Project title

New approaches to the discretization of partial differential equations.

Project Quality and Innovation

This project aims to develop new methods for the solution of those problems encountered in physics and engineering which can be formulated using partial differential equations, by combining and extending a number of existing methods.

Typical problems involving partial differential equations include boundary value problems:

$$Lu(x) = f(x), \quad (x \in \Omega), \quad Mu(x) = g(x), \quad (x \in \partial\Omega),$$

(for some region $\Omega \in \mathbb{R}^n$, and functions f, g and differential operators L, M), and eigenvalue problems:

$$Lu(x) = \lambda u(x), \quad (x \in \Omega), \quad Mu(x) = g(x), \quad (x \in \partial\Omega),$$

(where both the eigenvalues λ and the corresponding eigenfunctions u are to be found.)

Quite often, such problems are solved by using the Finite Element Method (FEM). Recently, a number of refinements of the theory of the Finite Element Method, based on ideas from differential geometry, have been developed. These are Discrete Exterior Calculus [44], and the Finite Element Exterior Calculus (FEEC) [29, 30]. These theories explain how certain types of discretization can cause numerical instability and, in the case of eigenvalue problems, *spurious modes* [35, 36], in other words, incorrect results. They also explain, in terms of differential forms and their discretization, why certain other types of discretization work well.

Other existing methods for the solution of problems involving partial differential equations use ideas from Clifford analysis, essentially, ideas from complex analysis which apply in higher dimensions. There is a large overlap between problems treated by FEM and those which can be solved by Clifford analysis, but some types of problem have traditionally been treated only by one of these two types of method. This project aims to extend the theory and methods of Discrete Exterior Calculus and FEEC to cover the types of problems which can be solved by the methods of Clifford analysis.

Background. In geometric algebras such as the Grassmann and Clifford algebras, the “numbers” embody the idea of *direction* as well as quantity, that is they answer the question “which way?” as well as “how much?” Examples of geometric algebras include the real numbers, the complex numbers, and real vector spaces with Grassmann or Clifford multiplication. The elements of geometric algebras are often called *hypercomplex numbers* or *multivectors* [55, 60]. Geometric algebras have been very important in the history of mathematics in the nineteenth and twentieth centuries, especially in the area of differential geometry, since the geometric algebra of *differential forms* is Grassmann’s *exterior algebra* [52].

The *Clifford algebras* [65, 60] 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 [58, 45]. Clifford algebras have been used in research leading to award-winning results such as the Atiyah-Singer index theorem [31] (M. Atiyah and Singer, Abel prize 2004) and the solution of the Kato square root problem [32] (A. McIntosh, Moyal medal 2002).

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 [31, 48]. The Dirac operator is essentially a type of directed derivative, generalizing the more familiar *gradient*, *divergence* and *curl* operators used in three dimensional calculus [55, 43]. Clifford analysis is essentially the study of the Dirac operator. The geometric calculus of Hestenes, Sobczyk and others, places Clifford analysis into the wider context of geometric algebras. An important advantage of geometric calculus in physics and engineering over traditional methods of vector and tensor calculus is the ability to formulate problems without resort to coordinates. An advantage of geometric calculus over differential geometry with exterior differential forms is that metric properties are incorporated naturally into the Clifford algebra.

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.

The idea of compatible (or *mimetic*) discretization [34, 72] 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 the Discrete Exterior Calculus of Desbrun et al. [44] is the use of discrete differential forms and exterior calculus, often using both primal and dual cell complexes ("meshes").

In Discrete Exterior Calculus [44], there are fundamental objects called *chains* and *cochains*. 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).

Finite Element Exterior Calculus [29, 30] essentially concentrates on discretizing the spaces involved in a problem, rather than the operators. This often results in problems being discretized over a single mesh. D. White, J. Koning and R. Rieben [73] recently formulated, implemented and tested a high order finite element compatible discretization method for Maxwell's electromagnetic equations, using only the primal mesh. Recently, M. Costabel and A. McIntosh have produced regularity results for certain integral operators [42] which can be used to explain the convergence of compatible discretization methods for Maxwell eigenvalue problems [36].

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, 45, 68]. Theoretical frameworks for discrete versions of Clifford analysis and geometric calculus have recently been developed, notably the work of N. Faustino [49, 50] and of the Clifford research group at Ghent University in Belgium [37], but these have been mainly oriented towards Finite Difference rather than Finite Element methods [53, 54].

Methodology. This project is split into two streams: a theory stream, and an implementation stream.

Theory stream. The aim of the theory stream is to create a theory of Finite Element Geometric Calculus (FEGC), based on combinations of Discrete Exterior Calculus, Finite Element Exterior Calculus, and Clifford analysis. There are two relatively straightforward approaches.

(1) The first approach is to extend the methods of Discrete Exterior Calculus to problems involving Dirac operators, essentially by discretizing the Dirac operator on a simplex in the context of function spaces appropriate to the solution of the problem. This approach takes an existing finite element space defined on cells, and ensure that Stokes' theorem holds exactly for the appropriate Dirac operator on each cell. The simplest case would be in for the vector derivative in Euclidean space, with each cell a simplex.

A first illustration of this approach is contained in the paper I wrote on the prospects for Finite Element Geometric Calculus [2], and presented at ICCA 9, the International Conference on Clifford Algebras and their Applications to Mathematical Physics, in Weimar, and at the International Council on Industrial and Applied Mathematics ICIAM, both in July 2011. This illustration follows.

Following Cnops [40, Chapter 3], we have, for a compact k-dimensional submanifold C of an m-dimensional manifold M, with boundary ∂C, and multivector-valued functions f and g,

$$\int_C \overline{f(x)} dM_k(x) g(x) \simeq \sum_j \overline{f(y_j)} v_k(T_j) g(y_j),$$

for some y_j near T_j, where $v_k(T) := \frac{1}{k!}(x_1 - x_0) \wedge \ldots \wedge (x_k - x_0)$, for the k-simplex T with vertices $x_0, \ldots, x_k$, where $\overline{x}$ is the main anti-involution of x in the relevant Clifford algebra, and where dM_k is defined via oriented k dimensional surface elements in M, or alternatively, via differential forms, or via Lebesgue measure. Also Stokes' theorem for the vector derivative, V_M on M, gives us

$$\int_{\partial C} \overline{f(x)} dM_{m-1}(x) g(x) = \int_C \overline{V_M f(x)} dM_m(x) g(x) + (-1)^m \int_C \overline{f(x)} dM_m(x) V_M g(x).$$

Setting $g \equiv 1$, so that $V_M g \equiv 0$, on a single m-dimensional simplex T with vertices $x_0, \ldots x_m$, and boundary ∂T consisting of faces $S_0, \ldots S_m$, we obtain

$$\sum_{j=0}^{m} \overline{f(y_j)} v_{m-1}(S_j) \simeq \overline{V_M f(y)} v_m(T), \tag{1}$$

for some y near T and y_j near S_j. We can use this to define the discrete vector derivative V_E of a multivector-valued affine function f on an m-simplex T in Euclidean space as:

$$V_E f(y) := \overline{v_m}(T)^{-1} \sum_{j=0}^{m} \overline{v_{m-1}}(S_j) \sum_{i \neq j} f(x_i)/m.$$

for any y in T, with x_i and S_j as per (1) above. We must then verify that this definition agrees with the usual definitions, and that Stokes' theorem holds for T as well as in the limit. Thus a function which is piecewise affine on simplices has a discrete vector derivative which is piecewise constant on these same simplices.

This exercise will be repeated with more sophisticated and higher order elements, including Whitney [74], Raviart-Thomas [66], and Nédélec [62, 63] elements. This will yield pairs of function spaces, which will then be compared to the spaces obtained by decomposition followed by discretization, as described in the second approach, below. This exercise will also be done for the the spinor Dirac and Hodge-Dirac operators on manifolds [40, Chap. 3]. The bulk of the theoretical work in the development of this type of discretization includes proving the consistency stability, and rates of convergence of the schemes corresponding to each such pair of function spaces.

(2) A second approach is to discretize equations involving the Dirac operator by using Hodge decomposition followed by the use of the existing techniques of Finite Element Exterior Calculus. This is the subject of my joint paper with Ari Stern [59, in preparation]. In the paper, we start with a closed and densely defined operator d on a Hilbert space W, such that $\mathrm{d}^2 = 0$, and perform an abstract Hodge decomposition on W. We also give the domain V, of d, a Hilbert space structure, and a corresponding Hodge decomposition. This leads to an abstract Poincaré inequality. We define the *abstract Hodge–Dirac operator* to be $\mathrm{D} = \mathrm{d} + \mathrm{d}^*$, where d^* is the adjoint of d with respect to the Hilbert space W. We consider a variational problem:
Find $(u, p) \in V \times \mathfrak{H}$ such that

$$\begin{aligned} \langle \mathrm{d}u, v \rangle + \langle u, \mathrm{d}v \rangle + \langle p, v \rangle &= \langle f, v \rangle\,, \quad && \forall v \in V, \\ \langle u, q \rangle &= 0, && \forall q \in \mathfrak{H}, \end{aligned} \tag{2}$$

where $\mathfrak{H} = \ker \mathrm{d} \cap (\mathrm{d}V)^{\perp_W}$. We prove that problem (2) is well-posed, and then use a bounded, commuting projection π_h from V to a finite dimensional subspace V_h, that is, $\pi_h \mathrm{d}v = \mathrm{d}\pi_h v$ for all $v \in V$. This projection discretizes our problem. We then prove that the discrete problem is well posed, and give error bounds as $h \to 0$. FEEC discretization uses smoothed projection operators [29, 39], and the project will investigate corresponding projection operators for use with the Hodge-Dirac operator. The role of variational crimes [56, 57] in FEGC will also be examined in detail.

Implementation stream. The implementation stream will develop practical methods based on the theory developed in the theory stream. The project will also investigate whether explicit calculation with Grassmann and Clifford algebras is useful in implementation, by interfacing the GluCat library, including PyClical [25] with Finite Element Exterior Calculus libraries such as FEMSTER/EMSolve [38, 73], FEniCS [51] and PyDEC [33], and using the combined software to implement numerical examples and conduct numerical experiments arising from the theory stream. This will be useful in a number of ways, firstly as a check on estimates arising from the theory stream, secondly, as a source of new ideas, and thirdly as open source software. The open-source software could be used to duplicate the results of this project, and also used as the basis of more robust software for the solution of practical problems.

Research Environment

ANU has an active world-class research environment in Pure Mathematics, as evidenced by its scoring 5 in the recent ARC ERA exercise. Ten of the academic staff of the MSI (P. Bouwknegt, C. Burden, A. Carey, M. Eastwood [48], A. Hassell, J. Huerta, A. Isaev, A. McIntosh [32], A. Rennie, and B. Wang) have published research which involves Clifford algebras or Dirac operators. M. Eastwood [47] and A. McIntosh [42] have also published research directly relevant to FEEC. Also, Computational Mathematics and High Performance Computing are key developing areas for ANU in the near future, as evidenced by the ARC Linkage project LP110200410 with Fujitsu Laboratories of Europe Limited. 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 their postdoctoral researchers), and external collaboration. External collaborators include A. Stern at Washington University, and the Clifford group in Portugal, including Uwe Kähler, who expressed great interest in the ideas of this project while I visited Weimar.

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 [25] and the Sage computer algebra system [69]. I also aim to use the algorithms and software to conduct "special topics" courses at the Honours level at ANU.

Feasibility and Benefit

Feasibility. The two approaches of the theory stream, along with the implementation stream, are highly feasible. A first illustration of the first approach is contained in the paper [2] and reproduced above. The second approach has been successful so far: the first step in this directions is the subject of the joint paper [59], in preparation with my colleague Ari Stern, who is very familiar with both Discrete Exterior Calculus and FEEC (e.g. [56, 57, 70, 71, 72]). The implementation stream is based on the interfacing of existing software, written in C++ and Python, and I am very familiar with both languages.

Benefit. Ideally, Finite Element Geometric Calculus (FEGC) would combine the techniques of FEEC with those of Clifford analysis on manifolds on a fundamental level.

The advantages of FEGC over FEEC alone could stem from the advantages of Clifford analysis over the use of differential forms in differential geometry and the formulation and solution of differential equations. These advantages could include: a unified treatment of problems in Euclidean, Projective and Conformal geometries; a more natural treatment of problems involving Dirac-type operators and their inverses; a more natural treatment of problems involving multivector fields, especially mixed-grade fields, rather than treating these as collections of homogeneous differential forms; a different and possibly more natural treatment of the metric, as embodied in Clifford algebras on tangent or cotangent bundles; a more general and natural formulation of problems involving generalized Stokes' theorems, Green's functions and Cauchy integral formulas; greater economy of expression of some problems; and greater geometrical insight on the formulation of some problems.

Ideally, the problems which could be addressed by FEGC would include those currently treated by numerical methods for Clifford analysis [53, 54], as well as the problems treated by FEEC. The problems which would initially yield the most insight on how to develop FEGC, could be those currently treated by both methods. Such problems include boundary and initial value problems, such as the Poisson problem, Stokes' equations, Maxwell's equations, and the equations of elasticity.

Success in this project would:

- Improve our understanding of the relationship between continuous problems involving Dirac operators and discrete versions of these problems.
- Improve our understanding of the stability of discretization of these problems, and circumstances in which spurious modes may arise in eigenvalue problems involving Dirac operators, eg. [28].
- Lead to improved methods of solution for these problems, and lead to a better understanding of how well these methods work in practice.
- Provide open-source software for use in duplicating results, and as a basis for software to be used in solving practical problems.

References

[28] H. Almanasreh, S. Salomonson, and N. Svanstedt *Stabilized Finite Element Method for the Radial Dirac Equation.* arXiv:1111.6263v2 [math-ph].

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

[30] D. N. Arnold, R. S. Falk and R. Winther, *Finite element exterior calculus: from Hodge theory to numerical stability.* Bull. Amer. Math. Soc. (N.S.), 47, 2010, pp. 281-354.

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

[32] 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, no. 7, 2001, pp. 601-606.

[33] N. Bell, A. N. Hirani, *PyDEC: Software and Algorithms for Discretization of Exterior Calculus* arXiv:1103.3076v2 [cs.NA], 2012.

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

[35] D. Boffi, F. Brezzi, and L. Gastaldi, *On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form.* Mathematics of Computation, 69:229, pp. 121-140, 2000.

[36] 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.

[37] 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.

[38] P. Castillo, R. Rieben, and D. White, *FEMSTER: An object-oriented class library of higher order discrete differential forms.* ACM Trans. Math. Software 31, 2005, pp. 425-457.

[39] S .H. Christiansen and R. Winther, *Smoothed projections in finite element exterior calculus.* Math. Comp. 77, no. 262, 2008, pp. 813-829.

[40] J. Cnops, *An Introduction to Dirac Operators on Manifolds.* Progress in Mathematical Physics, Birkhäuser, Boston, 2002.

[41] 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.

[42] 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.

[43] 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.

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

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

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

[47] M. G. Eastwood, *A complex from linear elasticity.* In: Slovák, Jan and Čadek, Martin (eds.): Proceedings of the 19th Winter School "Geometry and Physics". Circolo Matematico di Palermo, Palermo, 2000. pp. 23-29

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

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

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

[51] FEniCS Project. `http://fenicsproject.org/` (as at March 2012).

[52] 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.

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

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

[55] 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.

[56] M. Holst and A. Stern, *Geometric variational crimes: Hilbert complexes, finite element exterior calculus, and problems on hypersurfaces.* arXiv:1005.4455v1 [math.NA], 2010.

[57] M. Holst and A. Stern, *Semilinear mixed problems on Hilbert complexes and their numerical approximation.* Found. Comput. Math. DOI: 10.1007/s10208-011-9110-8, 2012.

[58] 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.

[59] **P. Leopardi** and A. Stern, *The abstract Hodge-Dirac operator and its stable discretization*, in preparation, to be presented at the International Workshop on Operator Theory and Applications at UNSW in July 2012.

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

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

[62] J. C. Nédélec, Mixed finite elements in R^3. Numer. Math. 35, 1980, pp. 315-341.

[63] J. C. Nédélec, A new family of mixed finite elements in R^3. Numer. Math. 50, 1986, pp. 57-81.

[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] P. Raviart and J. Thomas, *A mixed finite element method for 2nd order elliptic problems.* Mathematical Aspects of the Finite Element Method, I. Galligani and E. Mayera, eds. Lecture Notes in Mathematics, vol. 606. Springer Verlag, Berlin, Germany, 1977, pp. 293-315.

[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] A. Stern, Y. Tong, M. Desbrun, and J E. Marsden, *Variational integrators for Maxwell's equations with sources.* PIERS Online, 4 (7), 711-715. Previously appeared in PIERS Proceedings, 443-447, July 2-6, Cambridge, USA 2008.

[71] A. Stern, Y. Tong, M. Desbrun, and J E. Marsden, *Geometric computational electrodynamics with variational integrators and discrete differential forms.* arXiv:0707.4470v3 [math.NA], 2009.

[72] A. Stern, *Geometric discretization of Lagrangian mechanics and field theories.* Ph.D. thesis, California Institute of Technology, 2009.

[73] 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.

[74] H. Whitney, *Geometric Integration Theory.* Princeton University Press, Princeton, NJ, 1957.