Discrete Exterior Calculus

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Introduction

■ From Discrete to Continuous . . .

- Discrete geometry and numerical algorithms have traditionally been concerned with convergence in the continuous limit.
- However, convergence considerations alone are inadequate, since many discrete objects converge to the same continuous object. How should we choose between them?
- Local convergence properties yield little information about long term behavior, since errors exponentially accumulate in many problems of interest.
- Tendency to resort to continuous theory, by use of interpolation, and by restricting the theory to a finite dimensional function space.

Introduction

■ . . . and back to the Discrete

- In practice, much of our understanding of complex dynamical systems is derived from numerical simulations.
- Increasing need to study numerical algorithms and discrete geometry as intrinsically discrete dynamical systems in their own right.
- Wish to develop canonical discretizations that exhibit discrete analogues of desirable properties of continuous systems.
- Systematic development of the mathematical infrastructure and physical principles for the study of discrete geometry and geometric integration.

Introduction to Computational Geometric Mechanics

Geometric Mechanics

- Differential geometric and symmetry techniques applied to the study of Lagrangian and Hamiltonian mechanics.

Computational Geometric Mechanics

- Constructing computational algorithms using ideas from geometric mechanics.
- Variational integrators based on discretizing Hamilton's principle, automatically symplectic and momentum preserving.

Missing pieces

- Discrete Exterior Calculus
- Discrete Connections on Principal Bundles

Introduction to Computational Geometric Mechanics

Motivation for a Discrete Exterior Calculus

- Differential Operators in terms of Combinatorial Operations on Simplicial Complexes and Dual Cell Complexes.
- Mathematical foundation of Computational Geometric Mechanics.
- Natural Derivations of Discrete Conservation Laws.
- Natural Discretizations of Div, Grad, and Curl.

Motivation for a Discrete Theory of Connections

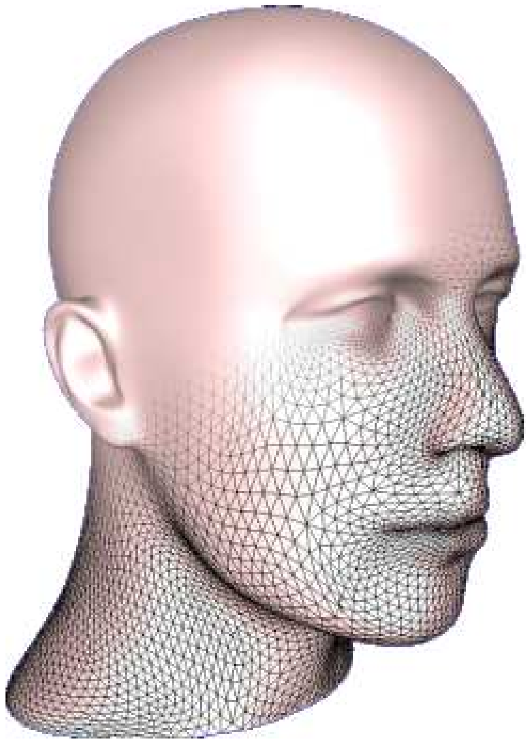
- Essential for a Discrete Theory of Lagrangian Reduction.
- Applications to geometric control of formations.
- Discrete analogues of Riemannian manifolds, Levi-Civita connections, and curvatures.

Discrete Exterior Calculus

Discrete Geometry and Computer Graphics

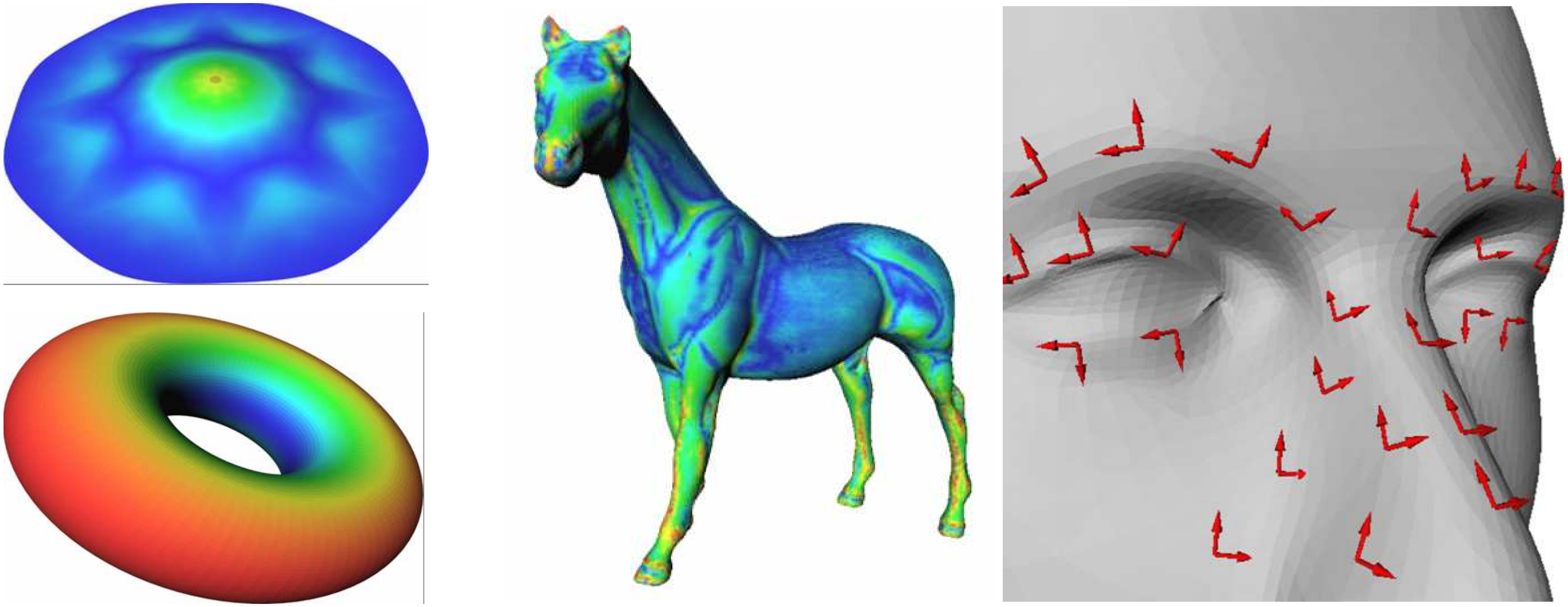
Motivation

- Desire robust computation on discrete meshes.
- Many applications require differential geometric concepts:
  - PDE based Image Processing on Curved Surfaces.
  - Smoothing, simplification, and remeshing of triangulated surfaces.
- Little consensus on how to compute basic surface properties like normals and curvature.



Discrete Geometry and Computer Graphics

- Mean, Gaussian, and Principal Curvatures



Introduction

Essential Aspects of Discrete Exterior Calculus

- Primal and Dual Complexes
- Differential Forms and Exterior Derivative
- Hodge Star and Codifferential
- Maps between One Forms and Vector Fields
- Wedge Product
- Contraction and Lie Derivative
- Discrete Poincaré Lemma

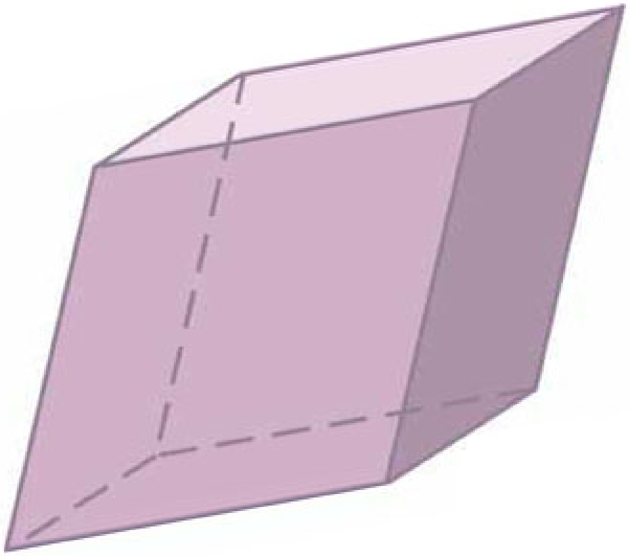
Applications

- Vector Calculus, Divergence, Curl and Laplace-Beltrami

Introduction

What is a differential form?

- A **differential form** of degree k is a smooth antisymmetric multilinear map that takes k vectors to $\mathbb{R}$.
- An example of this is the **determinant**, which measures the **signed volume** of a k-dimensional parallelepiped spanned by k-vectors.



Exterior Calculus

Natural Generalization of Vector Calculus

- Divergence

$$\nabla \cdot F = *d\left(*F^\flat\right)$$

- Gradient

$$\nabla f = (df)^\#$$

- Curl

$$\nabla \times F = \left[*\left(dF^\flat\right)\right]^\#$$

Mimetic Difference Schemes

Support-Operators Method

- Developed at Los Alamos National Laboratory, by J.M. Hyman and M. Shashkov.
- Based on the following properties of divergence, gradient and curl,

$$\mathbf{div}\ \overrightarrow{W} = \lim_{V \to 0} \frac{\oint_{\partial V} \left(\overrightarrow{W}, \overrightarrow{n} \right) dS}{V},$$

$$\left(\mathbf{grad}\ u,\ \overrightarrow{k} \right) = \frac{\partial u}{\partial k},$$

$$\left(\overrightarrow{n}, \mathbf{curl}\ \overrightarrow{A} \right) = \lim_{S \to 0} \frac{\oint_{l} \left(\overrightarrow{A}, \overrightarrow{l} \right) dl}{S}.$$

- Results in finite difference stencils on primal-dual logically rectangular meshes.

Computational Electromagnetism

Electromagnetic Field Quantities

Quantity	Form	Degree	Units	Vector/Scalar
Electric Field Intensity	E	1-form	V	$\mathbf{E}$
Magnetic Field Intensity	H	1-form	A	$\mathbf{H}$
Electric Flux Density	D	2-form	C	$\mathbf{D}$
Magnetic Flux Density	B	2-form	Wb	$\mathbf{B}$
Electric Current Density	J	2-form	A	$\mathbf{J}$
Electric Charge Density	ρ	3-form	C	q

Computational Electromagnetism

Maxwell's Equations

Vector Calculus	Differential Forms	Name
$\frac{\partial B}{\partial t} + \nabla \times E = 0$	$\frac{\partial B}{\partial t} + \mathbf{d}E = 0$	Faraday
$\frac{\partial D}{\partial t} - \nabla \times H = J$	$\frac{\partial D}{\partial t} - \mathbf{d}H = J$	Ampère
$\nabla \cdot D = \rho$	$\mathbf{d}D = \rho$	Gauss
$\nabla \cdot B = 0$	$\mathbf{d}B = 0$	Gauss
$D = \epsilon E$	$D = *(\epsilon E)$	Constitutive law
$B = \mu H$	$B = *(\mu H)$	Constitutive law

- Natural decomposition of equations into:
  - **conservation laws** involving metric-free operations.
  - **constitutive relations** involving metric-dependent operators.

Computational Electromagnetism

Exact Sequences and Spectral Properties

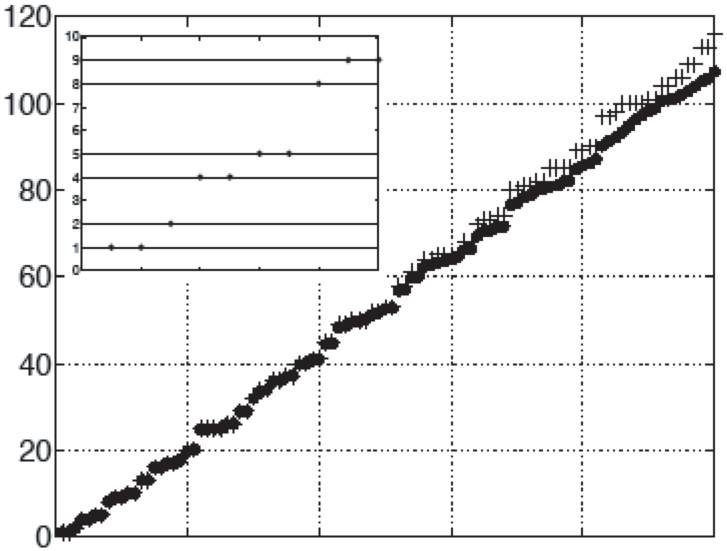
- Compatible discretizations of differential operators preserve the exact sequence properties of the corresponding continuous operators.

$$\mathbb{R} \hookrightarrow H^1(\Omega) \xrightarrow{\text{grad}} H^1(\text{curl}, \Omega) \xrightarrow{\text{curl}} H^1(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega, \mathbb{R}) \longrightarrow 0$$

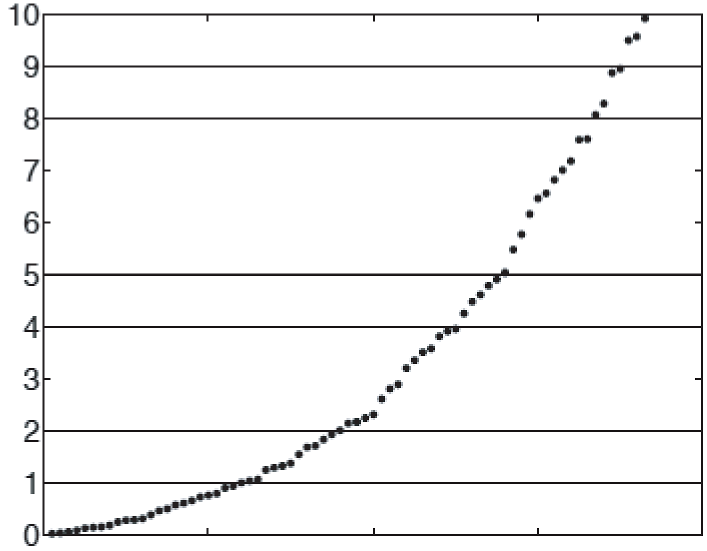
- These exactness properties turn out to be important in ensuring that the corresponding numerical schemes are stable.
- In computing the modes of an electromagnetic cavity, compatible discretizations yield more accurate eigenvalues.

Computational Electromagnetism

Exact Sequences and Spectral Properties



Computed using edge elements (compatible discretization)



Computed using linear finite elements

Computational Electromagnetism

Exact Sequence

$$\mathbb{R} \hookrightarrow H^1(\Omega) \xrightarrow{\text{grad}} H^1(\text{curl}, \Omega) \xrightarrow{\text{curl}} H^1(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega, \mathbb{R}) \longrightarrow 0$$

Helmholtz-Hodge Decomposition

- Decompose a vector field into **Divergence Free**, **Curl Free**, and **Harmonic** components.

Hodge Decomposition of Differential Forms

- The generalization of the Helmholtz-Hodge decomposition to differential forms is given by,

$$\Omega^k(M) = \mathbf{d}\Omega^{k-1}(M) \oplus \delta\Omega^{k+1}(M) \oplus \mathcal{H}^k$$

- For manifolds without boundary, **d** and δ are dual under the inner product on forms given by,

$$\langle \alpha^k, \beta^k \rangle = \int_M \alpha \wedge *\beta$$

- This comes from the Generalized Stokes' theorem,

$$\langle \mathbf{d}\alpha, \beta \rangle = \langle \alpha, \delta\beta \rangle + \int_{\partial M} \alpha \wedge *\beta$$

Motivation

Motivating Application

- Laplace-Beltrami Operator

Relevant Formalism

- Primal and Dual Complexes
- Differential Forms and Exterior Derivative
- Hodge Star and Codifferential

Primal and Dual Complexes

Why bother?

- Essential for capturing the inherent geometry of the problem.
- In geometric mechanics, we have to conscious of whether an object is in the tangent bundle or the cotangent bundle.
- While we can identify these spaces through the metric, we do this naïvely at our own peril.
- This results in a corresponding distinction at the level of discrete mechanics, where objects may be naturally primal or dual.

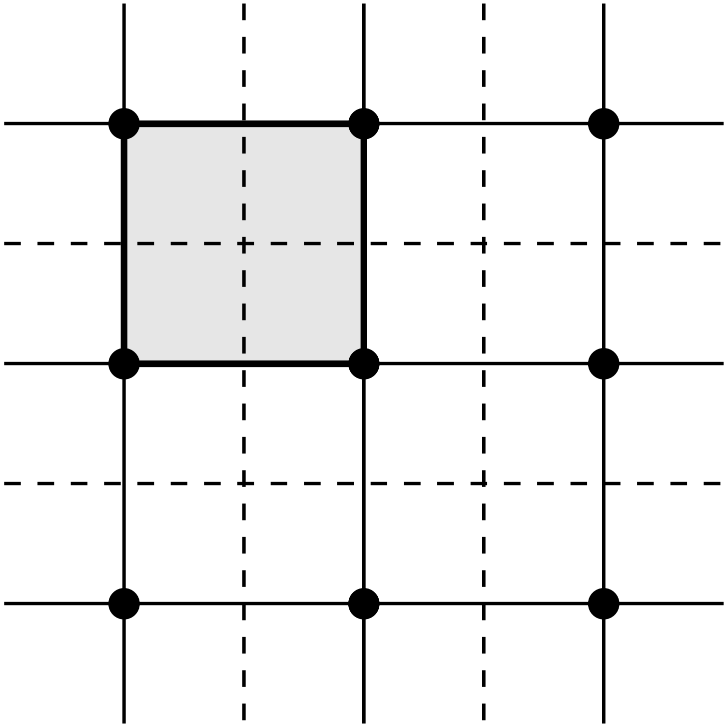
A new idea?

- Arises implicitly or explicitly in various schemes, including finite volume, finite element and finite difference methods.

Primal and Dual Meshes in FV, FE, FD Methods

Finite Volume Method

- Explicit use of two staggered discretization grids.

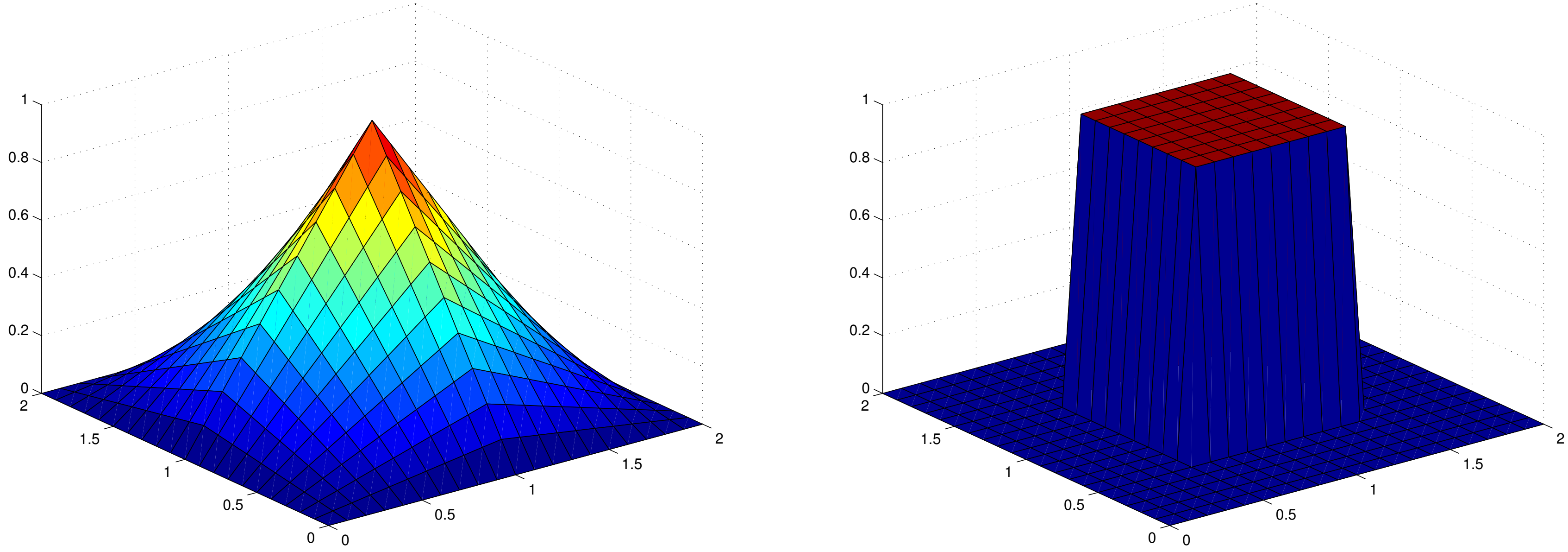


- Voronoi dual mesh obtained by associating to each point the volume that is closer to that point than any other point.

Primal and Dual Meshes in FV, FE, FD Methods

Finite Element Method

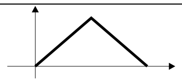
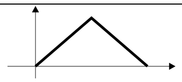
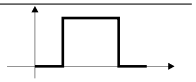
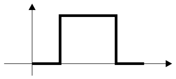
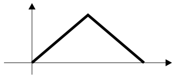
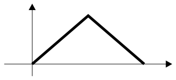
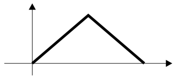
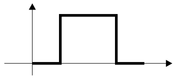
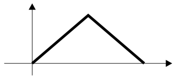
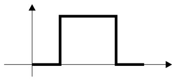
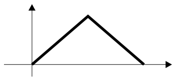
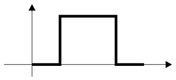
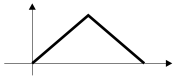
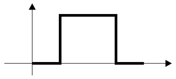
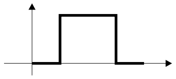
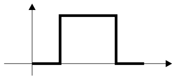
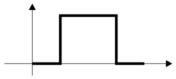
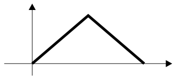
- Can arise implicitly by choice of shape functions.



- Application to computational electromagnetism hints at underlying geometry, since the choice of shape functions for field quantities depend on duality relations between the various field variables.

Primal and Dual Meshes in FV, FE, FD Methods

Computational Electromagnetism using Finite Elements

Field component	Variable x	Variable y	Variable t
ϕ			
A_x			
A_y			
E_x			
E_y			
B_z			

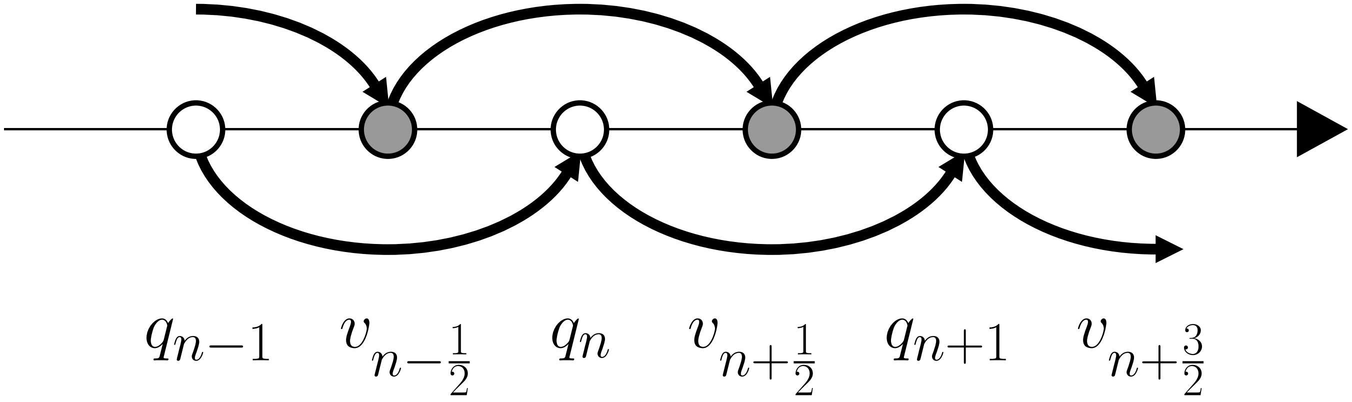
- The choice of tensor product shape functions in two dimensional Cartesian traverse magnetic (TM) model.

Primal and Dual Meshes in FV, FE, FD Methods

Finite Difference Method

- Primal and dual meshes arise in integration schemes such as the Verlet leapfrog method.

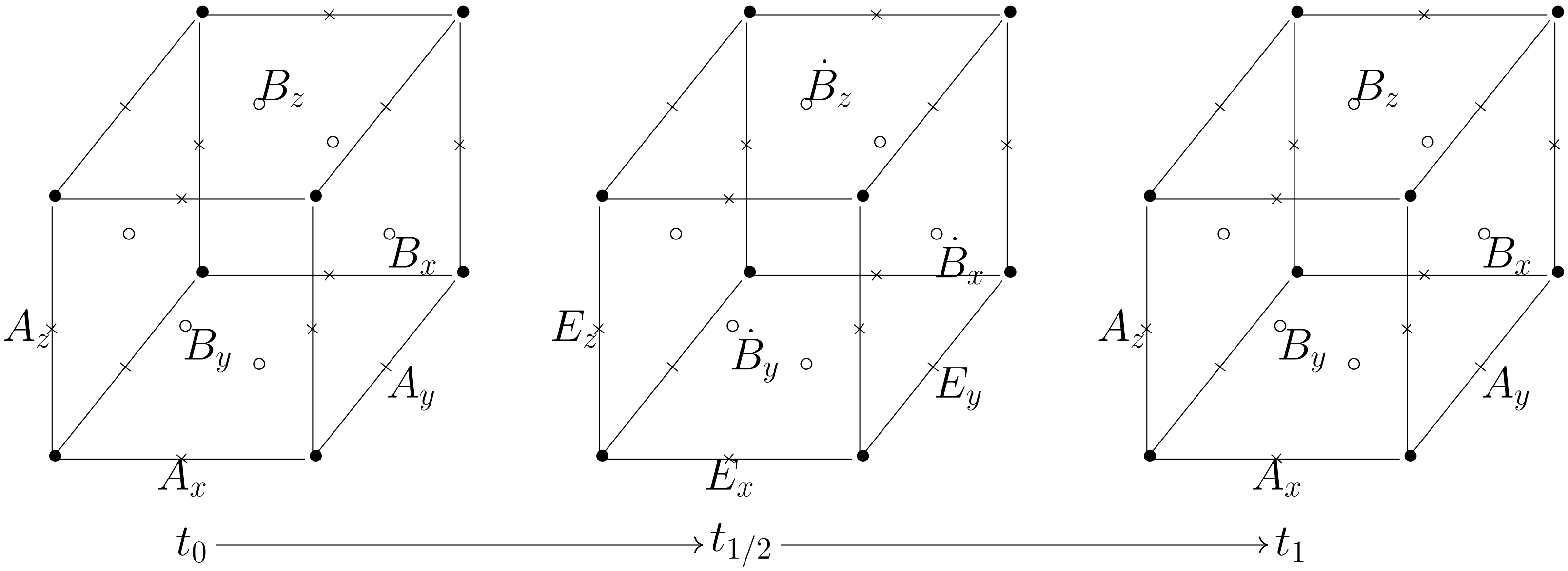
$$
\begin{aligned}
v_{n+\frac{1}{2}} &= v_{n-\frac{1}{2}} + \frac{f_n}{m}\Delta t \\
q_{n+1} &= q_n + v_{n+\frac{1}{2}}\Delta t
\end{aligned}
$$



Primal and Dual Meshes in FV, FE, FD Methods

Finite Difference Method

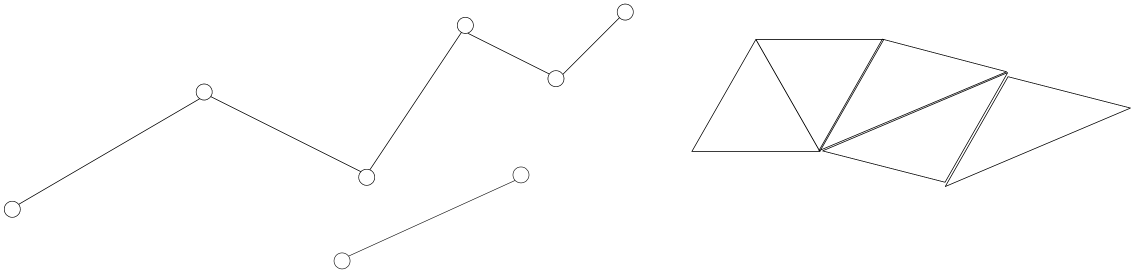
- Staggered Meshes in Space-time used in the Constrained Transport (CT) Method for Magnetohydrodynamics, implemented in ZEUS-2D.



Primal Simplicial Complex

Simplices

- A **k-simplex** is the convex span of $k+1$ linearly independent vectors.
- A **k-chain** is a formal sum of k-simplices.
- The group of k-chains is denoted $C_k(K)$.
- Example of chains,



Primal Simplicial Complex

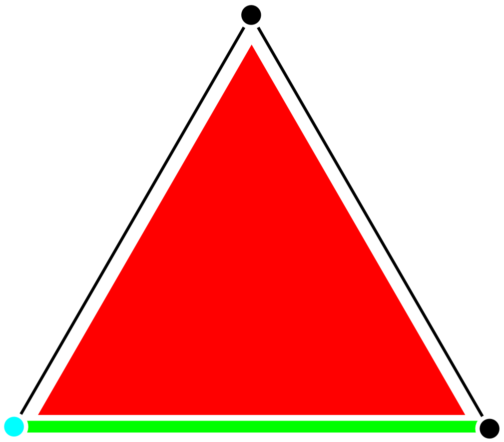
Simplicial Complex

- A **Simplicial Complex** K is a collection of simplices such that:
  - every face of a simplex of K is in K.
  - the intersection of any two simplices of K is a face of each of them.

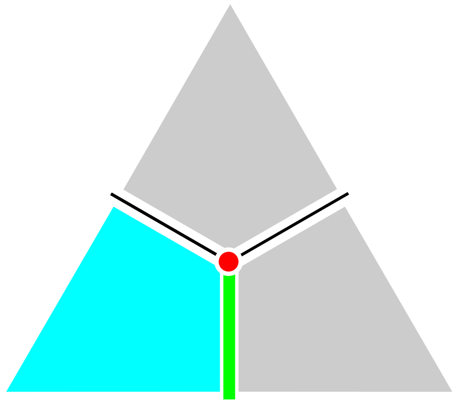
Simplicial Triangulation

- A **Simplicial Triangulation** of a polytope $|K|$ is a simplicial complex K such that the union of the simplices of K recover the polytope $|K|$.

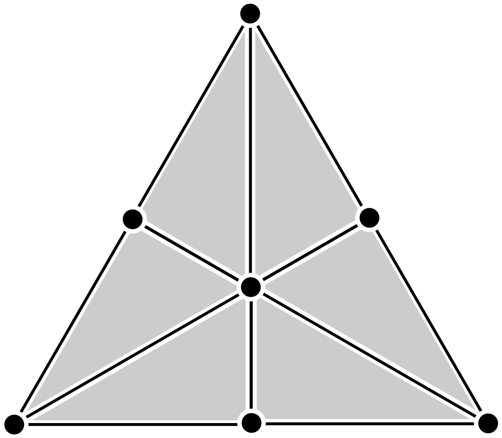
Primal and Dual Complexes



Primal Mesh



Dual Mesh



Subdivision

- The **Dual Mesh** is defined in terms of a **Discrete Poincaré Duality Operator**.
- The Dual Mesh to a Simplicial Triangulation is not Simplicial, but is a submesh of the **First Subdivision**.

Dual Cell Complex

Constructing the Dual Complex

- The **circumcentric duality operator** is given by

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

- Associates a k-simplex to a $(n-k)$-cell.
- Satisfies the property,

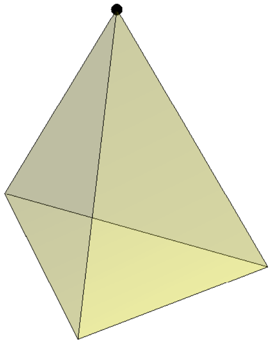
$$\star\star(\sigma^k) = (-1)^{k(n-k)}\sigma^k.$$

- Will be used in constructing the **Hodge Star** for discrete differential forms.

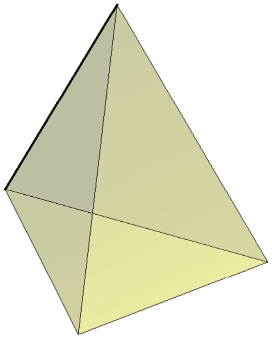
Examples of Primal Simplices and Dual Cells

- **Primal Simplex**

σ^0, 0-simplex

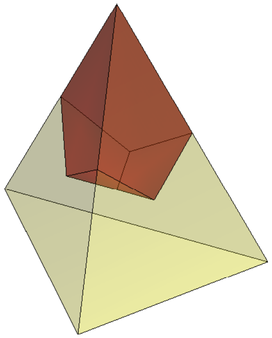


σ^1, 1-simplex

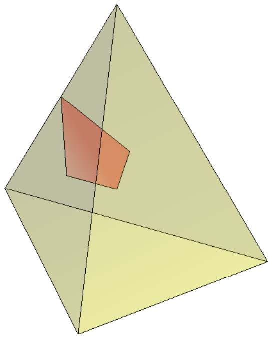


- **Dual Cell**

$\star\sigma^0$, 3-cell



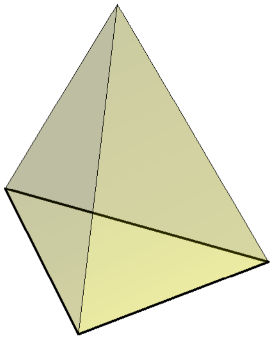
$\star\sigma^1$, 2-cell



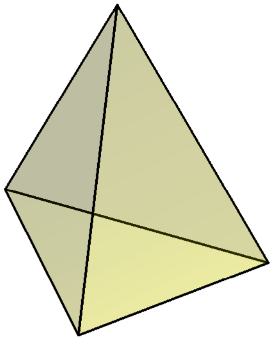
Examples of Primal Simplices and Dual Cells

- **Primal Simplex**

σ^2, 2-simplex

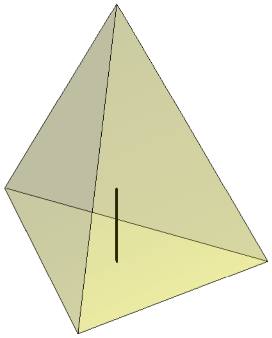


σ^3, 3-simplex

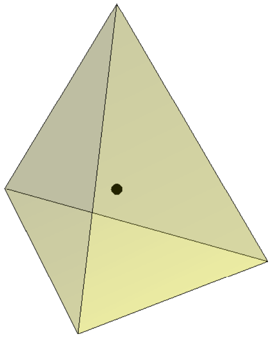


- **Dual Cell**

$\star\sigma^2$, 1-cell



$\star\sigma^3$, 0-cell



Differential Forms and Exterior Derivative

Cochains and Differential Forms

- A **Discrete Differential Form** is a cochain on the simplicial complex. That is,
$$\Omega_d^k(K) = C^k(K;\mathbb{R}) = Hom(C_k(K),\mathbb{R}).$$
- It is a *linear functional* on simplices, and it defined by assigning a number to each simplex.
- To discretize a continuous differential form into a discrete differential form, we assign a number to each simplex by integration,
$$\langle \alpha_d^k, \sigma^k \rangle = \int_{\sigma^k} \alpha^k.$$
- After the discretization step, we can discard the continuous differential form.

Differential Forms and Exterior Derivative

Exterior Derivative

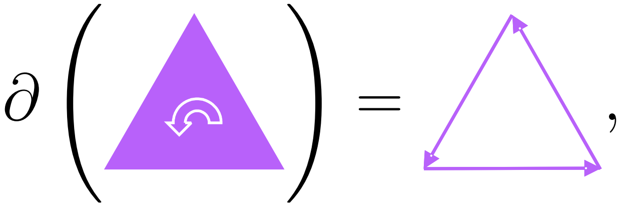
- The **Exterior Derivative** is defined by using the Generalized Stokes Theorem,

$$\langle \mathbf{d}\alpha^k, \sigma^{k+1} \rangle = \langle \alpha^k, \partial\sigma^{k+1} \rangle.$$

where the **boundary** operator $\partial_k : C_k(K) \rightarrow C_{k-1}(K)$ is given by,

$$\partial_k \sigma_k = \partial\left([v_0, v_1, \ldots, v_k]\right) = \sum_{i=0}^{k} (-1)^i [v_0, \ldots, \hat{v}_i, \ldots, v_p]$$

- As an example,



where clearly, orientation must be carefully taken into account.

Simplicial Algebraic Topology

Boundary and Chain Complex

- The **boundary** operator $\partial_p : C_p\left(K;\mathbb{Z}\right) \to C_{p-1}\left(K;\mathbb{Z}\right)$ is given by,

$$\partial_p \sigma_p = \partial\left(\langle v_0, v_1, \ldots, v_p\rangle\right) = \sum_{i=0}^{p} (-1)^i \langle v_0, \ldots, \hat{v}_i, \ldots, v_p\rangle$$

- On a simplicial complex of dimension n, we have the **chain complex** given by,

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

Simplicial Algebraic Topology

Coboundary and Cochain Complex

- Consider the dual space to the space of chains, the **cochain group**, $C_p^*(K) := C^p(K) = Hom\left(C_p(K), \mathbb{R}\right)$.
- The **coboundary** operator $d^p : C^p(K) \to C^{p+1}(K)$ defined by duality to the boundary operator,

$$\left\langle d^p c^p, c_{p+1} \right\rangle = \left\langle c^p, \partial_{p+1} c_{p+1} \right\rangle$$

- This induces the **cochain complex**,

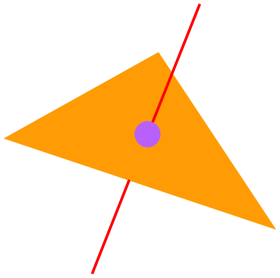
$$\begin{tikzcd} 0 & C^n(K) \arrow[l] & \ldots \arrow[l, "d^{n-1}"'] & C^p(K) \arrow[l, "d^p"'] & \ldots \arrow[l, "d^{p-1}"'] & C^0(K) \arrow[l, "d^0"'] & 0 \arrow[l] \end{tikzcd}$$

Hodge Star and Codifferential

Hodge Star

- The **discrete Hodge Star** is a map $* : \Omega_d^k(K) \longrightarrow \Omega_d^{n-k}(\star K)$. For a k-simplex σ^k and a discrete k-form α^k,

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



Codifferential

- The **discrete codifferential operator** $\delta : \Omega_d^{k+1}(K) \rightarrow \Omega_d^k(K)$ is defined by $\delta(\Omega_d^0(K)) = 0$ and on $(k+1)$-discrete forms to be,

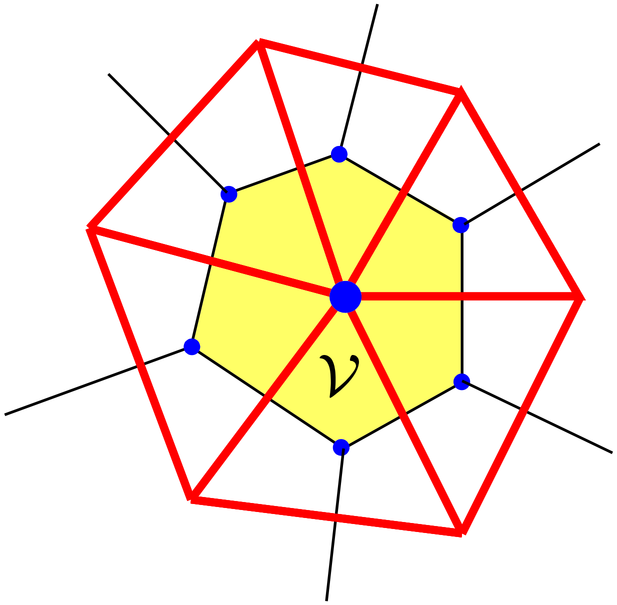
$$\delta\beta = (-1)^{nk+1} * \mathbf{d} * \beta \, .$$

Application

Laplace-Beltrami

- The **Laplace-Beltrami** operator is a special case of the more general Laplace-deRham operator $\Delta = \mathbf{d}\delta + \delta\mathbf{d}$.

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



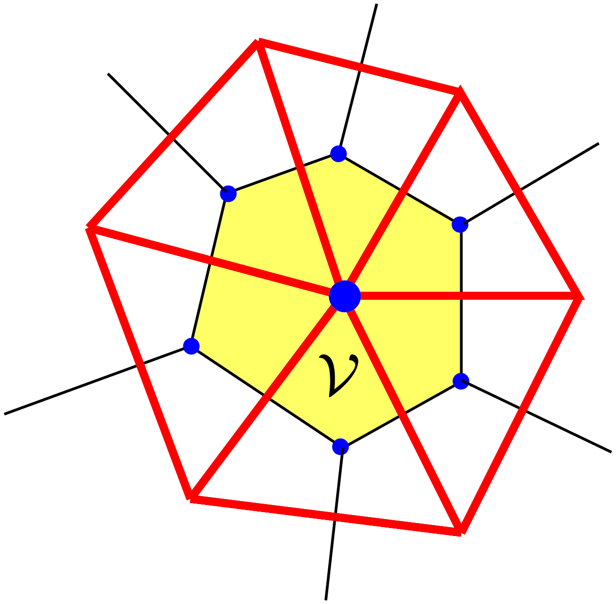
Application

Laplace-Beltrami

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

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

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



- This recovers a formula involving cotangents found by Meyer *et al.*using a variational approach.

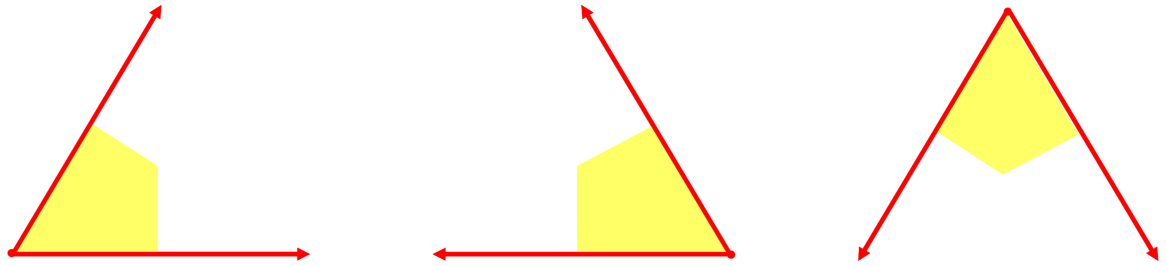
Wedge Product

Definition

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle$$

$$= \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|} \alpha \smile \beta(\tau(\sigma^{k+l}))$$

- Terms in a 1-1 wedge,



- Purely combinatorial definition of the wedge product.
- Also comes in a dual-dual variant.

Wedge Product

Properties

- Anti-commutative
- Leibniz Rule
- Associative for closed forms

Wedge Product and Associativity

Definition

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle$$

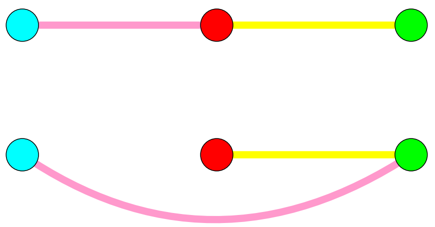
$$= \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|} \alpha \smile \beta(\tau(\sigma^{k+l}))$$

Non-associative

- Arises from difference in stencil.

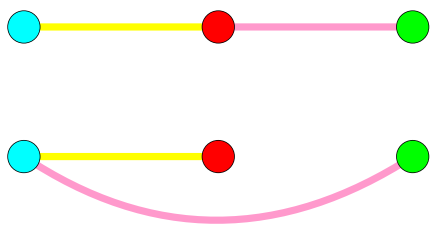
$$\alpha \wedge (\beta \wedge \gamma)$$

$$\sum \alpha \smile (\sum \beta \smile \gamma)$$



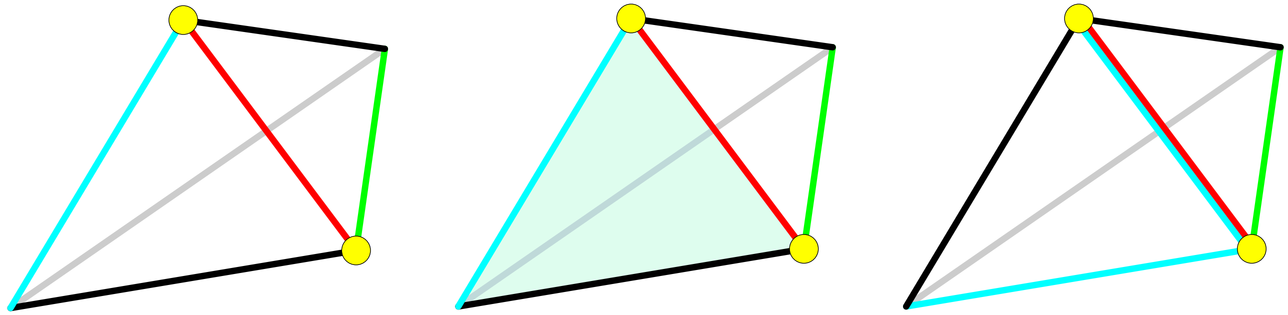
$$(\alpha \wedge \beta) \wedge \gamma$$

$$(\sum \alpha \smile \beta) \smile \sum \gamma$$



Associative for Closed Forms

- Since forms are closed, can rewrite sum so that the forms are all evaluated at a common vertex.



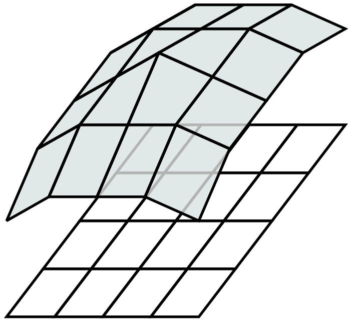
- Then, both sides can be written as,

$$\langle \alpha \wedge \beta \wedge \gamma, \sigma^{k+l+m} \rangle = \sum_{i=0}^{k+l+m} \sum_{\tau \in S^{k+l+m}} \alpha \smile \beta \smile \gamma$$

- Associativity important for showing that the algebraic definitions of contraction and Lie derivative are $\wedge$-antiderivations.

Multisymplectic Geometry

Geometry and Variational Mechanics



- **Base space** $\mathcal{X}$. The independent variables, typically $(n+1)$-spacetime, denoted by $(x^0, \ldots, x^n)$.
- **Configuration bundle**. $\pi : Y \to \mathcal{X}$.
- **Configuration** $q : \mathcal{X} \to Y$. Gives the field variables over each spacetime point.
- **First jet extension** J^1Y. Consists of the first partials of the field variables with respect to the independent variables.
- **Lagrangian density** $L : J^1Y \to \Omega^{n+1}(\mathcal{X})$.
- **Action integral** $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1q)$.
- **Hamilton's principle** $\delta\mathcal{S} = 0$.

Variational Formulation of Harmonic Functions

Inner Product for Differential Forms

- Need an inner product for forms,

$$\langle\langle \alpha, \beta \rangle\rangle = \int_M \alpha \wedge *\beta.$$

- At a discrete level, this involves a primal-dual wedge product, which we only have for the case of primal k forms and dual $(n-k)$-forms,

$$\begin{aligned}\langle \alpha^k \wedge *\beta^k, V_{\sigma^k} \rangle &= \frac{|V_{\sigma^k}|}{|\sigma^k||\star\sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle *\beta^k, \star\sigma^k \rangle \\ &= \frac{1}{n} \frac{|\star\sigma^k|}{|\sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle \beta^k, \sigma^k \rangle.\end{aligned}$$

Variational Formulation of Harmonic Functions

Discrete Variational Principle

- A discrete Harmonic function is a stationary point of the following discrete Lagrangian,

$$L = \sum_{\sigma^1 \in K} \langle \mathbf{d}f \wedge *\mathbf{d}f, V_{\sigma^1} \rangle .$$

- The corresponding Euler-Lagrange equation is,

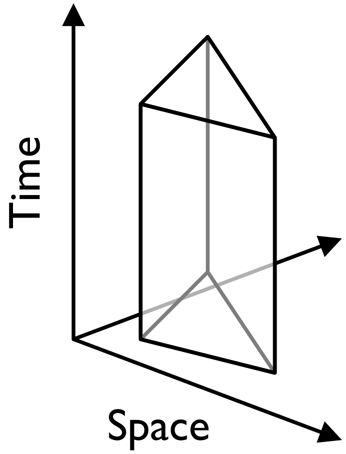
$$\sum_{\sigma^1 = [v_1, v_0] \succ v_0} \frac{2}{n} \frac{|\star \sigma^1|}{|\sigma^1|} \langle \mathbf{d}f, \sigma^1 \rangle = 0.$$

- This means that the variational formulation of discrete Harmonic functions is equivalent to the formulation in terms of the Laplace-Beltrami operator.

Discrete Electromagnetism

Discrete Formulation

- Covariant formulation using the 4-vector potential as the fundamental variable.
- 3+1 tensor product discretization, $K \otimes \mathbb{N}$.
- Lorentzian metric structure causes the Laplace-Beltrami operator to be a hyperbolic operator as opposed to an elliptic operator.
- Equivalent expressions when applying discretization at the level of the variational principle, and at the level of the equations.



- Discretizing either the Euler-Lagrange equations or the Lagrangian using DEC yields the same Discrete Euler-Lagrange equations.

Discrete Electromagnetism

Hodge Star for Prismal Complexes in Lorentzian Space

- The Hodge star $*$ is defined by the expression,

$$\alpha \wedge *\beta = \langle\!\langle \alpha, \beta \rangle\!\rangle \mathbf{v}\,,$$

and depends on the metric in particular.

- The **Discrete Hodge Star in Lorentzian Space** is given by,

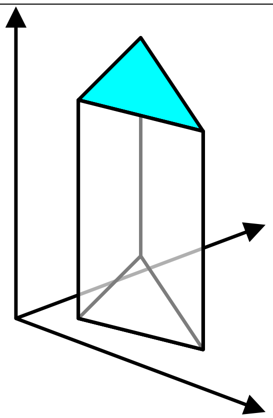
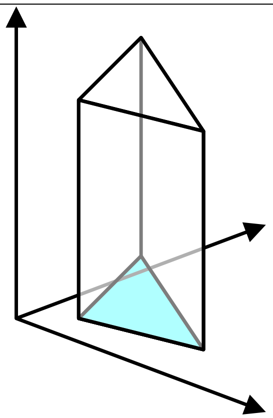
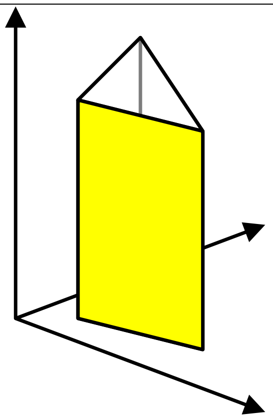
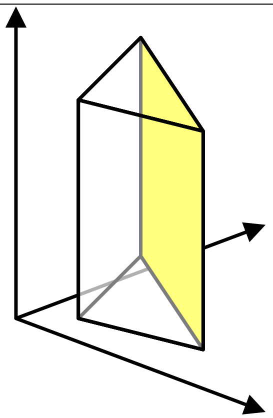
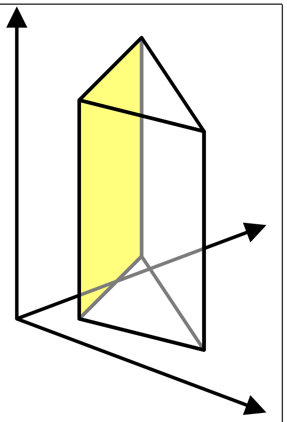
$$\frac{1}{|\star\,\sigma^k|}\langle *\alpha^k, \star\sigma^k\rangle = \kappa(\sigma^k)\frac{1}{|\sigma^k|}\langle \alpha^k, \sigma^k\rangle,$$

where $|\cdot|$ stands for the volume and $\kappa(\sigma^k)$ is the **causality sign** of the simplex σ^k.

Discrete Electromagnetism

Causality Sign

- The **causality sign** $\kappa(\sigma^k)$ arises from the pseudo-Riemannian metric structure of Lorentzian space-time. It is defined to be $+1$ if all the edges of the simplex are spacelike, and -1 otherwise.

σ^2					
$\kappa(\sigma^2)$	$+1$	$+1$	-1	-1	-1

Discretization and Variational Principles

Open question

- Does discretization using Discrete Exterior Calculus commute with the derivation of equations from variational principles using the Calculus of Variations?

$$\begin{tikzcd}
\begin{array}{c}\textbf{Lagrangian}\\ L : TQ \to \mathbb{R}\end{array} \arrow[r, "DEC"] \arrow[d] & \begin{array}{c}\textbf{Discrete Lagrangian}\\ L_d : Q \times Q \to \mathbb{R}\end{array} \arrow[d] \\
\begin{array}{c}\textbf{Euler-Lagrange}\\ \mathcal{EL} : T^2Q \to T^*Q\end{array} \arrow[r, "DEC"] & \begin{array}{c}\textbf{Discrete Euler-Lagrange}\\ \mathcal{EL}_d : Q^3 \to T^*Q\end{array}
\end{tikzcd}$$

- For harmonic functions, and electromagnetism, these two operations commute, but is it true in general?

Motivation

Motivating Application

- Divergence Operator

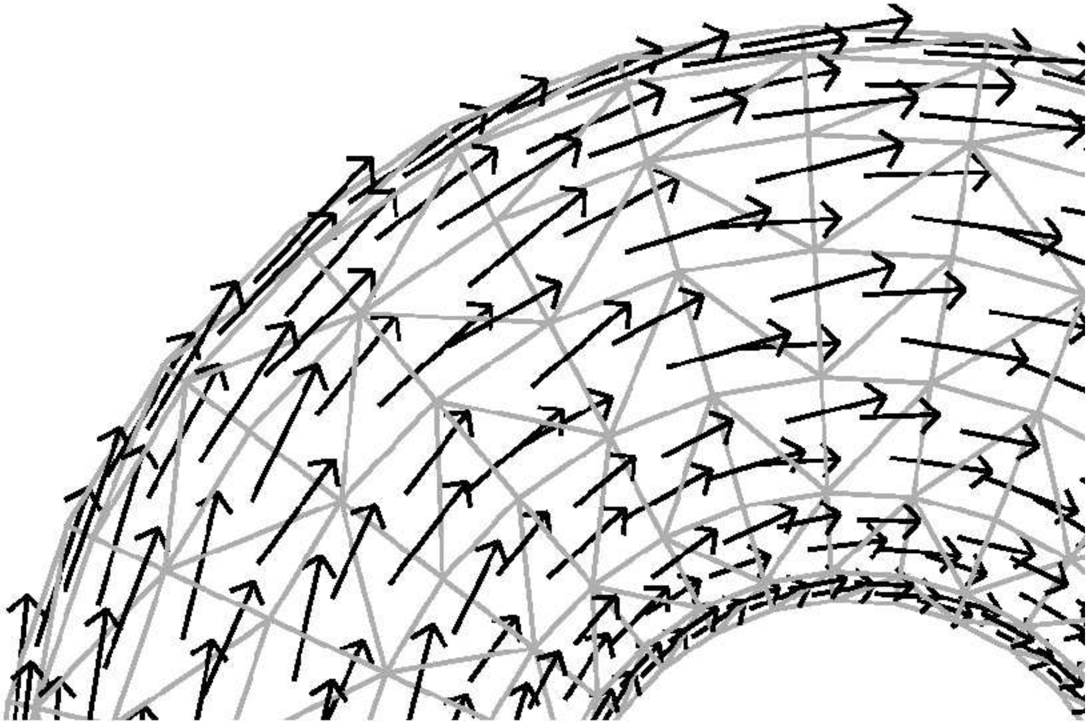
Relevant Formalism

- Maps between One-Forms and Vector Fields

Maps between One-Forms and Vector Fields

Discrete Vector Fields

- A **dual discrete vector field** X on a simplicial complex K is a map from the dual vertices to $\mathbb{R}^N$ such that its value on each dual vertex is tangential to the corresponding primal n-simplex.



Maps between One-Forms and Vector Fields

Discrete Flat operator

- The **discrete flat operator on a dual vector field** $\flat : \mathfrak{X}_d(\star K) \rightarrow \Omega^1_d(K)$ is given by,

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

  where $X \cdot \vec{\sigma}^1$ is the usual dot product of vectors in $\mathbb{R}^N$ and $\vec{\sigma}^1$ stands for the vector corresponding to σ^1 and with the same orientation. The sum is over all σ^n containing the edge σ^1.

Application

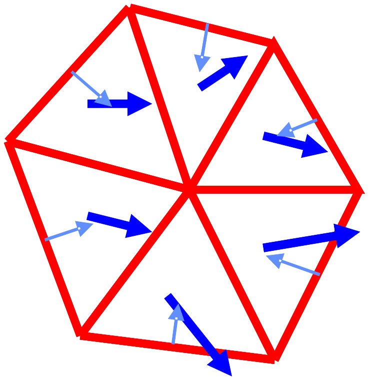
Divergence

- Recall the definition of the divergence in terms of flat, and codifferential,

$$\mathrm{div}(\mathbf{X}) = -\delta X^\flat\,.$$

This can then be expressed in terms of the Hodge star, the exterior derivative, and the flat,

$$\begin{aligned}\frac{1}{|\sigma^0|}\langle \mathrm{div}(X), \sigma^0\rangle &= \frac{1}{|\star\sigma^0|}\langle * * \mathbf{d} * X^\flat, \star\sigma^0\rangle \\ &= \frac{1}{|\star\sigma^0|}\langle \mathbf{d} * X^\flat, \star\sigma^0\rangle \\ &= \frac{1}{|\star\sigma^0|}\langle *X^\flat, \partial(\star\sigma^0)\rangle\end{aligned}$$

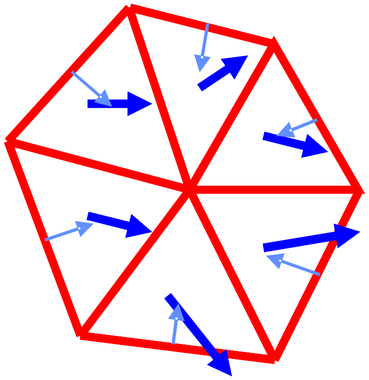


Application

Divergence

- But,

$$\partial(\star\sigma^0) = \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1.$$



Thus,

$$\frac{1}{|\sigma^0|}\langle \mathrm{div}(X), \sigma^0 \rangle = \frac{1}{|\star\sigma^0|}\langle * X^\flat, \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1 \rangle$$
$$= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \langle * X^\flat, \star\sigma^1 \rangle$$

Application

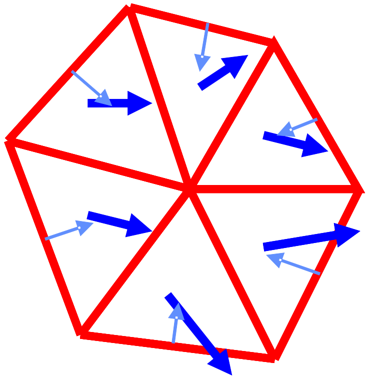
Divergence

$$= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|} \langle X^\flat, \sigma^1 \rangle$$

$$= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|} \sum_{\sigma^2 \succ \sigma^1} \frac{|\star\sigma^1 \cap \sigma^2|}{|\star\sigma^1|} X \cdot \vec{\sigma}^1$$

$$= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \sum_{\sigma^2 \succ \sigma^1} \frac{|\star\sigma^1 \cap \sigma^2|}{|\star\sigma^1|} X \cdot \vec{\sigma}^1$$

$$= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} |\star\sigma^1| \left(X \cdot \frac{\vec{\sigma}^1}{|\sigma^1|} \right).$$



Contraction

Algebraic

- The contraction operator can be expressed in the continuous case in terms of the Hodge star, wedge product and flat,

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

We then define the discrete contraction operator using the above formula, but with the discrete Hodge, wedge and flat substituted.

Dynamic

- Alternatively, contraction can be defined dynamically in terms of the extrusion of a simplex by a vector field,

$$\int_S i_X \beta = \frac{d}{dt}\bigg|_{t=0} \int_{E_X^t(S)} \beta.$$

Lie Derivative

Algebraic

- The Lie Derivative can be expressed by the following homotopy formula,

$$\pounds_{\mathbf{X}}\omega = \mathbf{i}_{\mathbf{X}}\mathbf{d}\omega + \mathbf{d}\mathbf{i}_{\mathbf{X}}\omega\,.$$

  We then define the discrete Lie derivative in terms of the discrete contraction and discrete exterior derivative.

Dynamic

- Alternatively, the Lie derivative can be defined dynamically as,

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

  Where S_t is the surface S advected by the time t flow of the vector field X.

Discrete Poincaré Lemma

Theorem

- In a generalized star-shaped region, given a closed cochain α^{k+1}, that is to say, $\mathbf{d}\alpha^{k+1} = 0$, there exists a cochain β^k such that $\mathbf{d}\beta^k = \alpha^{k+1}$.

Idea behind proof

- Construct a generalized cone operator $p : C_k(K) \to C_{k+1}(K)$, that is well-defined, and satisfies the condition,

$$\partial p + p\partial = I.$$

- Construct the cocone operator $H : \Omega_d^{k+1}(K) \to \Omega_d^k(K)$,

$$\langle H\alpha^{k+1}, \sigma^k \rangle = \langle \alpha^{k+1}, p\sigma^k \rangle.$$

- Then, $H\mathbf{d} + \mathbf{d}H = I$, and $\beta^k = H\alpha^{k+1}$.

Discrete Poincaré Lemma

Construction of the Cone Operator

- To define $p(\sigma^k)$, we consider $\sigma^{k+1} \succ \sigma^k$, such that σ^{k+1} and σ^k are consistently oriented. Then by applying the identity,

$$p\partial + \partial p = I,$$

to σ^{k+1} and setting,

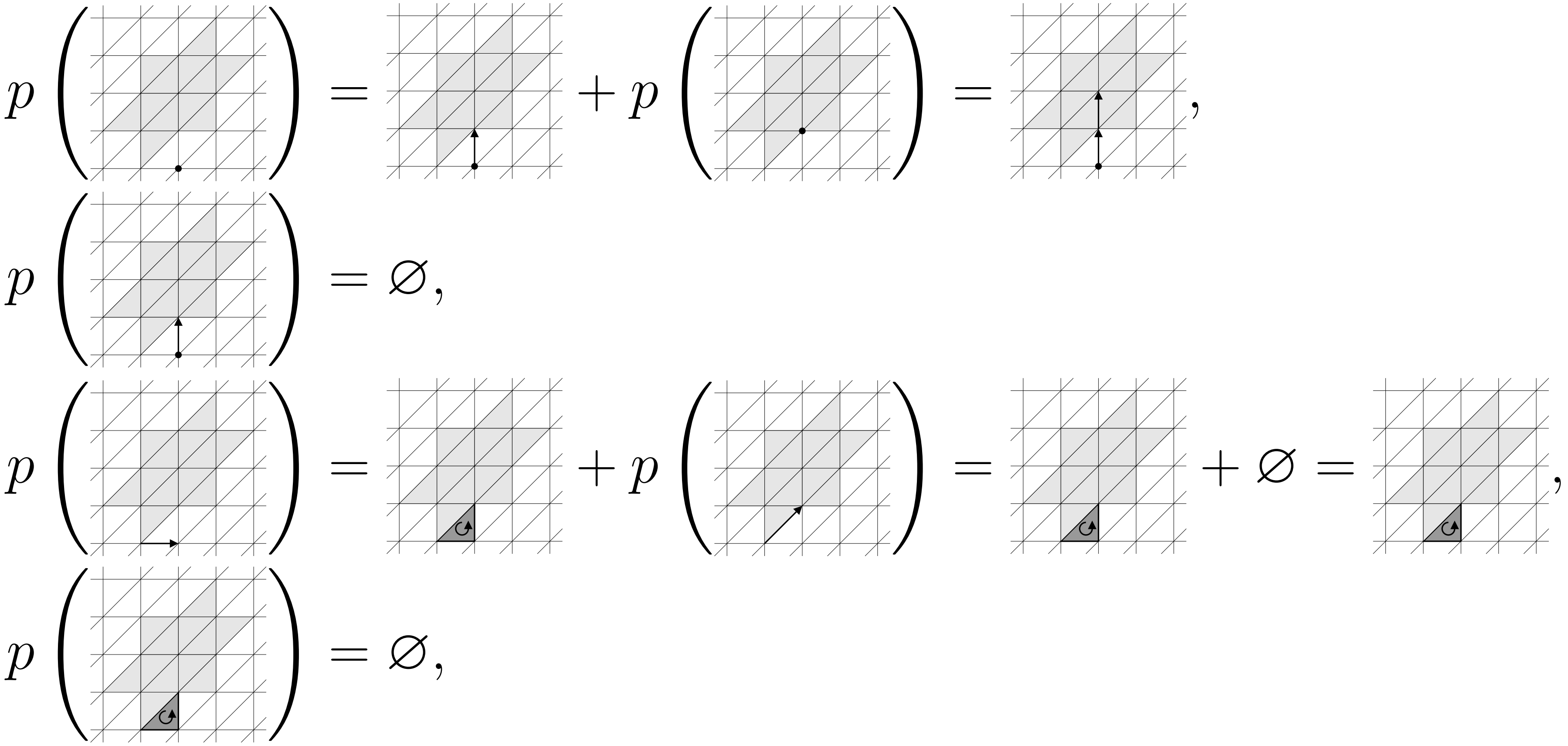
$$p(\sigma^{k+1}) = \varnothing,$$

we obtain,

$$p(\sigma^k) = \sigma^{k+1} - p(\partial\sigma^{k+1} - \sigma^k).$$

Discrete Poincaré Lemma

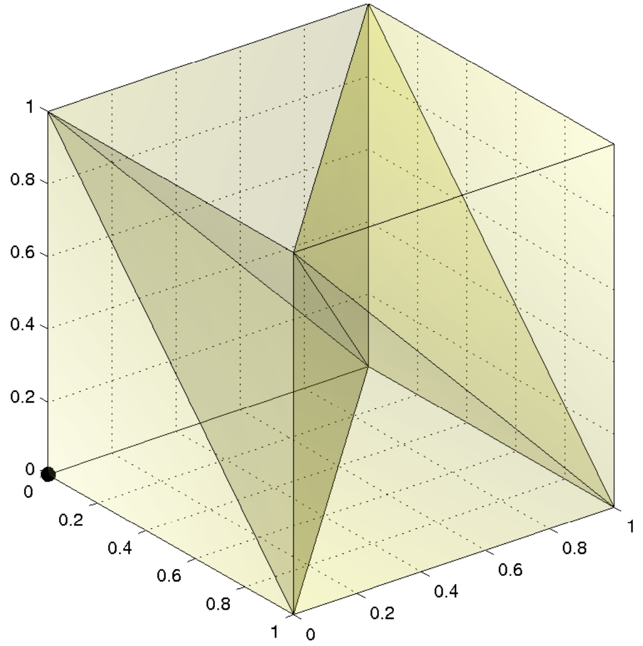
Example of Generalized Cone Operator

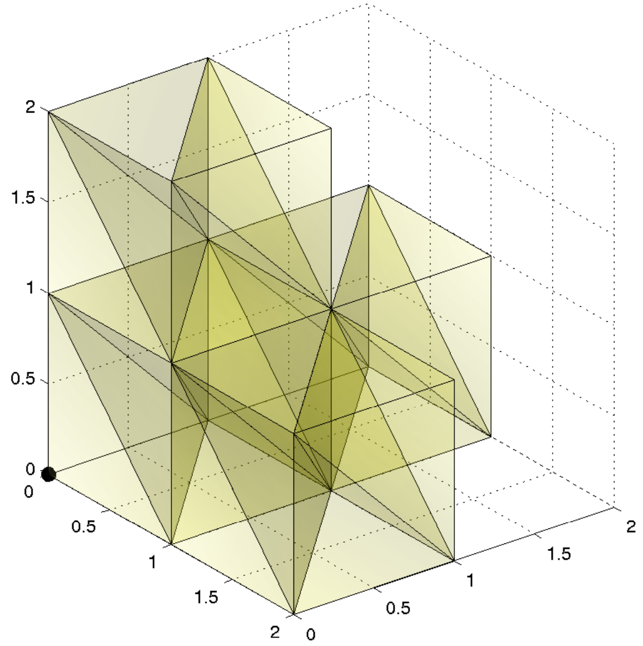


Discrete Poincaré Lemma

Global results

- The Discrete Poincaré Lemma holds globally for a regular triangulation of $\mathbb{R}^2$.
- The Discrete Poincaré Lemma holds globally for a regular tetrahedralization of $\mathbb{R}^3$.





Discrete Curvatures from Geometric Identities

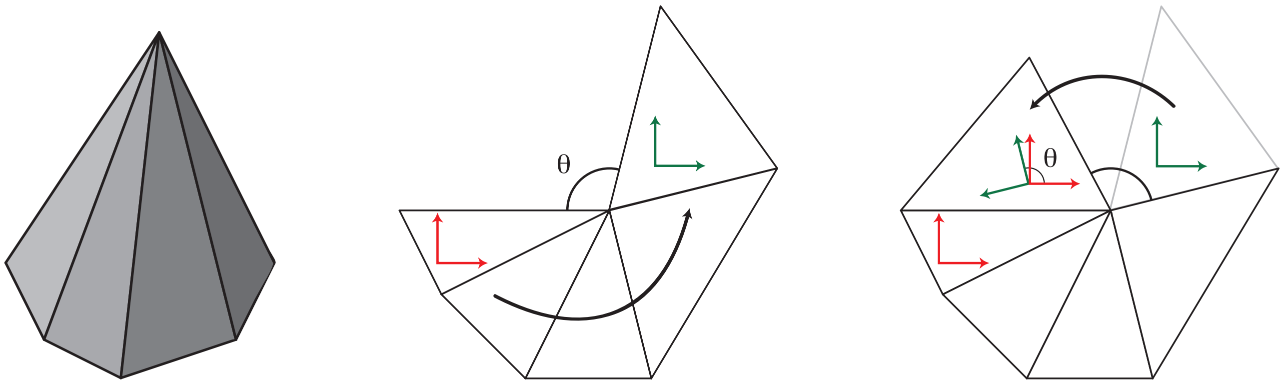
Discrete Gauß Curvature

- The discrete expression for the Gauß curvature can be derived from the Gauß–Bonnet theorem, and is given by

$$\int_D K dA = \sum_{p \in D} K_p \,,$$

where K_p is the **angle defect** at a point p, given by

$$K_p = 2\pi - \sum_i \theta_i \,.$$



Discrete Connection Form

Definition

A **Discrete Connection Form** is a continuous map,

$$\mathcal{A}_d : Q \times Q \to G,$$

such that,

- $\mathcal{A}_d$ is G-equivariant.

$$\mathcal{A}_d \circ L_g = I_g \circ \mathcal{A}_d.$$

This is the discrete analogue of the statement, $\mathcal{A} \circ L_g = Ad_g \circ \mathcal{A}$.

- $\mathcal{A}_d$ induces a splitting of the Discrete Atiyah sequence.

$$\mathcal{A}_d(i_q(g)) = g.$$

This is the discrete analogue of the statement, $\mathcal{A}(\xi_Q) = \xi$.

Discrete Atiyah Sequence

Discrete Atiyah Sequence

$$\begin{tikzcd}
0 \arrow[r] & \tilde{G} \arrow[r, shift left, "i"] \arrow[d, equal, "1_{\tilde{G}}"'] & (Q \times Q)/G \arrow[l, dashed, shift left, "(\pi_1{,}\mathcal{A}_d)"] \arrow[r, shift left, "(\pi{,}\pi)"] \arrow[d, "\alpha_{\mathcal{A}_d}"] & S \times S \arrow[l, dashed, shift left, "(\cdot{,}\cdot)^h"] \arrow[r] \arrow[d, equal, "1_{S\times S}"] & 0 \\
0 \arrow[r] & \tilde{G} \arrow[r, shift left, "i_1"] & \tilde{G} \oplus (S \times S) \arrow[l, dashed, shift left, "\pi_1"] \arrow[r, shift left, "\pi_2"] & S \times S \arrow[l, dashed, shift left, "i_2"] \arrow[r] & 0
\end{tikzcd}$$

Maps

- $i : \tilde{G} \to (Q \times Q)/G$, where,

$$i([q, g]_G) = [q, gq]_G.$$

- $(\pi, \pi) : (Q \times Q)/G \to S \times S$, where,

$$(\pi, \pi)([q_0, q_1]_G) = (\pi q_0, \pi q_1).$$

Discrete Levi-Civita Connection

Discrete Riemannian manifold

- Cartan's persective: Bundle of oriented orthonormal frames over a manifold as a principal $SO(n)$ bundle.
- Semidiscretize by discretizing manifold with a simplicial complex, but keeping the group $SO(n)$ continuous.
- Associate with each n-simplex a metric tensor g.

Constructing the Levi-Civita connection

- The Levi-Civita connection is a $SO(n)$-valued **dual one-form**.
- This element of $SO(n)$ transforms the frame associated with a n-simplex into the frame associated with an adjacent n-simplex, and is assigned to the codimension-one face common to both simplices.

Example

Discrete Mechanical Connection

- $\mathcal{A}_d : Q \times Q \to G$ defined on a G-invariant neighborhood of the diagonal by $\mathcal{A}_d(q_0, q_1) = e$ iff $\mathbf{J}_d(q_0, q_1) = 0$, and extended by,

$$\mathcal{A}_d(g_0 q_0, g_1 q_1) = g_1 g_0^{-1}.$$

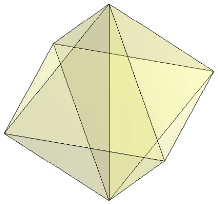
- This is consistent with the discrete horizontal space obtained by pulling-back the continuous horizontal space associated with the mechanical connection by the fibre derivatives.

$$\begin{tikzcd}
(Q \times Q, \mathbf{J}_d) \arrow[r, "\mathbb{F}L_d"] & (T^*Q, \mathbf{J}) \\
 & (TQ, \mathbf{J}_L) \arrow[u, "\mathbb{F}L"']
\end{tikzcd}$$

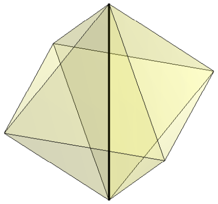
Discrete Levi-Civita Connection

Curvature

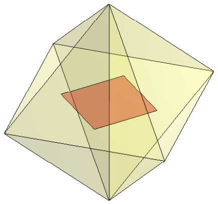
- Curvature is a dual two-form, and is associated with the dual of a codimension-two simplex, given by $\star\sigma^{n-2}$.



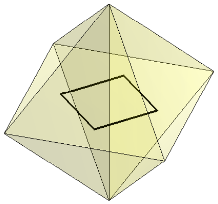
Simplicial Complex, K



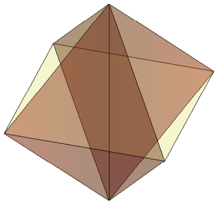
$n-2$ primal simplex, σ^{n-2}



2 dual cell, $\star\sigma^{n-2}$



1 dual chain, $\partial\star\sigma^{n-2}$



$n-1$ primal chain, $\star\partial\star\sigma^{n-2}$

- The curvature $\mathcal{B}$ of the discrete Levi-Civita connection is given by,

$$\langle \mathcal{B}, \star\sigma^{n-2}\rangle = \langle \mathbf{d}A, \star\sigma^{n-2}\rangle = \langle A, \partial\star\sigma^{n-2}\rangle.$$

Global and Local Embeddings

Global Embeddings

- While it is computationally more convenient to have a global embedding of the simplicial complex into a higher dimensional ambient space to account for non-flat manifolds, it is not necessary.

Local Embeddings

- It suffices to have an abstract simplicial complex along with a metric on vertices, $d : K^{(0)} \times K^{(0)} \longrightarrow \mathbb{R}$, such that the usual metric axioms hold.
- This allows us to embed each n-simplex locally into $\mathbb{R}^n$, and thereby compute all the necessary metric dependent quantities in our formulation.

Conclusion

Summary

- Incorporates discrete forms, vector fields, and related operators
- Construction of canonical discrete differential operators
- Applications to Laplace-Beltrami operator, Harmonic maps, Electromagnetism, and Curvature