Lewis, A. McIntosh, P. Tchamitchian, *The solution of Kato's conjectures.* C. R. Acad. Sci. Paris Sér. I Math. 332 (2001), no. 7, pp. 601-606.

[37] N. Bell, A. N. Hirani, *PyDEC: Software and Algorithms for Discretization of Exterior Calculus* arXiv:1103.3076v1 [cs.NA], 2011.

[38] P. Bochev and J. Hyman, *Principles of Mimetic Discretizations of Differential Operators.* Compatible Spatial Discretizations, Springer, 2006, pp. 89-119.

[39] D. Boffi, M. Costabel, M. Dauge, L. Demkowicz, R. Hiptmair, *Discrete compactness for the p-version of discrete differential forms.* arXiv:0909.5079v4 [math.NA], 2009.

[40] J. M. Borwein and P. B. Borwein, *Class number three Ramanujan type series for* $1/\pi$. Journal of Computational and Applied Mathematics, 46:1-2, 1993, pp. 281-290.

[41] F. Brackx, H. De Schepper, F. Sommen and L. Van de Voorde, *Discrete Clifford analysis: a germ of function theory,* Hypercomplex Analysis. Birkhauser, 2009, pp. 37–53.

[42] J. H. Bruinier and F. Strömberg, *Computation of harmonic weak Maass forms.* arXiv:1101.3190v1 [math.NT] 2011.

[43] 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.

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

[45] M. Costabel and A. McIntosh, *On Bogovskiĭ and regularized Poincaré integral operators for de Rham complexes on Lipschitz domains.* Mathematische Zeitschrift, 265:2, 2010, pp. 297-320.

[46] R. Delanghe, F. Sommen, and V. Souček, *Clifford algebra and spinor-valued functions. A function theory for the Dirac operator.* Mathematics and its Applications, 53. Kluwer Academic Publishers Group, Dordrecht, 1992.

[47] M. Desbrun, A. N. Hirani, M. Leok and J. E. Marsden, *Discrete exterior calculus.* arXiv:math/0508341v2 [math.DG]. 2005.

[48] C. Doran and A. Lasenby, *Geometric Algebra for Physicists.* Cambridge University Press, 2003.

[49] L. Dorst and D. Fontijne. *Geometric Algebra for Computer Science.* 2009.

[50] M. G. Eastwood and J. Ryan, *Aspects of Dirac Operators in Analysis.* Milan J. Math. 75 (2007) pp. 91-116.

[51] N. Faustino, U. Kahler and F. Sommen, *Discrete Dirac operators in Clifford analysis.* Advances in Applied Clifford Algebras, 17 (2007), pp. 451-467.

[52] N. Faustino, *Discrete Clifford analysis.* PhD thesis, Universidade de Aveiro, 2009.

[53] FEniCS Project. `http://www.fenics.org`

[54] D. Fontijne. *Gaigen 2: A Geometric Algebra Implementation Generator.* In GPCE06. ACM, 2006.

[55] L. Fousse, G. Hanrot, V. Lefèvre, P. Pélissier, and P. Zimmermann, *MPFR: A multiple-precision binary floating-point library with correct rounding.* ACM Trans. Math. Softw. 33:2, 2007, Article 13.

[56] H. Grassmann, *Extension theory.* Translated from the 1896 German original by L.C. Kannenberg. History of Mathematics, 19. American Mathematical Society, Providence, RI; London Mathematical Society, London, 2000.

[57] D. Hestenes, *A unified language for mathematics and physics.* Clifford algebras and their applications in mathematical physics (Canterbury, 1985), pp. 1-23, Reidel, Dordrecht, 1986.

[58] N. J. Higham, *Accuracy and Stability of Numerical Algorithms,* Second Edition. SIAM, 2002.

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

[60] R. S. Krausshar, *Generalized analytic automorphic forms in hypercomplex spaces.* Birkhäuser, 2004.

[61] J. Lasenby, A. Lasenby and C. Doran, *A Unified Mathematical Language for Physics and Engineering in the 21st Century.* Phil. Trans. R. Soc. A: Mathematical, Physical and Engineering Sciences, 358:1765, 2000, pp. 21-39.

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

[63] R. Mikkola and P. Lounesto, *Computer-aided vector algebra.* International Journal of Mathematical Education in Science and Technology 14:5, 1983, pp. 573-578.

[64] C. Perwass and D. Hildenbrand, *Aspects of Geometric Algebra in Euclidean, Projective and Conformal Space.* Technical report, University of Kiel, 2004.

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

[66] K. Shoemake, *Animating rotation with quaternion curves.* Computer Graphics (Proc. Siggraph 85) 19:3, 1985, pp. 245-254.

[67] G. Sobczyk, *Simplicial Calculus with Geometric Algebra,* in Clifford Algebras and Their Applications in Mathematical Physics, A. Micali, R. Boudet, and J. Helmstetter (eds), Kluwer Academic Publishers, Dordrecht, 1992.

[68] G. Sobczyk and O. L. Sanchez, *Fundamental Theorem of Calculus.* arXiv:0809.4526v1 [math.HO] 2008.

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

[70] W. Stein, *Modular Forms, a Computational Approach* with an appendix by P. E. Gunnells. AMS, 2007.

[71] D. White, J. Koning, and R. Rieben, *Development and application of compatible discretizations of Maxwell's equations,* Compatible Discretization of Partial Differential Equations. Springer-Verlag, 2006, pp. 209-234.