

Can compatible discretization, finite element methods, and discrete Clifford analysis be fruitfully combined?

Paul Leopardi

Mathematical Sciences Institute, Australian National University.
For presentation at ICCA, Weimar, 2011.

12 July 2011



AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics
and Statistics of Complex Systems



Acknowledgements

R. Sören Krausshar (TU Darmstadt).

Ari Stern (UCSD).

Chris Doran (Geomerics).

Australian Research Council.

Australian Mathematical Sciences Institute.

Australian National University.

Subjects with parallel 40+ year histories

Finite Element Method

M. Zlámal, *On the finite element method*. Numer. Math., 12, 1968, pp. 394-409.

Clifford analysis

D. Hestenes, *Multivector calculus*. J. Math. Anal. and Appl., 24:2, 1968, pp. 313-325.

More recent developments

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

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

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

Calls for Finite Element Geometric Calculus

At AGACSE, Amsterdam, 2010:

Chris Doran calls for a Geometric Algebra version of Discrete Exterior Calculus:

“We MUST develop a GA version of this theory.”

(Thoughts from the front line: Current issues in real-time graphics and areas where Geometric Algebra can help.)

David Hestenes asks for Geometric Calculus to be applied to the differential geometry of the Finite Elements Method:

“Challenges: II. Finite Element differential geometry”

(The shape of differential geometry with Geometric Calculus.)

Topics

- ▶ Related previous work
 - ▶ Geometric Calculus / Clifford analysis.
 - ▶ Compatible discretization
- ▶ Finite Element Geometric Calculus (FEGC)
 - ▶ FEGC via Hodge Decomposition
 - ▶ FEGC via Dirac operator on finite element spaces

Grassmann, Clifford and Geometric Algebras

Clifford algebras can be constructed on any vector space with a quadratic form including tangent spaces on orientable manifolds with a metric.

Geometric Algebra, a “unified language for physics and engineering,” uses the exterior (Grassmann) product and the geometric (Clifford) product, as well as contractions, on the same underlying tangent space, with the quadratic form defined by the metric.

$$xy = x \wedge y + x \cdot y.$$

(Porteous 1995; Lounesto 1997; Lasenby, Lasenby and Doran 2000; Cnops 2002)

Clifford analysis and Geometric Calculus

Clifford algebras are a natural setting for Dirac operators, such as the vector derivative.

Clifford analysis (CA) studies the Dirac operator and its kernel in various contexts, including smooth manifolds, finding structures, functions and relationships analogous to complex analysis.

Geometric Calculus (GC) encompasses both Clifford analysis and the use of exterior derivatives and differential forms on embedded orientable manifolds with arbitrary metric signatures.

(Sobczyk 1992; Delanghe 2001; Cnops 2002; Doran and Lasenby 2003; Eastwood and Ryan 2007)

Some successes of Clifford analysis

Generalizations of the Cauchy-Riemann operator, the Cauchy integral theorem and holomorphic function theory

(Lounesto 1997; Cnops 2002; Gürlebeck, K. Habetha, and W. Sprössig 2008; others).

Solution of Kato's square root problem (McIntosh 1985; Auscher, Hofmann, Lacey,

McIntosh and Tchamitchian 2002; Axelsson, Keith and McIntosh 2006).

Generalized series expansions, generating functions, kernels, and special functions including orthogonal polynomials

(Delanghe 2001; Gürlebeck, K. Habetha, and W. Sprössig 2008; Malonek and Tomaz 2008; others).

Maxwell's equations (Chantaveerod, Seagar, and Angkaew 2007; Krausshar, Cação and Constaes 2009; Constaes, Faustino and Krausshar 2011; others) and Navier Stokes' equations

(Gürlebeck,, A. Hommel, U. Kähler 2006; Krausshar and Constaes 2008; others).

Discrete Clifford analysis

Mostly uses finite difference methods, lattices and umbral calculus. Lattice frameworks for the Dirac-Kähler operator date to the 1980s (Becher and Joos 1982; Jourjine 1986).

Gürlebeck and Sprössig worked on finite differences and discrete Dirac operators (1997 and later).

The PhD thesis of Nelson Faustino (2009) combines the finite element exterior algebra with umbral calculus and discrete Dirac operators, including operators on lattices (Forgy and Schreiber 2004; Faustino and Kähler 2007; Faustino, Kähler and Sommen 2007).

These methods have been further developed by Faustino and by the Clifford research group at Ghent University (Brackx, De Schepper, Sommen and Van de Voorde 2009; Faustino 2010; Faustino and Ren (in proof)).

Geometric Calculus and Clifford analysis on cell complexes

Multivectors provide a natural data structure for simplices and other cells, chains, complexes, and mixed grade differential forms

(Lundholm and Svensson 2009).

It has been known for quite some time how Geometric Calculus and Clifford analysis, relate to differential forms (Hestenes 1993) and to cell complexes.

The directed integral can be defined as the limit of a sum defined on cell complexes.

The vector derivative can be defined as a limit of a directed integral over the boundary of a simplex, in such a way that Stokes' theorem holds.

(Sobczyk 1992; Cnops 2002; Doran and Lasenby 2003; Sobczyk and Sanchez 2008).

Variational principles and Noether's theorem

Variational principle: Abstract trajectory that makes some functional stationary.

Example: Hamilton's Principle of Stationary Action.

Noether's Theorem: *Symmetries* in the equations describing a variational principle are equivalent to *conservation laws*.

(Noether 1918; Vujanovic and Jones 1989; Frankel 2004)

Principles of compatible discretization

Compatible (or *mimetic*) discretization creates 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.

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.

(Hiptmair 2001; Bochev and Hyman 2006; Arnold Falk and Winther 2006; He and Teixeira 2006)

Some aspects of compatible discretization

These 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.

Simplicial *chains* and *cochains* are discrete objects which correspond in some continuous limit to domains of integration and to differential forms, respectively.

Various concepts of chains and cochains arise in homology theory and the foundations of geometry (Whitney 1937; Eilenberg 1944).

(Hiptmair 2001; Bochev and Hyman 2006; Arnold Falk and Winther 2006; He and Teixeira 2006)

Discrete Exterior Calculus

These compatible discretization methods focus on the discretization of operators via simplicial complexes.

Often both a primal and a *dual mesh* is used, to simplify or even diagonalize the discrete Hodge star operator.

Much effort is put into the definition of the dual mesh and the Hodge star, to optimize performance for particular problems.

(Hiptmair 2001; Bochev and Hyman 2006; Arnold Falk and Winther 2006; He and Teixeira 2006)

Finite Element Method

The Finite Element Method solves boundary value problems based on partial differential equations.

The original problem in a Hilbert space of functions is put into variational form, and is mapped into a problem defined on a finite dimensional function space, whose basis consists of functions supported in small regions, such as simplices.

(Iserles 1996; Braess 2001).

Finite Element Exterior Calculus (FEEC)

FEEC discretizes spaces rather than operators. It is based on the Finite Element Method over Hilbert complexes. These are cochain complexes where the relevant vector spaces are Hilbert spaces.

For the de Rham complex, FEEC uses Hodge decomposition, the exterior derivative and differential forms.

The numerical stability of the FEEC discretization depends on the existence of a bounded cochain projection from a Hilbert complex to a subcomplex. FEEC uses smoothed projections to obtain this numerical stability.

(Arnold, Falk and Winther 2006, 2010; Christiansen and Winther 2008)

Applications to Maxwell's equations

White, Koning and Rieben recently (2006) successfully formulated, implemented and tested a high order finite element compatible discretization method for Maxwell's electromagnetic equations based on the concepts of FEEC.

This method is incorporated into the the EMSolve package from Lawrence Livermore National Laboratory.

What would FEGC look like?

Finite Element Geometric Calculus (FEGC) should combine the techniques of Finite Element Exterior Calculus (FEEC) with those of Geometric Calculus / Clifford analysis on manifolds (GC/CA) on a fundamental level.

The problems to be addressed by FEGC could include those currently treated by numerical methods for GC/CA, as well as the problems treated by FEEC.

Problems currently treated by both methods, such as the Poisson problem, Stokes' equations, Maxwell's equations, and the equations of elasticity, should initially yield the most insight on how to develop FEGC.

Possible advantages of FEGC over FEEC

1. Unified treatment of problems in Euclidean, Projective and Conformal geometries.
2. More natural treatment of problems involving Dirac-type operators and their inverses.
3. More natural treatment of problems involving multivector fields, especially mixed-grade fields, rather than treating these as collections of homogeneous differential forms.
4. Different and possibly more natural treatment of the metric, via Clifford algebras on tangent or cotangent bundles.
5. More general and natural formulation of problems involving Stokes' theorems, Green's functions, Cauchy integral formulas.
6. Greater economy of expression of some problems.
7. Greater geometrical insight in formulating some problems.

FEGC via Hodge Decomposition

A viable approach is to discretize boundary value problems involving the multivector-valued fields and Dirac operators by using Hodge decomposition followed by the existing techniques of FEEC.

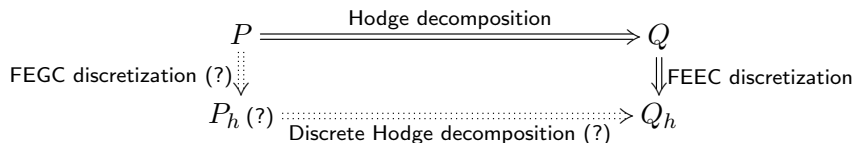
The Hodge Dirac operator is decomposed into operators defined in terms of the exterior derivative and Hodge star.

Using the weak formulation eliminates the explicit use of the Hodge star in favour of the use of inner products.

Very recently, Stern has essentially shown that this approach to discretizing the Hodge Dirac operator works (Private communication).

“Notional commutative diagram” for FEGC

Instead of Hodge decomposition of problem P into problem Q followed by FEEC discretization into problem Q_h , it may be possible to perform “FEGC discretization” into problem P_h followed by “discrete Hodge decomposition” into problem Q_h :



Dirac operators on Finite Element spaces

One possible guide to what “FEGC discretization” might look like is to take 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.

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

$$v_k(T) := \frac{1}{k!} (x_1 - x_0) \wedge \dots \wedge (x_k - x_0),$$

for the k -simplex T with vertices x_0, \dots, x_k , where \bar{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.

(Cnops 2002)

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 $V_M g \equiv 0$, gives us

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

(Cnops 2002)

On a single m -dimensional simplex T with vertices x_0, \dots, x_m , and boundary ∂T consisting of faces S_0, \dots, S_m , we obtain

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

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 .

(Cnops 2002)

We must then verify that this definition agrees with the usual definitions, and that Stokes' theorem holds for T , and in the limit.

This exercise could be repeated with more sophisticated and higher order elements, such as Whitney (1957), Raviart-Thomas (1977), and Nédélec (1980,1986).

This would yield pairs of function spaces, which could then be compared to the appropriate direct sums of the spaces obtained by decomposition followed by discretization.

The bulk of the theoretical work in the development of FEGC discretization may be in proving consistency and stability, and in proving bounds for rates of convergence for each such pair of function spaces.

Geometric Algebra computation within FEGC

Explicit calculation with Grassmann and Clifford algebras may be useful in the implementation of a FEGC scheme.

One way to investigate this would be to interface Geometric Algebra packages and libraries, such as the GluCat library and PyCliCal (L. 2001) with FEEC and DEC libraries, such as EMSolve (White, Koning, and Rieben 2006), FEniCS and PyDEC (Bell, Hirani 2011).

Meanwhile, conformal geometric algebra has been used in the formulation and solution of deformation problems, using Finite Element methods, by researchers in TU Darmstadt

(Brendel, Kalbe, Hildenbrand, and Schfer 2008).