Discrete Exterior Calculus : Applications in Mechanics and Computer Science

Anil N. Hirani

Control and Dynamical Systems

California Institute of Technology

hirani@caltech.edu

http://www.cs.caltech.edu/~hirani

Compatible Spatial Discretizations for Partial Differential Equations

IMA, May 11-15, 2004

(Based on my Ph.D thesis, available at above website)

What is Discrete Exterior Calculus (DEC) ?

- *Exterior Calculus* :
  - Generalization of vector calculus to nonlinear manifolds.
  - Operators and objects for full tensor analysis on manifolds.
  - Many theorems connecting the operators and objects.
- *Discrete Exterior Calculus* :
  - Discretization of EC for use in computations.
  - Coordinate-free, i.e operators defined without coordinates.
  - Discrete versions of the theorems from smooth theory.

DEC is calculus, differential geometry, and tensor analysis on discrete spaces. We aim to *preserve*, in discrete case, the *structure* of smooth theory.

DEC Results

- Provides framework for numerics on non-flat, simplicial meshes and their duals.
- Unlike FEM, DEC is coordinate-free, tensor analysis on discrete meshes.
- DEC introduces discrete vector fields, as separate from discrete differential forms, allowing for moving meshes.
- Many theorems from smooth exterior calculus have discrete counterparts.
- Well-known discrete formulas are reproduced by DEC.
- DEC also clarifies the role of Riemannian metric in numerics.

Objects of DEC

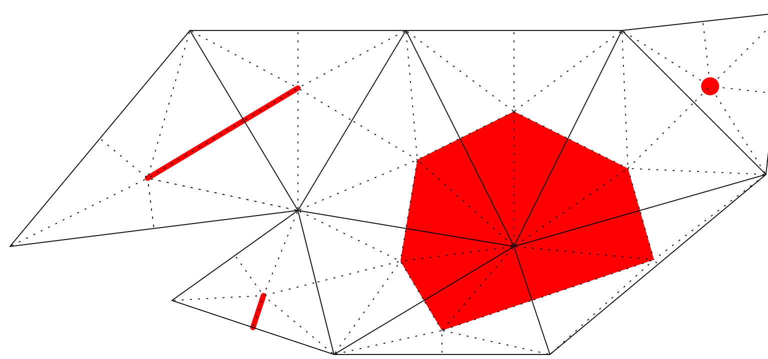
Exterior Calculus	*Examples*	*Discrete Exterior Calculus*
Manifolds	Surface, $\mathrm{SO}(3)$, $\mathbb{RP}^2$, $G(k,n)$	Simplicial complex and its dual
Differential forms	$\mathbf{d}f$, $\mathbf{d}x \wedge \mathbf{d}y \wedge \mathbf{d}z$, vorticity, force	Numbers on oriented mesh elements or their duals
Vector fields	Velocity	Vectors on primal or dual vertices
Other tensors	Stress tensor, metric tensor	Tensor product of 1-forms ?

Operators of DEC

- Hodge star ($*$) relates complementary forms.
- Flat ($\flat$), sharp ($\sharp$) relate vector fields to 1-forms.
- Exterior derivative ($\mathbf{d}$) raises degree of forms.
- $\flat$,$\sharp$ and $*$ are used to define grad, curl, Δ, and δ, adjoint of $\mathbf{d}$.
- Wedge product ($\wedge$) combines k and l forms into $(k+l)$-forms.
- Interior product ($\mathbf{i}_X$) combines forms and vector fields
- Lie derivative ($\pounds_X$) computes derivative of tensors along flows of X.

Primal Simplicial Complex and its Dual

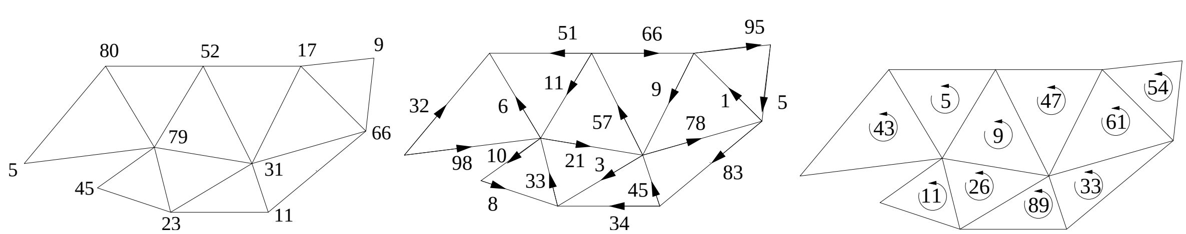
- Orientable simplicial complex and its dual discretizes manifolds in DEC, as in modern computational electromagnetism.
- Reminiscent of staggered meshes of many numerical methods.
- We use circumcentric dual, though barycentric can be used as well.
- Example of primal and dual meshes in 2D. The mesh need not lie in a plane :



Primal mesh is solid lines, dashed lines is circumcentric subdivision, thick gray are some dual elements.

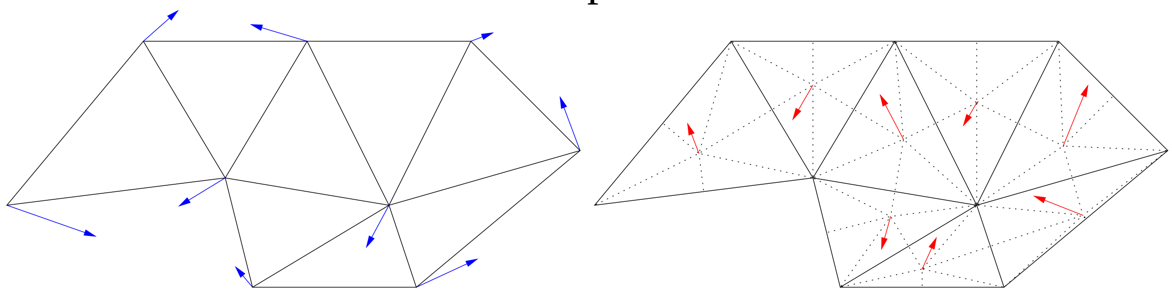
Discrete Differential Forms

- The usual definition used in this field, i.e. a *primal discrete p-form* is a homomorphism from the chain group $C_p(K;\mathbb{R})$ to the additive group $\mathbb{R}$. Example of a discrete 0-form, 1-form and 2-form are numbers on oriented mesh elements :

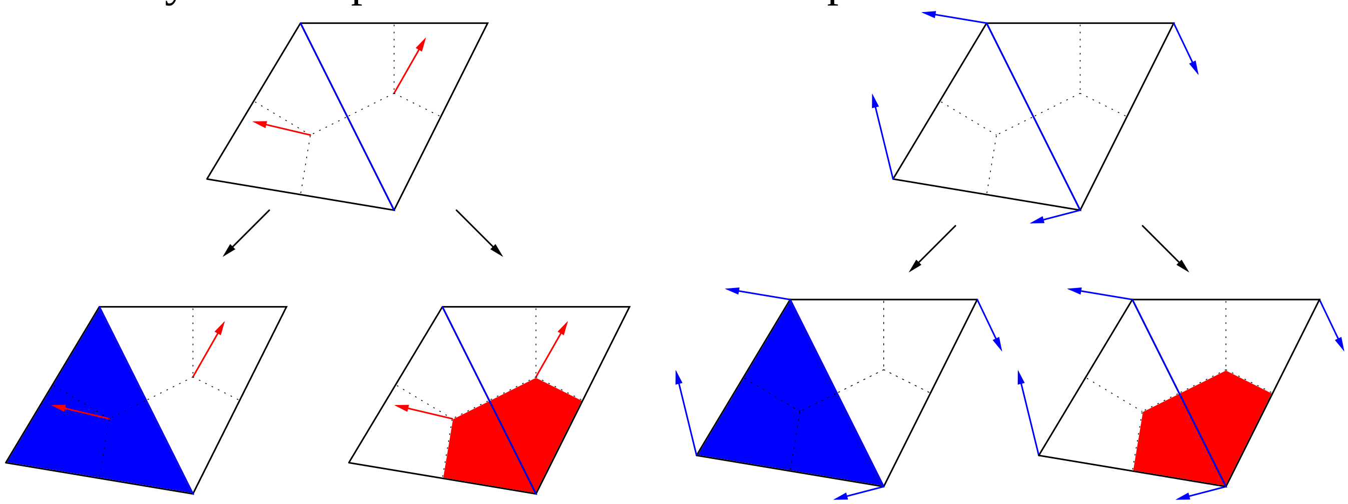


Discrete Vector Fields

- Two types : discrete primal vector field is on primal vertices and discrete dual vector field is on n-simplices :



- Then they are interpolated to build discrete operators :



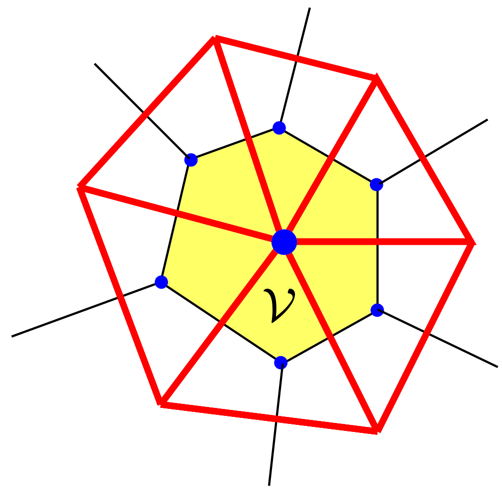
Separation of Forms and Vector Fields

- 1-forms and vector fields are related via metric.
- In $\mathbb{R}^3$, dimensions of spaces of 1-forms, 2-forms and vector fields is 3.
- But they shouldn't be identified in a general theory since : $(\pounds_X \alpha)^\sharp \neq \pounds_X(\alpha^\sharp)$ and $(*(\pounds_X \beta))^\sharp \neq \pounds_X((*\beta)^\sharp)$ i.e. Lie derivative does not commute with sharp, etc.
- This separation is useful, for example, in magnetohydrodynamics or moving conductors problems in electromagnetism.

Example Operator : Discrete Laplace-Beltrami

- Discrete Laplacian in flat space is easy. Just add the discrete second derivatives in each coordinate direction. But what to do on a piecewise linear triangle mesh ? First define *discrete Laplace-Beltrami* by the smooth definition $\Delta = \mathbf{d}\delta + \delta\mathbf{d}$.

- Then use definitions of discrete δ, $\mathbf{d}$ and $*$:



$$\begin{aligned}
\frac{1}{|\sigma^0|}\langle \Delta f, \sigma^0\rangle &= -\langle \delta\mathbf{d} f, \sigma^0\rangle \\
&= -\langle *\mathbf{d} * \mathbf{d} f, \sigma^0\rangle \\
&= -\frac{1}{|\star\sigma^0|}\langle \mathbf{d} * \mathbf{d} f, \star\sigma^0\rangle \\
&= -\frac{1}{|\star\sigma^0|}\langle *\mathbf{d} f, \partial(\star\sigma^0)\rangle
\end{aligned}$$

$$\begin{aligned}
&= -\frac{1}{|\star\sigma^0|}\langle *\mathbf{d} f, \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\langle *\mathbf{d} f, \star\sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\langle \mathbf{d} f, \sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}(f(v) - f(\sigma^0))
\end{aligned}$$

- This formula involves values at a vertex and its neighbors, volume of dual of the vertex, and lengths of primal edges σ^1 incident on the vertex, and the dual edges $\star\sigma^1$.

- This is identical to the cotangents based formula found by Meyer et al, 2002, using a variational approach.

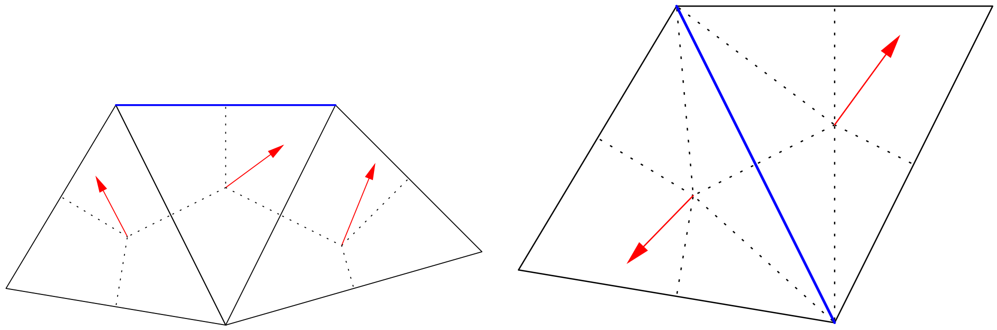
Example Operator : Discrete Flat

- Maps vector fields to 1-forms, used for example to define vorticity as $\mathbf{d}u^\flat$, for spatial fluid velocity vector field of u.
- Define *discrete primal-primal-dual flat* to be

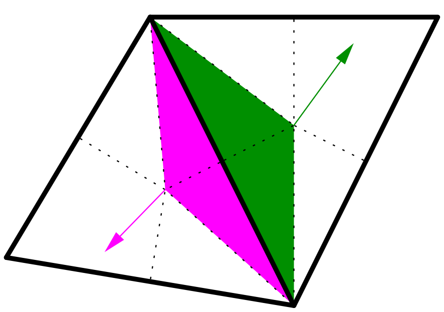
$$\langle X^\flat, \sigma^1 \rangle = \sum_{\sigma^n \succ \sigma^1} \frac{|\star\sigma^1 \cap \sigma^n|}{|\star\sigma^1|} X(\star\sigma^n) \cdot \vec{\sigma}^1 \,.$$

  where left hand side is evaluation on an edge σ^1 and the sum on right is over all n-simplices σ^n containing edge σ^1.

- For smooth vector field X and e a straight edge, $\int_e X^\flat = X \cdot \vec{e}$. What value of X should be used in discrete case ? In the easy case below, the smooth definition gives the answer. But the answer for the interesting case below, is to take a weighted sum of the two vectors.



Easy case　　　　Interesting case



- Weighting factor $=$ area of one small shaded triangle divided by total area of small shaded triangles.
- Equivalent to fraction of dual edge in each triangle.
- This is the *unique* choice that makes discrete divergence theorem true.

Example Operator : Discrete Interior Product

- Combines a p-form and a vector field to give a $(p-1)$-form.
- *Example Usage:* Hamiltonian vector field on manifold satisfies

$$\mathbf{i}_X \Omega = \mathbf{d} H$$

- Define *discrete interior product* algebraically using following

  Lemma. *Given a smooth manifold M of dimension n and a vector field $X \in \mathfrak{X}(M)$ and a k-form $\alpha \in \Omega^k(M)$ we have that*

$$\mathbf{i}_X \alpha = (-1)^{k(n-k)} * (*\alpha \wedge X^\flat) \, .$$

- Since we know how to discretize Hodge star, wedge and flat, this discretizes interior product.
- A different, dynamic definition is based on the discretization of following Lemma. This idea is due to Bossavit, 2003.

  Lemma.

$$\int_S \mathbf{i}_X \beta = \left. \frac{d}{dt} \right|_{t=0} \int_{E_X(S,t)} \beta \, .$$

  Proof Sketch: Prove instead that

$$\int_0^t \left[\int_{S_\tau} \mathbf{i}_X \beta \right] d\tau = \int_{E_X(S,t)} \beta \, .$$

  To prove the above, take coordinates on S and carry them along with the flow and define the transversal coordinate to be the flow of X.

- Here S is a $(k-1)$-manifold, β is a k-form, $E_X(S,t)$ is the extrusion, along containing manifold, of S by the flow of the vector field X for time t. Note that extrusion yields a manifold of dimension one higher than the extruded manifold.
- Since discrete forms are obtained from smooth ones by integration, this definition makes sense as a discretization.

Example Operator : Discrete Lie Derivative

- Derivative of a tensor β along the flow of a vector field X is written $\pounds_X \beta$. For example for a function f, $\pounds_X f = \nabla f \cdot X$.
- Define *discrete Lie derivative* algebraically using Cartan's Homotopy formula

$$\pounds_X \omega := \mathbf{i}_X \mathbf{d}\omega + \mathbf{d}\mathbf{i}_X \omega \,.$$

- Define it dynamically using the following lemma :

  Lemma. *If at time t, submanifold S is carried to S_t by the flow of X, then:*

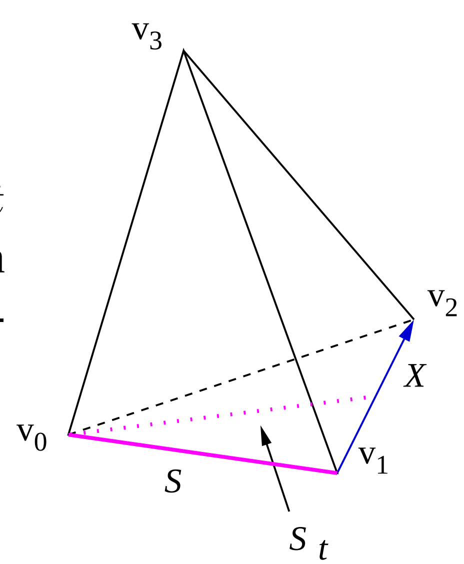
$$\int_S \pounds_X \beta = \left.\frac{d}{dt}\right|_{t=0} \int_{S_t} \beta$$

  Proof Sketch: First show that for any $\tau \le t$

$$F_\tau^*(\pounds_X \beta) = \frac{d}{d\tau} F_\tau^* \beta \,.$$

  Then integrate both sides from 0 to t and use the fact that $F_0^* \beta = \beta$.

- Dotted line shows edge $[v_0, v_1]$ at time t as it is dragged by vector field X. Then $\langle \pounds_X \alpha, [v_0, v_1] \rangle$ requires the value of α at intermediate positions.



Applications

Image matching and nonlinear waves

- Image matching can be posed as finding geodesics on group of diffeomorphisms. Resulting equations arise in nonlinear waves in fluids also.
- Averaged Template Matching Equations for image matching in a form suitable for DEC implementation are :

$$\frac{\partial}{\partial t}\mathbf{v}^\flat + \pounds_{\mathbf{u}}\mathbf{v}^\flat + \mathbf{v}^\flat \operatorname{div}\mathbf{u} = 0\,.$$

Thin shell dynamics

- If $\varphi : \bar{\Omega} \mapsto \Omega$ is a deformation map and a diffeomorphism, $\bar{\mathrm{S}}$ and S are shape operators, in reference and deformed, and $\bar{H}$ and H are mean curvatures, define bending energy as a change in shape operator : $[\mathrm{Tr}(\varphi^*\mathrm{S}) - \mathrm{Tr}(\bar{\mathrm{S}})]^2 = 4(H \circ \varphi - \bar{H})^2$
- Comparison of shape operators possible only because of :

$$\mathrm{Tr}(\varphi^*\mathrm{S}) = \varphi^*\,\mathrm{Tr}(\mathrm{S}) = \mathrm{Tr}(\mathrm{S}) \circ \varphi = 2(H \circ \varphi)\,.$$

- Discretize the bending energy using mean curvature on edges.

Discrete Hodge decomposition

- In the smooth case, vector fields can be decomposed as

$$\xi = \nabla u + \nabla \times \mathbf{v} + \mathbf{h}$$

- Given a discrete 3D dual vector field defined per tetrahedron, we give its Hodge decomposition. This has direct application to computational incompressible fluid mechanics. We also find the potentials and so vector field processing possible : strengths of vortices and sources and sinks can be adjusted.