Discrete Exterior Calculus

Thesis by

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For

my parents Nirmal and Sati Hirani

my wife Bhavna and daughter Sankhya.

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Abstract

The language of modern mechanics is calculus on manifolds, and exterior calculus is an important part of that. It consists of objects like differential forms, general tensors and vector fields on manifolds, and operators that act on these. While the smooth exterior calculus has a long history going back to Cartan, Lie, Grassmann, Hodge, de Rham and many others, the need for a discrete calculus has been spurred on recently by the need to do computations.

This thesis presents the beginnings of a theory of *discrete exterior calculus* (DEC). This is motivated by potential applications in computational methods for field theories (elasticity, fluids, electromagnetism) and in areas of computer vision and computer graphics. One approach to approximating a smooth exterior calculus is to consider the given mesh as approximating some smooth manifold at least locally, and then defining the discrete operators by truncating the smooth ones. Another approach is to consider the discrete mesh as the only given thing and developing an entire calculus using only discrete combinatorial and geometric operations. The derivations may require that the objects on the discrete mesh, but not the mesh itself, are interpolated. It is this latter route that we have taken and this leads to a discrete exterior calculus.

Our theory includes not only discrete equivalents of differential forms, but also discrete vector fields and the operators acting on these objects. General tensors are not developed, though we suggest a possible way to do that towards the end. The presence of forms and vector fields allows us to address the various interactions between forms and vector fields which are important in applications. With a few exceptions, most previous attempts at discrete exterior calculus have addressed only differential forms, or vector fields as proxies for forms. We also show that the circumcentric dual of a simplicial complex plays a useful role in the metric dependent part of this theory. The importance of dual complexes in this field has been well understood, but with a few exceptions previous researchers have used barycentric duals.

The use of duals is reminiscent of the use of staggered meshes in computational mechanics. The appearance of dual complexes leads to a proliferation of the operators in the discrete theory. For example there are primal-primal, primal-dual etc. versions of many operators. This is of course unique to the discrete side. In many examples we find that the formulas derived from our discrete exterior calculus are identitical to the existing formulas in literature.

We define discrete differential forms in the usual way, as cochains on a simplicial complex. The discrete vector fields are defined as vector valued 0-forms, and they live either on the primal, or on the dual vertices.

We then define the operators that act on these objects, starting with discrete versions of the exterior derivative, codifferential and Hodge star for operating on forms. A discrete wedge product is defined for combining forms; discrete flat and sharp operators for going between vector fields and one forms; and discrete interior product operator and Lie derivatives for combining forms and vector fields. The sharp and flat allow us to define various vector calculus operators on simplicial meshes including a discrete Laplace-Beltrami operator.

Our development of the theory is formal in that we do not prove convergence to a smooth theory. We have tried instead to build a discrete calculus that is *self*-consistent and parallels the smooth theory. The discrete operator should be natural under pullbacks, when the smooth one is, important theorems like the discrete Stokes' theorem must be satisfied, and the operators should be local. We then use these operators to derive explicit formulas for discrete differential operators in specific cases. These cases include 2-surfaces in $\mathbb{R}^3$ built with irregular triangles, regular rectangular and hexagonal meshes in the plane, and tetrahedralization of domains in $\mathbb{R}^3$. At least in these simple but important examples we find that the formula derived from our discrete exterior calculus is identitical to the existing formula in the literature.

Numerical methods similar to those based on a discrete exterior calculus have been used in many physical problems, for example, in areas like electromagnetism, fluid mechanics and elasticity. This is due to the geometric content of many physical theories. In this thesis we give a glimpse into three fields of discrete, geometric computations, which we have developed without an exterior calculus framework. These are examples of areas which are likely to benefit from a working DEC. They include discrete shells, a Hodge type decomposition of discrete 3D vector fields on an irregular, simplicial mesh, and template matching.

One potential application of DEC is to variational problems. Such problems come equipped with a rich exterior calculus structure and so on the discrete level, such structures will be enhanced by the availability of a discrete exterior calculus. One of the objectives of this thesis is to fill this gap. An area for future work, is the relationship between multisymplectic geometry and DEC. There are many constraints in numerical algorithms that naturally involve differential forms, such as the divergence constraint for incompressibility of fluids. Another example is in electromagnetism since differential forms are naturally the fields in that subject, and some of Maxwell's equations are expressed in terms of the divergence and curl operations on these fields. Preserving, as in the mimetic differencing literature, such features directly on the discrete level is another one of the goals, overlapping with our goals for variational problems.

In future work we want to make a cleaner separation of metric independent and metric dependent parts of DEC. For example, the wedge product, pairing of forms and vector fields, interior product and Lie derivative, should all be metric independent. Divergence should depend on the metric, only through the appearance of volume form. The metric should play a role only in the definition of sharp and flat operators. In this thesis, we don't always make this distinction and sometimes use identities from smooth theory, where the metric dependence cancels. It is not clear that the same cancellation happens on the discrete side. In these cases we have also tried to give at least a partial development of a metric independent definition.

In this thesis we have tried to push a purely discrete point of view as far as possible. In fact, in various parts of the thesis we argue that this can only be pushed so far, and that interpolation is a useful device for developing DEC. For example, we found that interpolation of functions and vector fields is a very convenient device for understanding and deriving a discrete theory involving functions and vector fields. This naturally leads to the next step, that of interpolation of higher degree forms, for example using Whitney map. This is the methodology that is quite common in this field. In future work we intend to continue this interpolation point of view, especially in the context of the sharp, Lie derivative and interior product operators. Some preliminary ideas on this point of view are spread throughout the thesis.

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