Discrete Exterior Calculus

and the Averaged Template Matching Equations

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This talk is mostly based on my thesis :
Discrete Exterior Calculus
Caltech, 2003 (Hirani [2003])
supervised by Prof. Jerrold E.Marsden. Thesis available from my home page.

Main Points

- PDEs using differential forms and vector fields.
- Distinction between forms and vector fields.
- Examples : Template matching, Maxwell’s equations.

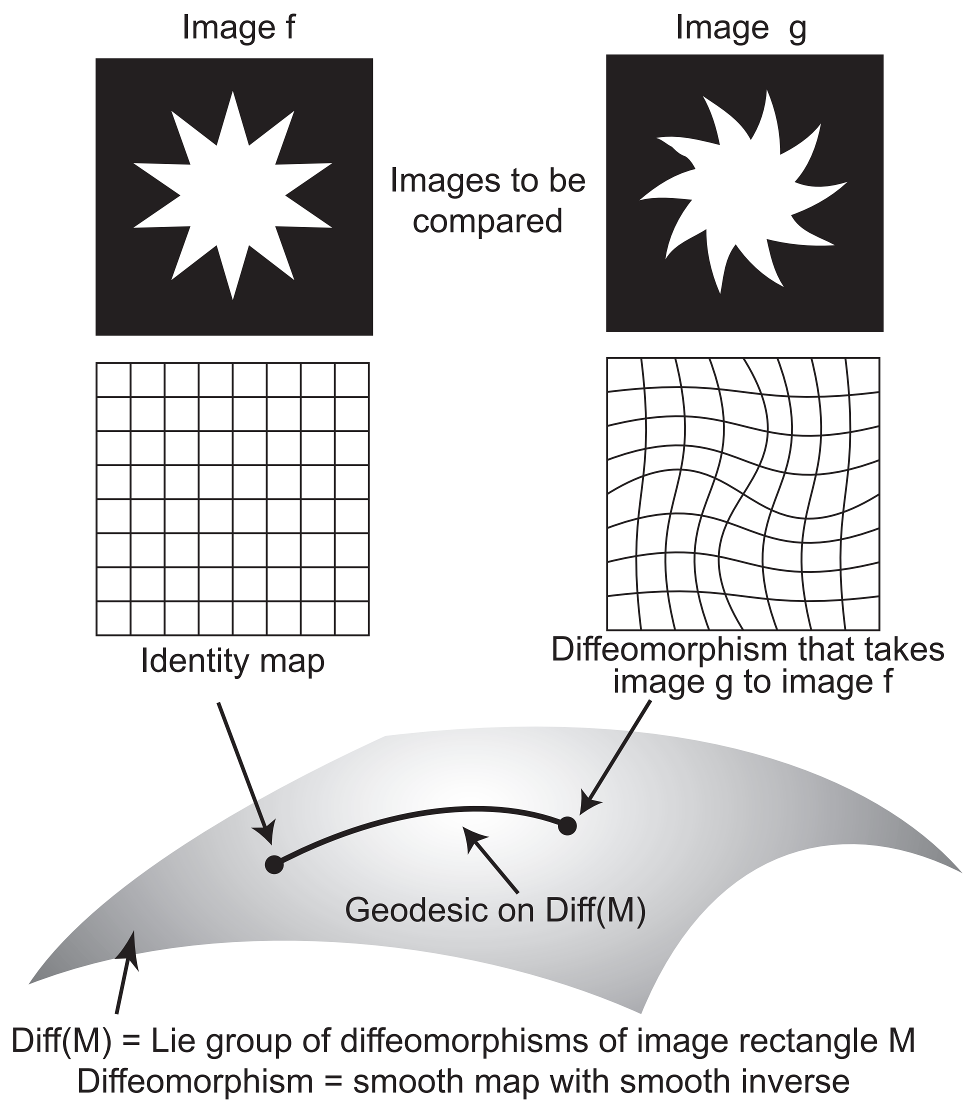
Introduction

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.
  - Operators defined without global 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.

Template Matching



Averaged Template Matching Equations

- Euler-Poincaré equation, called ATME (Hirani et al. [2001]).
- Nonlinear waves (IVP), work of Holm and Staley.
- BVP to IVP for ATME in 1D (Chapman et al. [2002]).
- DEC and irregular grids.

ATME in Div, Grad, Curl form

$$\frac{\partial}{\partial t}\mathbf{v} + (\nabla \cdot \mathbf{u})\mathbf{v} + \nabla(\mathbf{u} \cdot \mathbf{v}) + (\nabla \times \mathbf{v}) \times \mathbf{u} = 0 \,.$$

ATME in Lie derivative form

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

where $\mathbf{v} = (1 - \alpha^2 \Delta)\mathbf{u}$.

Objects of Exterior Calculus and DEC

Exterior Calculus	*Examples*	*Discrete Exterior Calculus*
Manifolds	Surface, $SO(3)$, $\mathbb{RP}^2$, $G(k, n)$	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 Exterior Calculus

Metric-dependent operators

- Hodge star ($*$) relates complementary forms
- Flat ($\flat$), sharp ($\sharp$) relate vector fields to forms
- These are used to define ∇, $\nabla\times$ and Δ.

Metric-independent operators

- Exterior derivative ($\mathbf{d}$)
- Wedge product ($\wedge$) to combine forms
- Interior product ($\mathbf{i}_X$) to combine forms and vector fields
- Lie derivative ($\pounds_X$) for derivatives along flows.

Review of Existing Results

Maxwell's Equations and DEC

- ***Differential k-forms***
  - Antisymmetric k-tensors on a manifold, M.
  - A k-form α at $p \in M$, $\alpha : T_pM \times \ldots \times T_pM \rightarrow \mathbb{R}$.
  - For submanifold S^k (dim = k) of M $\int_{S^k} \alpha \in \mathbb{R}$
- ***Exterior derivative*** (**d**), a differential operator subsuming all vector calculus operators, $\mathbf{d}\alpha$ is a $(k+1)$-form.
- ***Hodge star***, $(*)$, isomorphism between k-forms and $(n-k)$-forms.

Maxwell's Equations

Maxwell's equations in presence of an isotropic, linear, medium.

- Faraday's and Ampére's laws :

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0 \quad \text{(Faraday's law)}$$
$$-\partial_t \mathbf{D} + \nabla \times \mathbf{H} = \mathbf{J} \quad \text{(Ampére's law)}$$

- Constitutive relations :

$$\mathbf{D} = \epsilon \mathbf{E}$$
$$\mathbf{B} = \mu \mathbf{H}$$

E is electric field

D is electric induction

J is current density.

B is magnetic flux density

H is magnetic field

Fields versus Global Quantities

- **E** cannot be measured, its work along a curve can :

$$\int_c \mathbf{E} \cdot \dot{c} \, .$$

- **B** cannot be measured, its flux through a surface can :

$$\int_S \mathbf{B} \cdot \mathbf{n} \, .$$

- **E** and **B** depend on choice inner product.
- Curl, used in the two laws, also depends on metric.
- Why not use differential forms instead ?
- Electric field e is a 1-form and b a 2-form and

$$\int_c e = \int_c \mathbf{E} \cdot \dot{c} \qquad \int_S b = \int_S \mathbf{B} \cdot \mathbf{n}$$

Maxwell's using Differential Forms

$$\partial_t b + \mathbf{d}e = 0$$
$$-\partial_t d + \mathbf{d}h = j$$

$$d = *_\epsilon e$$
$$b = *_\mu h$$

e, h are 1-forms

b, d are 2-forms.

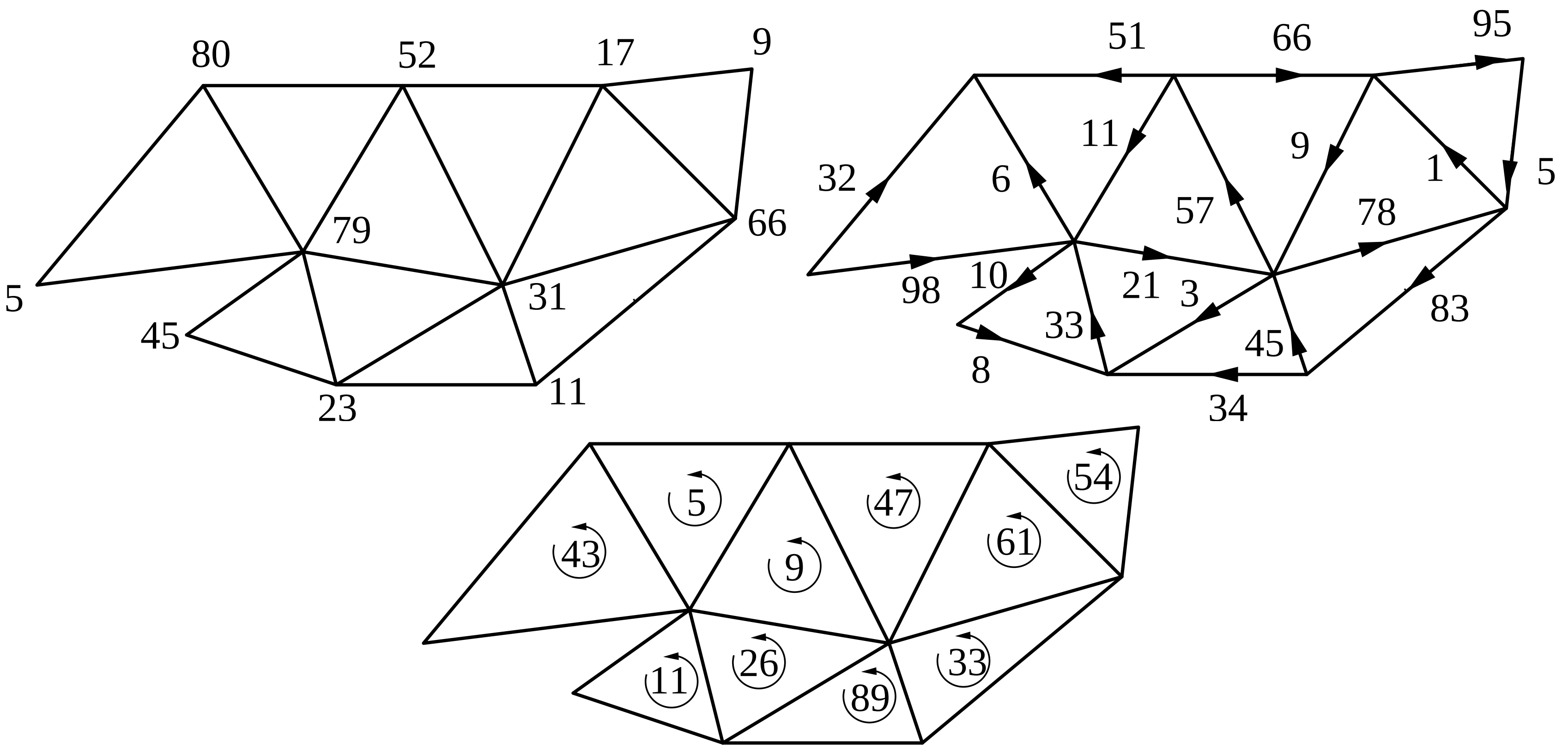
Discretizing Faraday's Law

$$\partial_t b + \mathbf{d}e = 0 \quad \text{(Start with differential forms)}$$

$$\partial_t \int_S b + \int_S \mathbf{d}e = 0 \quad \text{(Write in integral form)}$$

- For S, use all the facets of the tetrahedral mesh.
- This gives F (number of facets) DOF for b.
- Similarly there are E (number of edges) DOF for e.
- Semi-discrete Faraday's law in matrix form : $\partial_t \mathbf{b} + \mathbf{Re} = 0$.

Discrete Differential Forms



- A ***primal discrete p-form*** is a homomorphism from the chain group $C_p(K;\mathbb{R})$ to the additive group $\mathbb{R}$. Thus a discrete p-form is an element of $\mathrm{Hom}(C_p(K),\mathbb{R})$ the space of ***cochains***.
- In discrete Faraday's law, **b** is a discrete 2-form, and **e** is a discrete 1-form.

Discrete Exterior Derivative

- ***Smooth exterior derivative*** $\mathbf{d} : \Omega^p(M) \to \Omega^{p+1}(M)$. For example in $\mathbb{R}^2$, in coordinates:

$$\mathbf{d}f = \frac{\partial f}{\partial x}\mathbf{d}x + \frac{\partial f}{\partial y}\mathbf{d}y$$

- The boundary operator on chains gives a chain complex

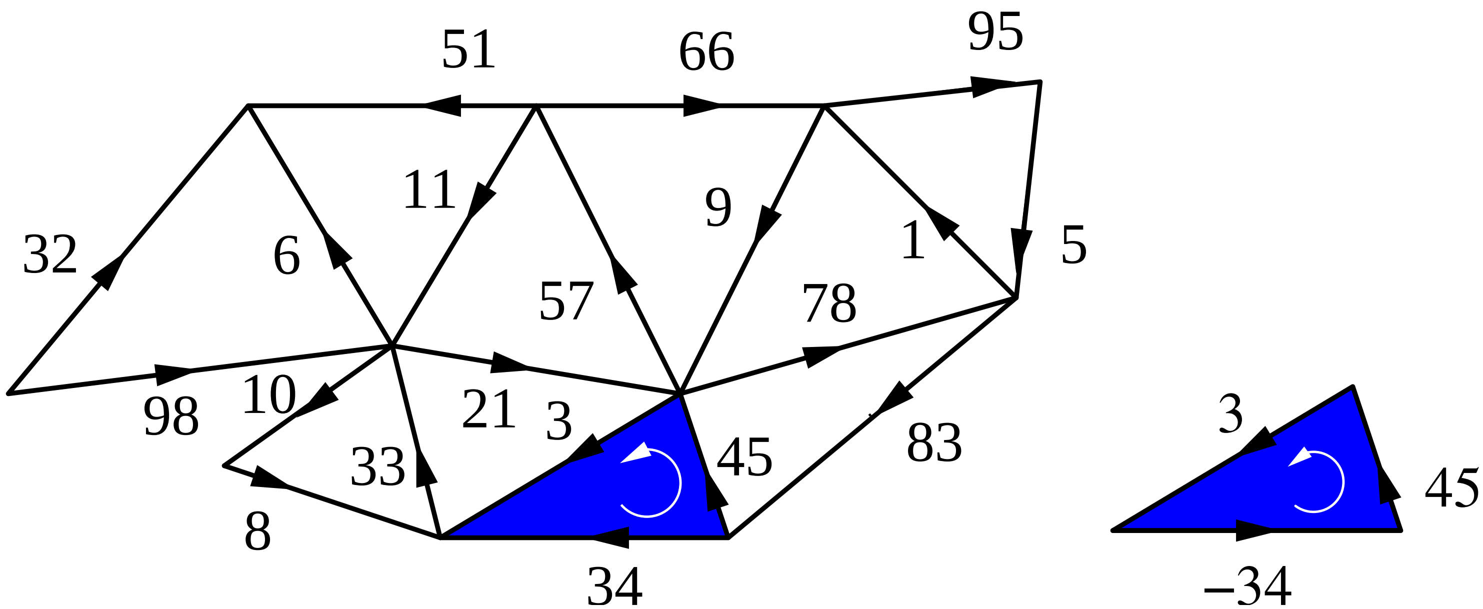
$$0 \longrightarrow C_n(K) \xrightarrow{\partial_n} \ldots \xrightarrow{\partial_{p+1}} C_p(K) \xrightarrow{\partial_p} \ldots \xrightarrow{\partial_1} C_0(K) \longrightarrow 0$$

- The co-boundary operator gives a co-chain complex

$$0 \longleftarrow C^n(K) \xleftarrow{\delta^{n-1}} \ldots \xleftarrow{\delta^p} C^p(K) \xleftarrow{\delta^{p-1}} \ldots \xleftarrow{\delta^0} C^0(K) \longleftarrow 0$$

- For a discrete form $\alpha^p \in C^p(K)$ and a chain $c_{p+1} \in C_{p+1}(K;\mathbb{R})$ the co-boundary operator δ^p is $\left\langle \delta^p \alpha^p, c_{p+1} \right\rangle = \left\langle \alpha^p, \partial_{p+1} c_{p+1} \right\rangle$
- Define ***discrete exterior derivative*** to be the co-boundary operator.

Discrete Exterior Derivative



- Just add up values shown on little triangle on right.
- Discrete **d** is the coboundary : $\langle \mathbf{d}\alpha^1, \sigma^2 \rangle = \langle \alpha^1, \partial\sigma^2 \rangle$
- Discrete Stokes' theorem is true by definition.
- $\mathbf{d} \circ \mathbf{d} = 0$.
- In discrete Faraday's law, $\partial_t \mathbf{b} + \mathbf{R}\mathbf{e}$, the matrix **R** is the discrete exterior derivative, **b** is a discrete 2-form and **e** is a discrete 1-form.

Discretizing Constitutive Laws

- Next we do a count, using constitutive equations :

$$d = *_\epsilon e$$
$$b = *_\mu h$$

- Recall that :
  - e is a 1-form while d is a 2-form
  - b is a 2-form while h is a 1-form
- e lives on edges and d lives on surfaces. Which surfaces in the mesh ? Need as many 2 dimensional surfaces as edges.
- Enter the dual mesh ...

Primal Simplicial Complex and its Dual

- If σ^p is p-simplex, $\star\sigma^p$ (dimension $n-p$) is its dual defined by

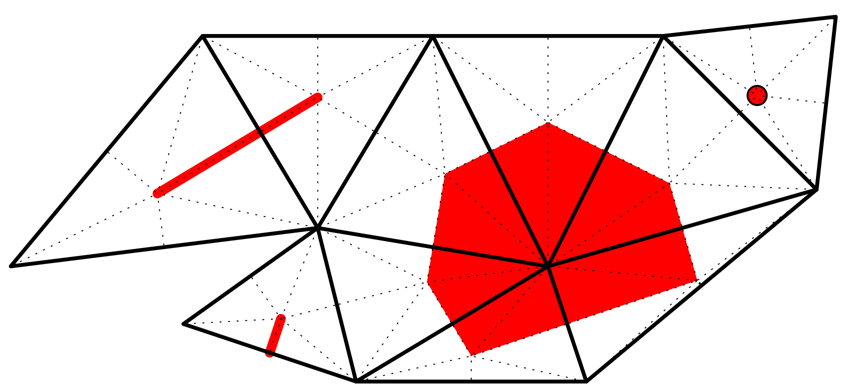
$$\star(\sigma^p) = \sum_{\sigma^p \prec \sigma^{p+1} \prec \ldots \prec \sigma^n} s_{\sigma^p,\ldots,\sigma^n}\left[c(\sigma^p), c(\sigma^{p+1}), \ldots, c(\sigma^n)\right]$$

where $s_{\sigma^p,\ldots,\sigma^n}$ is a sign given by a simple algorithm, $c(\sigma^k)$ is the circumcenter of σ^k.

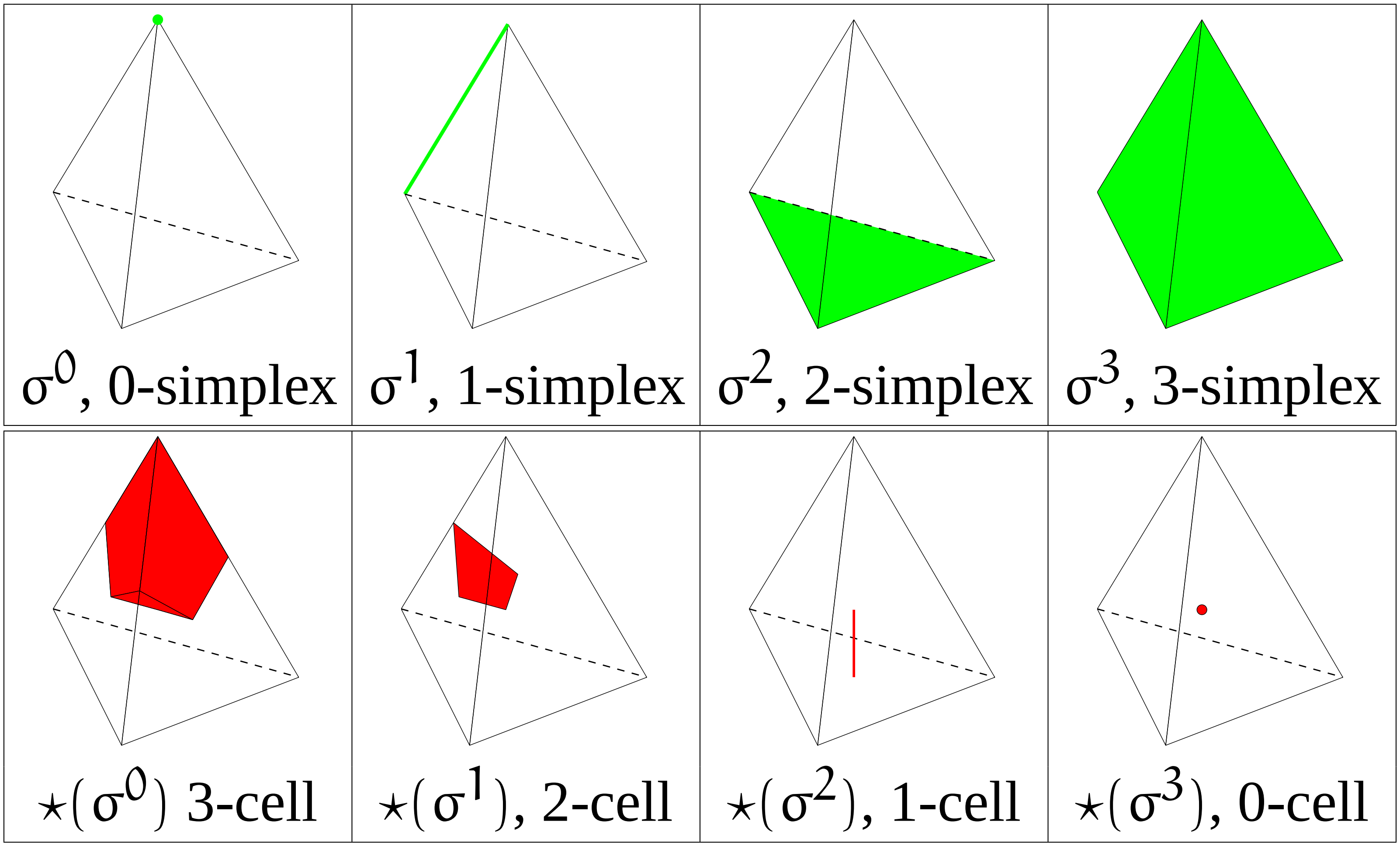
- Dual of dual is defined to be primal

$$\star\star(\sigma^p) = (-1)^{p(n-p)}\sigma^p$$

- We discovered a simple algorithm for orienting the dual.



Primal Simplicial Complex and its Dual



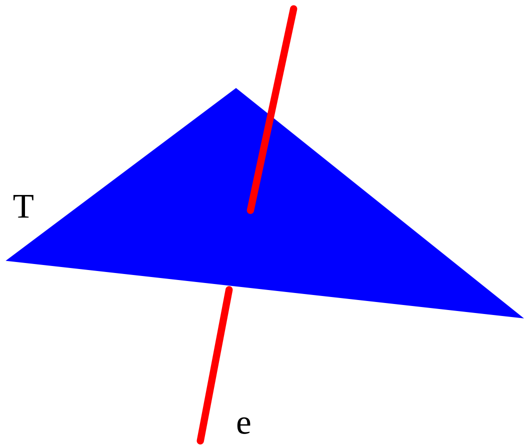
Discrete Hodge Star

- ***Smooth hodge star*** $* : \Omega^p(M) \rightarrow \Omega^{n-p}(M)$. Used, for example, to define codifferential which in turn appears in div, curl, Laplace-Beltrami. The codifferential is defined by $\delta\beta = (-1)^{np+1} * \mathbf{d} * \beta$.
- ***Discrete Hodge Star*** is an information transfer between primal and dual meshes and defined as :

$$\frac{1}{|\sigma^p|}\langle \alpha, \sigma^p \rangle = \frac{1}{|\star\, \sigma^p|}\langle *\alpha, \star\sigma^p \rangle\,.$$

- For example for a primal 2-form α, for $n = 3$:

$$\frac{1}{\text{Area}(T)}\langle \alpha, T \rangle = \frac{1}{\text{Length}(e)}\langle *\alpha, e \rangle\,.$$



Now on to New Stuff

What was Known Before DEC

- Forms should be used instead of proxy vector fields.
- Discrete forms are cochains on primal and dual meshes.
- Discrete exterior derivative is co-boundary operator.

What DEC Introduced

- Algorithm for orienting the dual mesh.
- Discrete wedge product.
- Reproduction of well-known formulas for Laplace-Beltrami etc.
- Vector fields as distinct from forms.
- Operators acting on vector fields (flat) or vector fields and forms together (contraction, Lie derivative).

History and Previous Work

- Physics : Tonti [2002]; Sen et al. [2000]; Schwalm et al. [1999]
- Computational Electromagnetism : Bossavit [2002, 2001]; Hiptmair [2001, 2002]; Teixeira [2001]; Gross and Kotiuga [2001]
- Mimetic Discretization : Robidoux and Steinberg [2003]; Hyman and Shashkov [1997a,b]
- Numerical Analysis : Nicolaides [1992]; Mattiussi [1997]; Arnold [2003]; Trapp [2004]
- Computer Graphics : Meyer et al. [2002]; Gu [2002]
- Mathematics : Dodziuk [1976]; Harrison [1993]; Dezin [1995]; Mitchell [1998]; Mansfield and Hydon [2001]
- Recent Work : Workshop ***Compatible Spatial Discretization of Partial Differential Equations***, May 11-15, 2004, Institute for Mathematics and its Applications (IMA), Minneapolis.

Contributions

Discrete Laplace-Beltrami

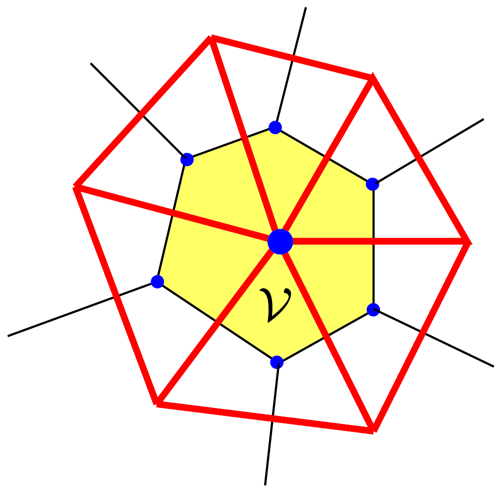
- With **d** and Hodge star, we can define Laplace-Beltrami.
- Define ***discrete Laplace-de Rham operator*** by the smooth definition $\Delta = \mathbf{d}\delta + \delta\mathbf{d}$.

$$\frac{1}{|\sigma^0|}\langle \Delta f, \sigma^0 \rangle = -\langle \delta \mathbf{d} f, \sigma^0 \rangle$$

$$= -\langle * \mathbf{d} * \mathbf{d} f, \sigma^0 \rangle$$

$$= -\frac{1}{|\star\sigma^0|}\langle \mathbf{d} * \mathbf{d} f, \star\sigma^0 \rangle$$

$$= -\frac{1}{|\star\sigma^0|}\langle * \mathbf{d} f, \partial(\star\sigma^0) \rangle$$



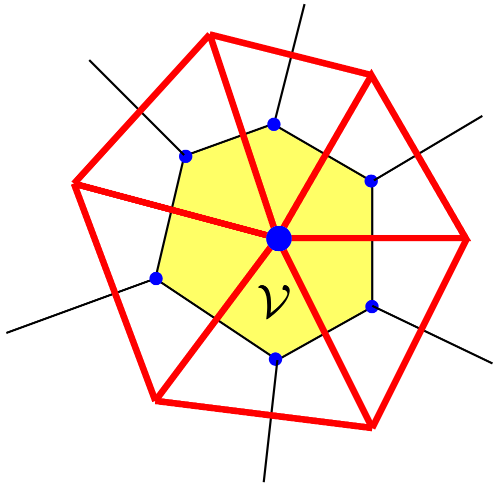
Discrete Laplace-Beltrami

$$= -\frac{1}{|\star\sigma^0|}\langle *\mathbf{d}f, \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1\rangle$$

$$= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0} \langle *\mathbf{d}f, \star\sigma^1\rangle$$

$$= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|}\langle \mathbf{d}f, \sigma^1\rangle$$

$$= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|}(f(v) - f(\sigma^0))$$



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

Moving Conductor and DEC

- Eddy current equation in vector field notation :

$$\sigma \partial_t \mathbf{A} + \nabla \times (\nu \nabla \times \mathbf{A}) = \mathbf{J}^s$$

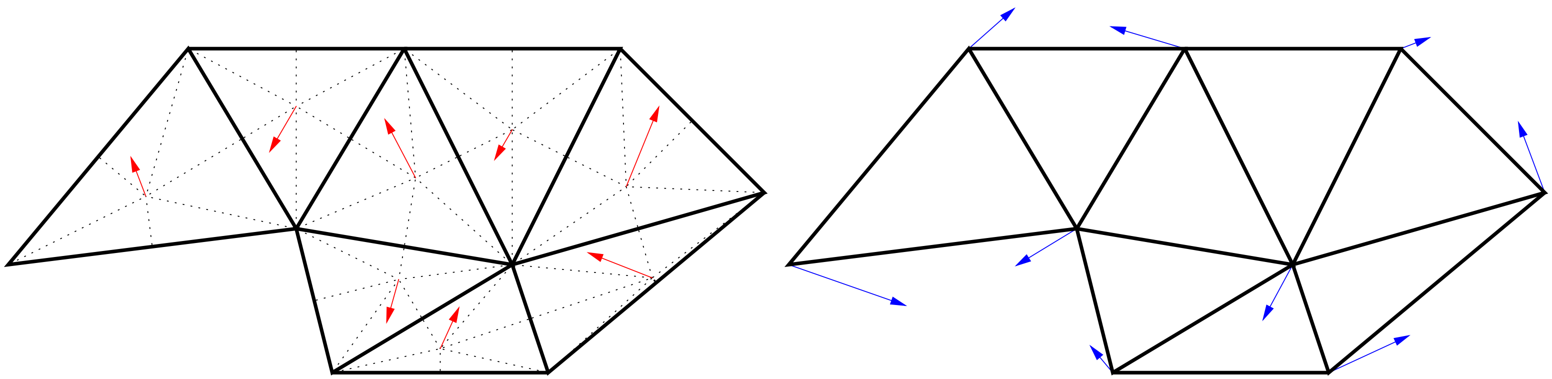
where $\mathbf{A} = -\int_0^t \mathbf{E}(s) ds$.

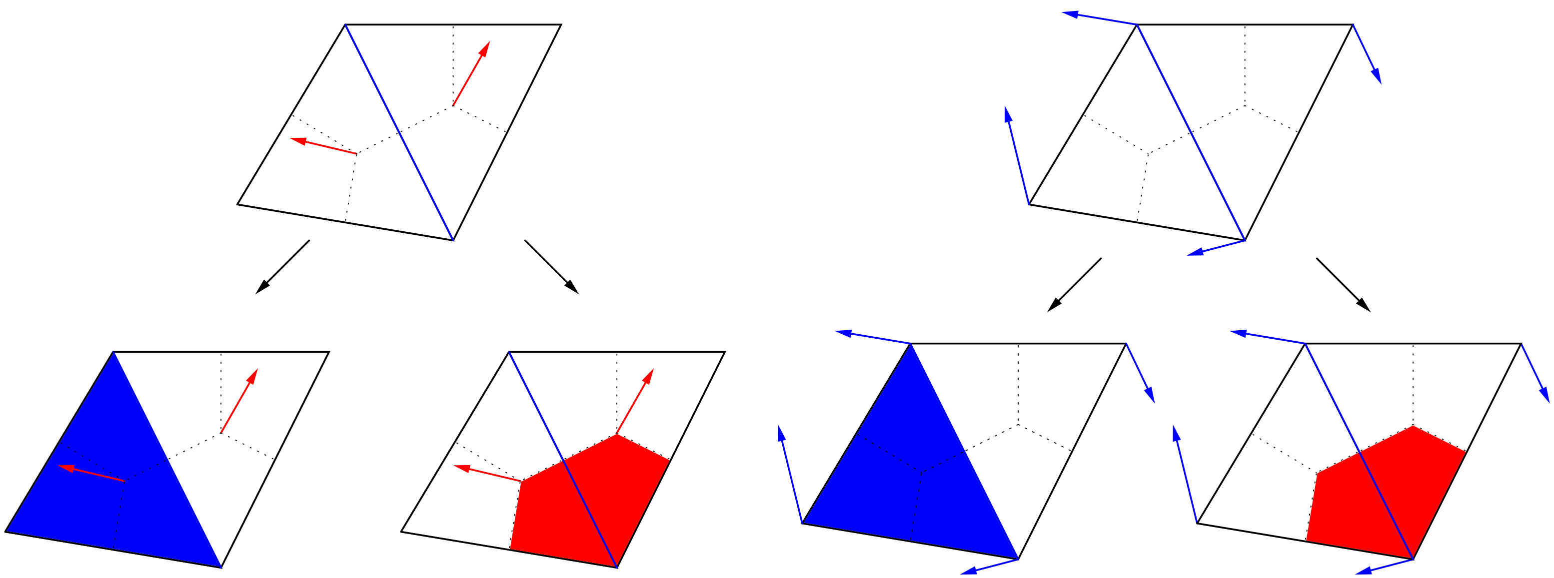
- If conductive material is moving with a velocity field **v**, the equation becomes :

$$\sigma(\partial_t \mathbf{A} - \mathbf{v} \times \mathbf{B}) + \nabla \times (\nu \nabla \times \mathbf{A}) = \mathbf{J}^s$$

- What is $\mathbf{v} \times B$ in terms of forms ?
- Hint : $F = q(E + \mathbf{v} \times B)$.
- $\mathbf{v} \times B$ is $\mathbf{i_v} b$.
- What is a good discretization of contraction ?
- First we need to introduce discrete vector fields.

Discrete Vector Fields





Distinction Between Forms and Vector Fields

- Vector fields are related to 1-forms and 2-forms via metric.
- In $\mathbb{R}^3$ we have :

Space	Representative	Dimension
0-forms	Scalar	1
1-forms	Row Vector	3
2-forms	Antisymmetric Matrix	3
3-forms	Volume form	1

- Thus in $\mathbb{R}^3$, 1-forms and 2-forms have same dimension (i.e 3), as vector fields.
- But they shouldn't be identified in a general theory since :

$$(\pounds_X \alpha)^\sharp \neq \pounds_X(\alpha^\sharp)$$
$$(*(\pounds_X \beta))^\sharp \neq \pounds_X((*\beta)^\sharp)$$

Interior Product (Contraction)

- ***Interior product*** $\mathbf{i}_X : \Omega^p(M) \to \Omega^{p-1}(M)$, lowers the degree of a form. For a vector field X and k-form α,

$$\mathbf{i}_X \alpha := \alpha(X, \ldots) \, .$$

Discrete Interior Product (1)

- Define ***discrete interior product*** of a discrete k-form α and a vector field X on an n-dimensional complex by :

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

- For example for 2-form $\alpha = b$ and vector field $X = \mathbf{v}$,

$$\mathbf{i}_{\mathbf{v}} b = *(*b \wedge \mathbf{v}^\flat) \, .$$

Discrete Interior Product (2)

- Another definition is based on the discretization of

Lemma.

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

- Example : contract 2-form b and vector field v in 3D :
  - Result is a 1-form.
  - Value of $\mathbf{i}_X \alpha$ on an edge ?
  - Edge sweeps out a surface depending on time.
  - Evaluate α on surface, take time derivative at 0.
  - But swept surface may not be a facet.
  - Leads us to interpolation of discrete forms.

Interpolation of Discrete Forms : Whitney Forms

- Whitney form is to discrete form, as linear basis function is to scalar function in finite elements.
- Built from the linear basis functions over simplex.
- Example : Whitney 1-forms in $\mathbb{R}^3$. There are 6, corresponding to edges of a tetrahedron.

$$\phi_{mn} = \phi_m \mathbf{d}\phi_n - \phi_n \mathbf{d}\phi_m \qquad \text{(invariant form)}$$
$$\phi_{mn} = \phi_m \nabla\phi_n - \phi_n \nabla\phi_m \qquad \text{(proxy form)}$$

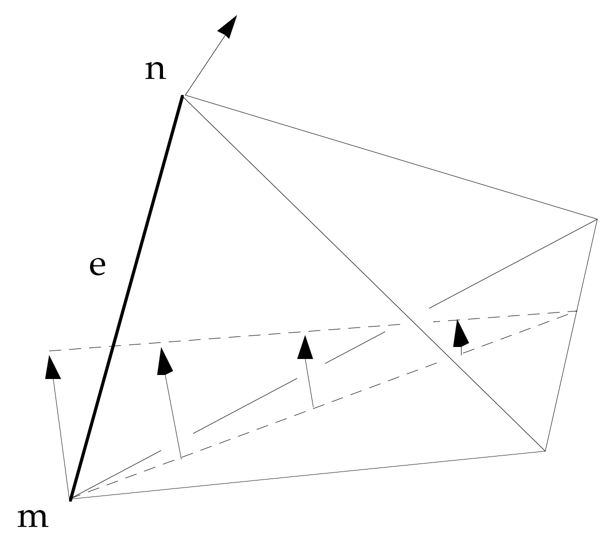


Figure from Bossavit [1998]

Euler Equations of Fluid and Template Matching

- Euler equations for homogenous, incompressible fluid of constant density 1, and with no body force :

$$\begin{aligned} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\nabla p \\ \nabla \cdot \mathbf{u} &= 0 \,. \end{aligned}$$

- Using differential forms :

$$\partial_t \mathbf{u} + \pounds_{\mathbf{u}} \mathbf{u}^\flat - \frac{1}{2}\mathbf{d}(\mathbf{u}^\flat(\mathbf{u})) = -\mathbf{d}p \,.$$

- Averaged Template Matching Equations :

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

- Thus we need discrete flat operator and discrete Lie derivative.

Lie Derivative

- Lie derivative of a tensor along a vector field is its derivative along the flow. No need for a metric on M. For a k-form α and vector field $X \in \mathfrak{X}(M)$:

$$\pounds_X \alpha := \left.\frac{d}{dt}\right|_{t=0} \varphi_t^* \alpha$$

where

$$(\varphi_t^* \alpha)|_p (v_1, \ldots, v_k) = \alpha|_{\varphi_t(p)} \big(T_p\varphi_t(v_1), \ldots, T_p\varphi_t(v_k)\big)$$

Discrete Lie Derivative (2 definitions)

- Define ***discrete Lie derivative*** algebraically using Cartan's Homotopy formula

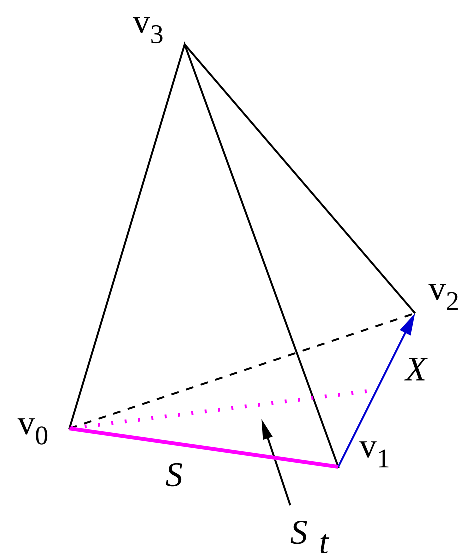
$$\pounds_X \omega := \mathbf{i}_X \mathbf{d}\omega + \mathbf{d}\mathbf{i}_X \omega\,.$$

- 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:*

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

- Dotted magenta 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.



Convergence and Stability

- See Dodziuk [1976]; Bossavit [2002]; Arnold [2003]; Garimella and Swartz [2003]; Xu [2003, 2004]; Trapp [2004] and slides of several talks at the IMA Hot Topics workshop : Compatible Spatial Discretizations of Partial Differential Equations. Also some new work by group at ZIB, Berlin.

Summary

- Discrete wedge product, sharp, flat, div, grad and curl have also been developed but were not discussed today.
- Well-known discrete formulas are reproduced by DEC.
- DEC distinguishes between forms and vector fields.
- DEC also clarifies the role of Riemannian metric in numerics on non-flat meshes (Hodge star, LB, flat and sharp).
- It is the first step towards a full tensor analysis on non-flat meshes.
- Vector fields allows for moving mesh applications.
- Discretizing the EC operators unifies diverse computational fields.
- DEC preserves some of the structure of smooth theory.

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