Towards Discrete Exterior Calculus and Discrete Mechanics for Numerical Relativity

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IPAM Workshop on Relativistic Astrophysics, May 2005.

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Geometry and Numerical Methods

Dynamical equations preserve structure

- Many continuous systems of interest have properties that are conserved by the flow:
  - Energy
  - Symmetries, Reversibility, Monotonicity
  - Momentum - Angular, Linear, Kelvin Circulation Theorem, Constraint Equations in Relativity
  - Symplectic Form
- At other times, the equations themselves are defined on a manifold, such as a Lie group, or more general configuration manifold of a mechanical system, and the discrete trajectory we compute should remain on this manifold, since the equations may not be well-defined off the surface.

Motivation: Geometric Integration

Main Goal of Geometric Integration:

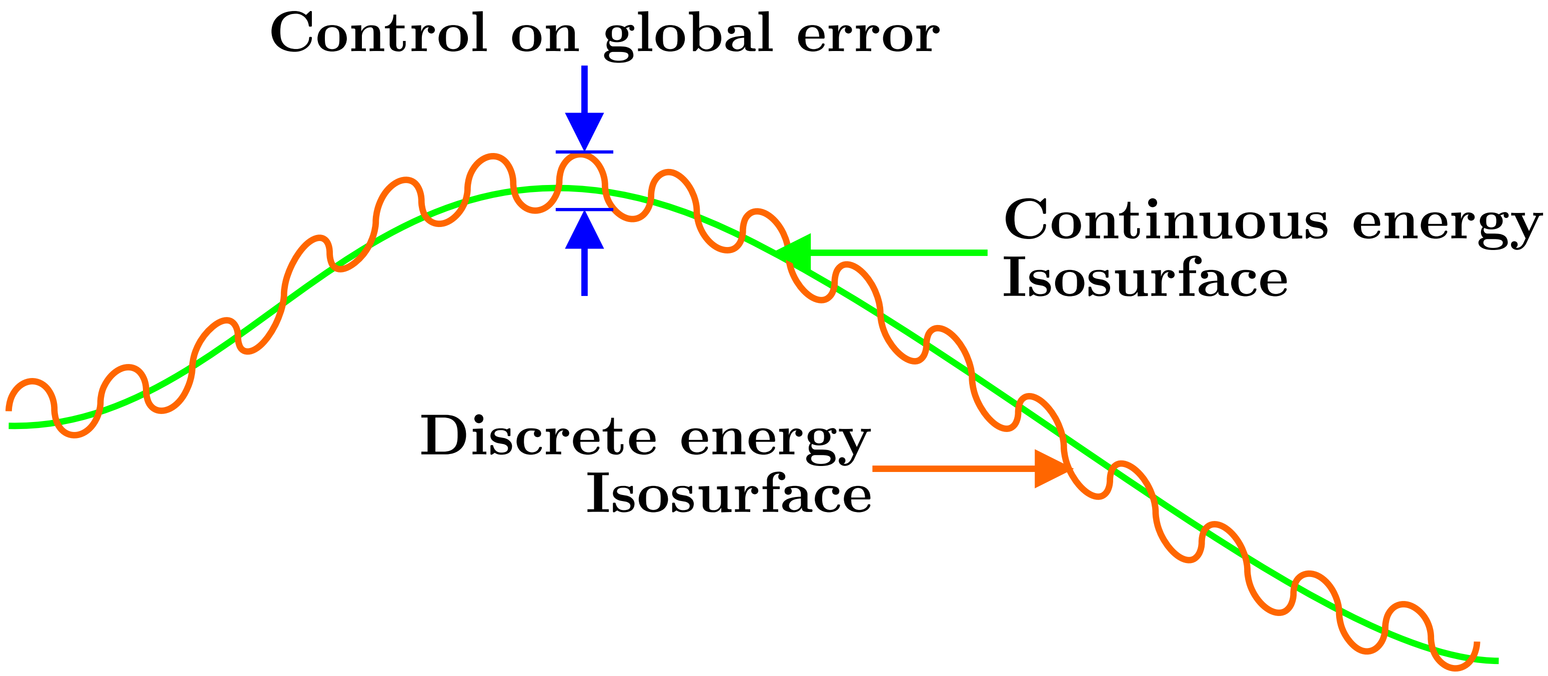
Structure preservation in order to reproduce long time behavior.

Role of Discrete Structure-Preservation:

Discrete conservation laws impart long time numerical stability to computations, since the structure-preserving algorithm exactly conserves a discrete quantity that is always close to the continuous quantity we are interested in.

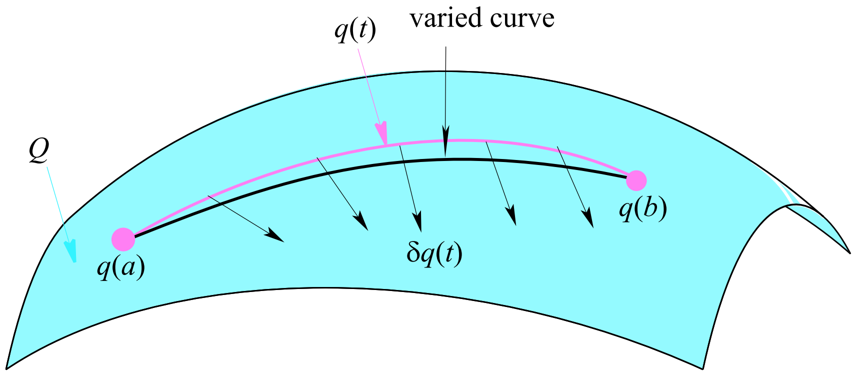
Geometric Integration: Energy Stability

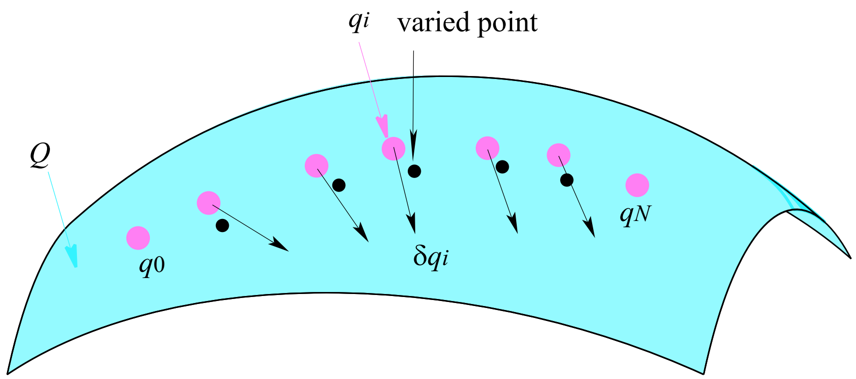
- Energy stability for symplectic integrators



Discrete Mechanics

Discrete Variational Principle





- **Discrete Lagrangian**

$$L_d \approx \int_0^h L\left(q(t), \dot{q}(t)\right) dt$$

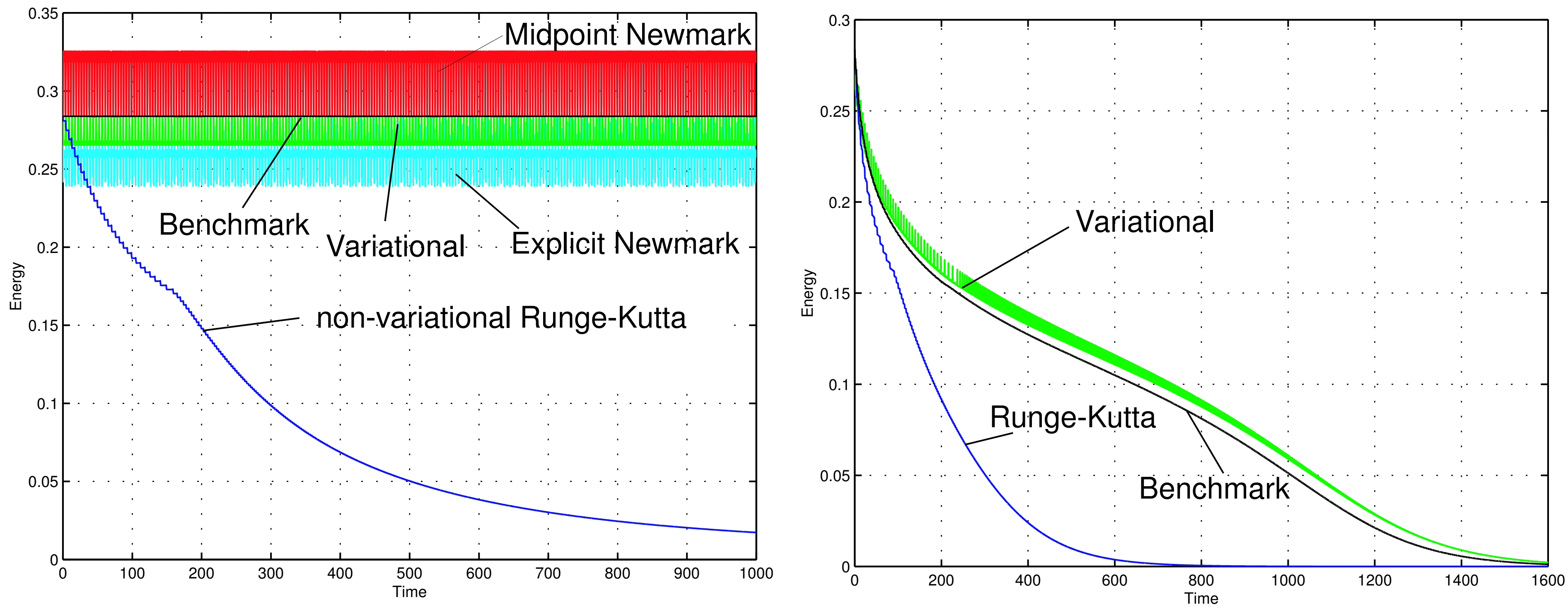
- **Discrete Euler-Lagrange equation**

$$D_2 L_d(q_0, q_1) + D_1 L_d(q_1, q_2) = 0$$

- The discrete flows are **symplectic** and **momentum** preserving.

Geometric Integration: Energy Stability

■ **Energy behavior for conservative and dissipative systems**

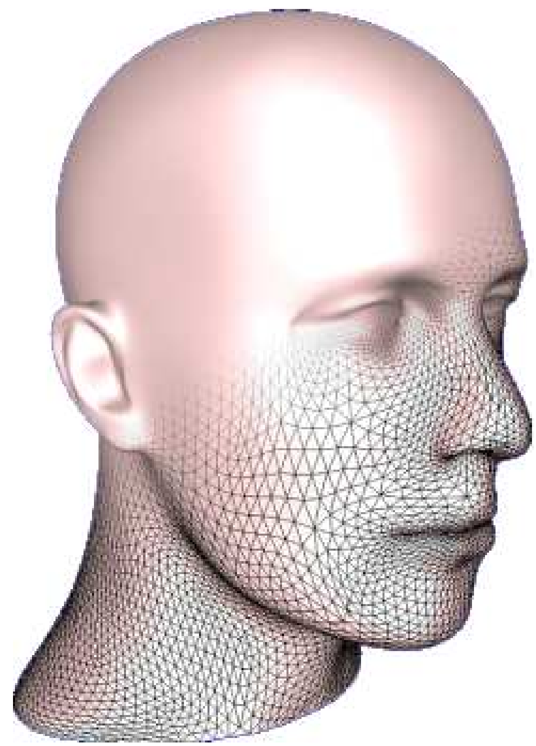


(a) Conservative mechanics (b) Dissipative mechanics

Discrete Geometry and Computer Graphics

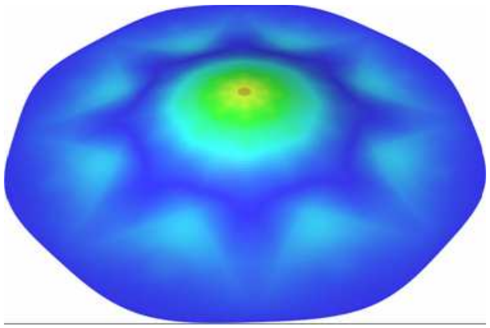
Motivation

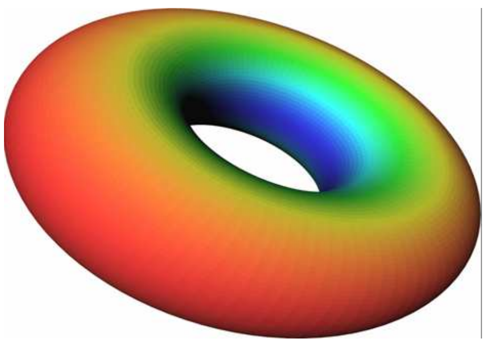
- Desire robust computation on discrete meshes.
- Many applications require differential geometric concepts:
  - PDE based Image Processing on Curved Surfaces.
  - Smoothing, simplification, and remeshing of triangulated surfaces.
- Little consensus on how to compute basic surface properties like normals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

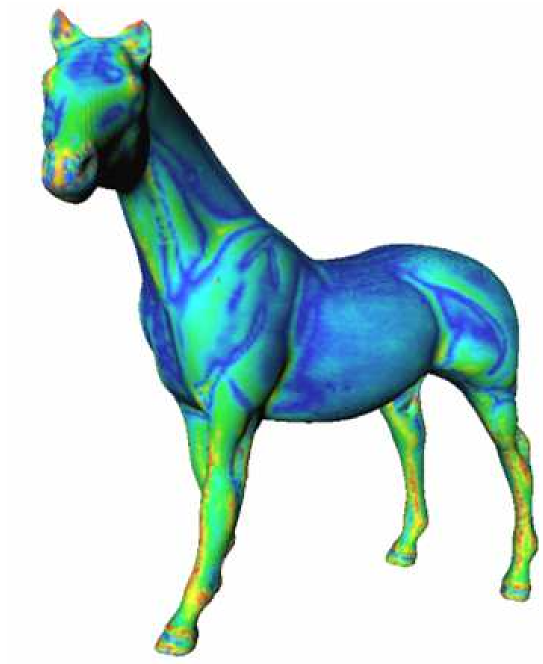


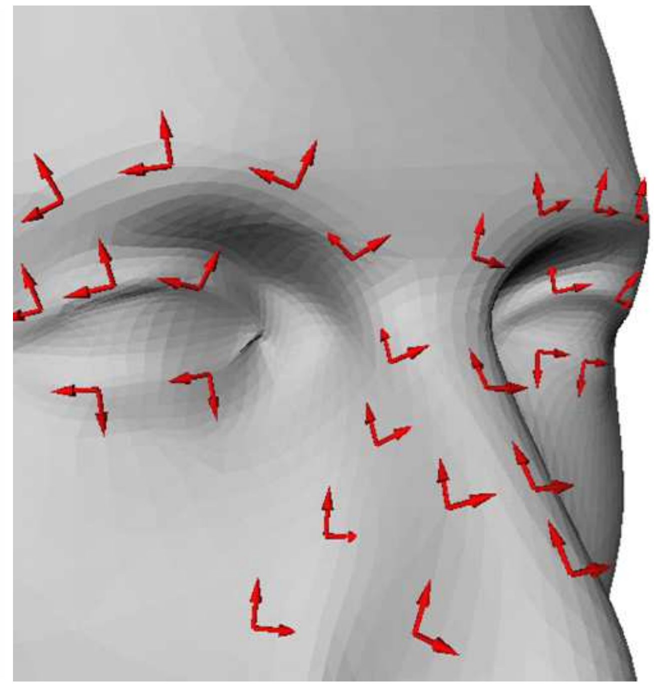
Discrete Geometry and Computer Graphics

■ Mean, Gaussian, and Principal Curvatures









Discrete Geometry and Accurate Simulation

Exact Sequences and Spectral Properties

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

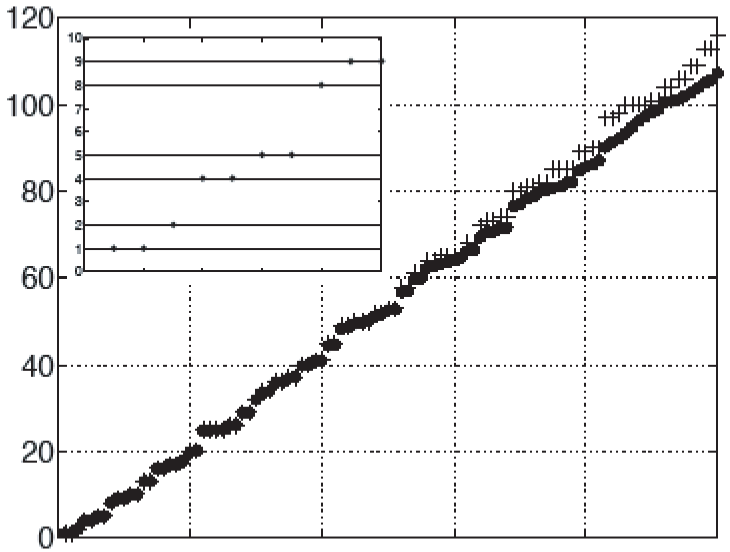
$$\mathbb{R} \hookrightarrow H^1(\Omega) \xrightarrow{\text{grad}} H^1(\text{curl}, \Omega) \xrightarrow{\text{curl}} H^1(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega, \mathbb{R}) \longrightarrow 0$$

- 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.

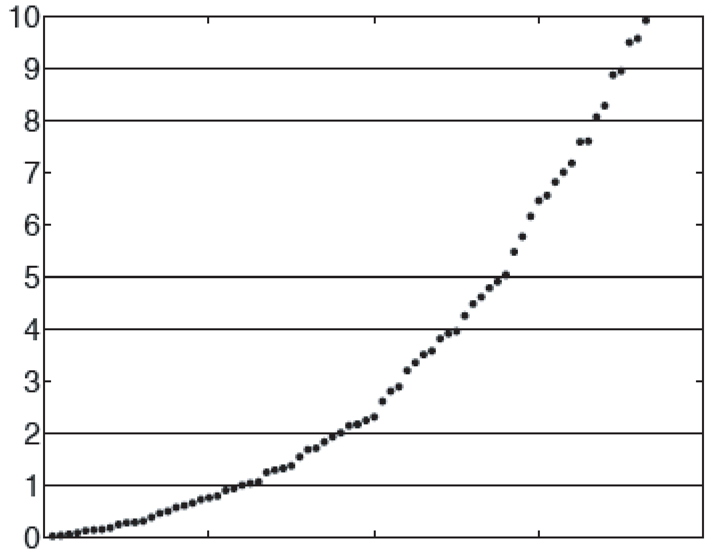
Discrete Geometry and Accurate Simulation

Exact Sequences and Spectral Properties

- Compatible discretization may be important for accurate prediction of gravitational wave modes.



Computed using edge elements (compatible discretization)



Computed using linear finite elements

Discrete Exterior Calculus

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.

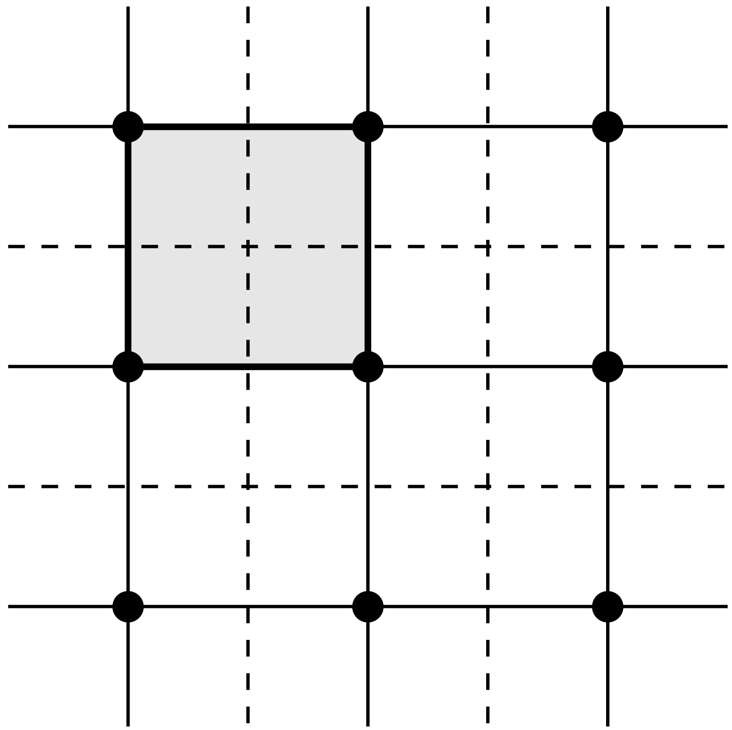
A new idea?

- 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.

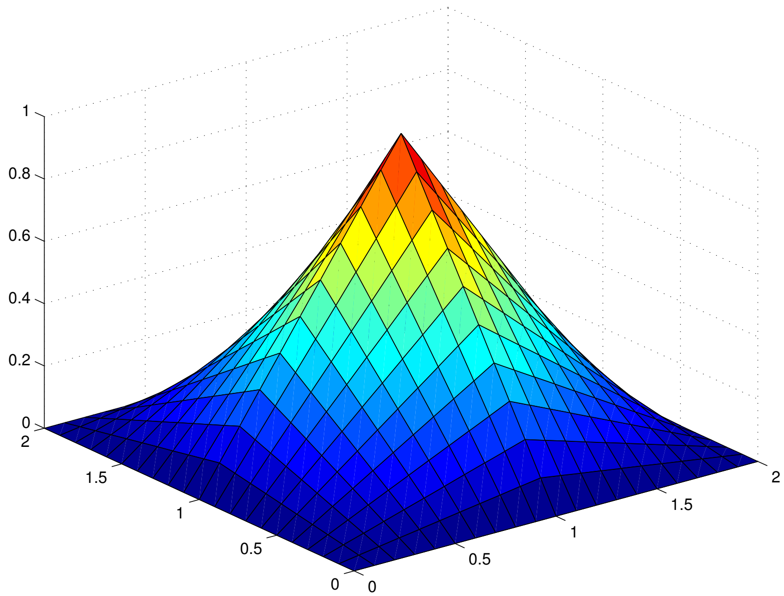


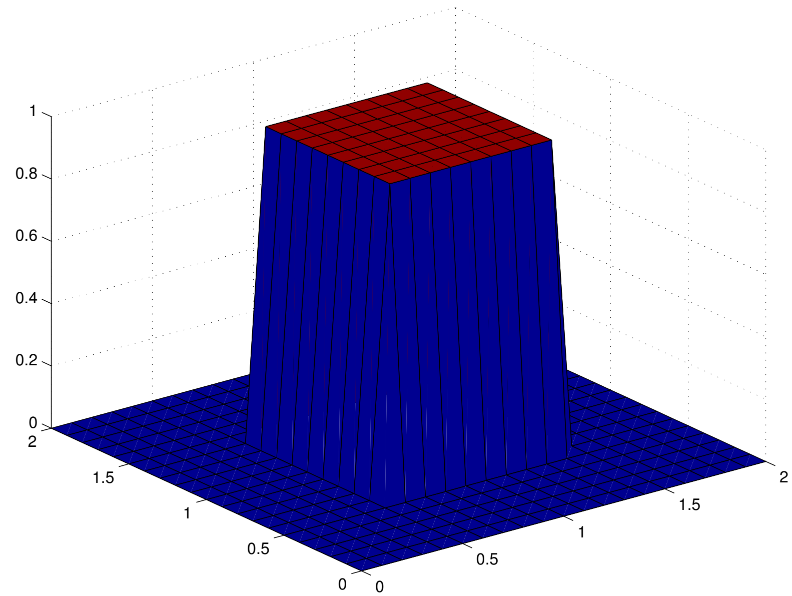
- Voronoi dual mesh obtained by associating to each point the volume that is closer to that point than any other point.

Primal and Dual Meshes in FV, FE, FD Methods

Finite Element Method

- Can arise implicitly by choice of shape functions.

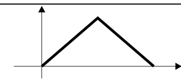
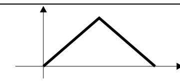
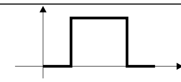
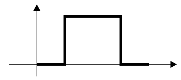
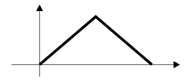
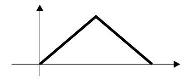
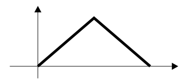
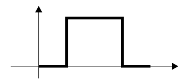
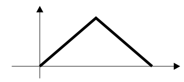
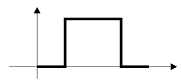
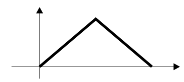
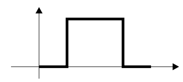
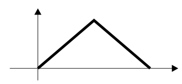
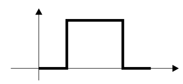
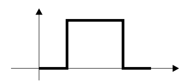
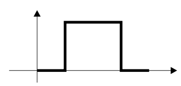
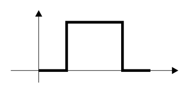
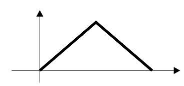




- Application to computational electromagnetism hints at underlying geometry, since the choice of shape functions for field quantities depend on duality relations between the various field variables.

Primal and Dual Meshes in FV, FE, FD Methods

Computational Electromagnetism using Finite Elements

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

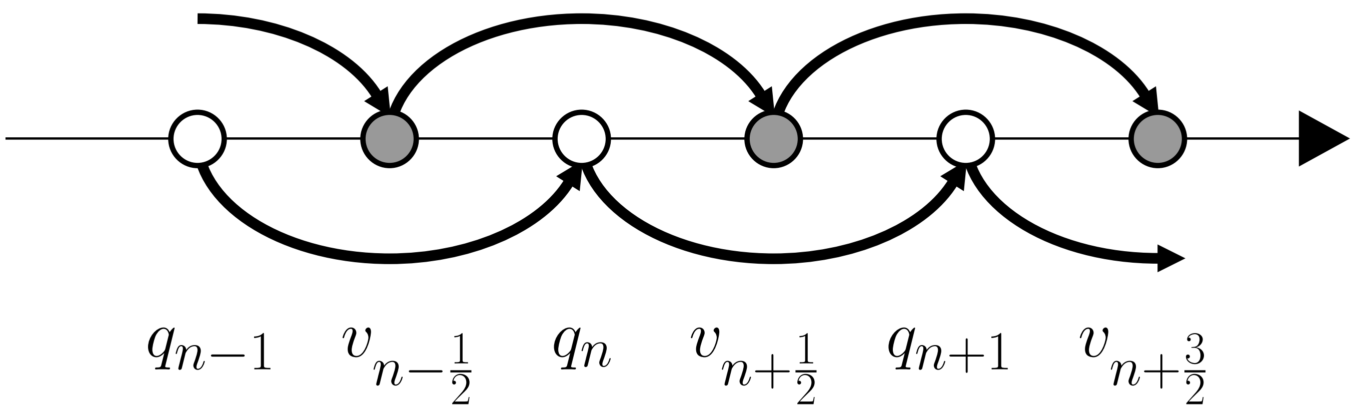
- The choice of tensor product shape functions in two dimensional Cartesian traverse magnetic (TM) model.

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.

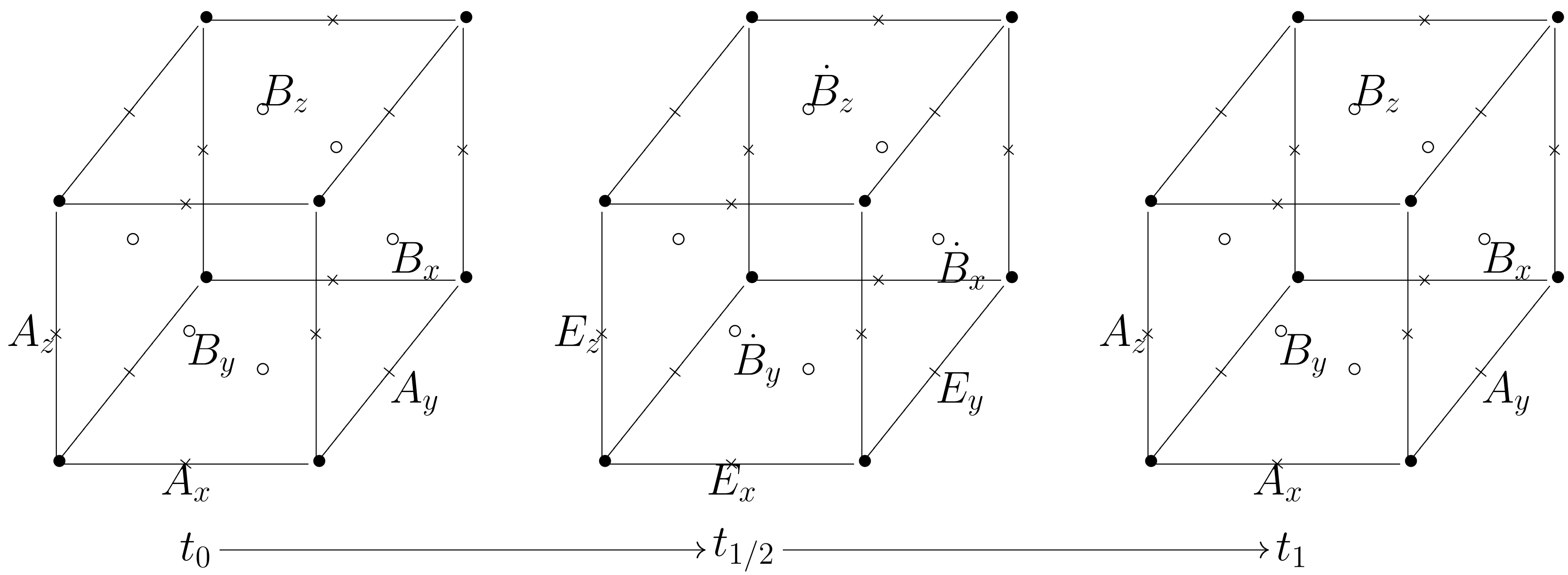
$$v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + \frac{f_n}{m}\Delta t$$
$$q_{n+1} = q_n + v_{n+\frac{1}{2}}\Delta t$$



Primal and Dual Meshes in FV, FE, FD Methods

Finite Difference Method

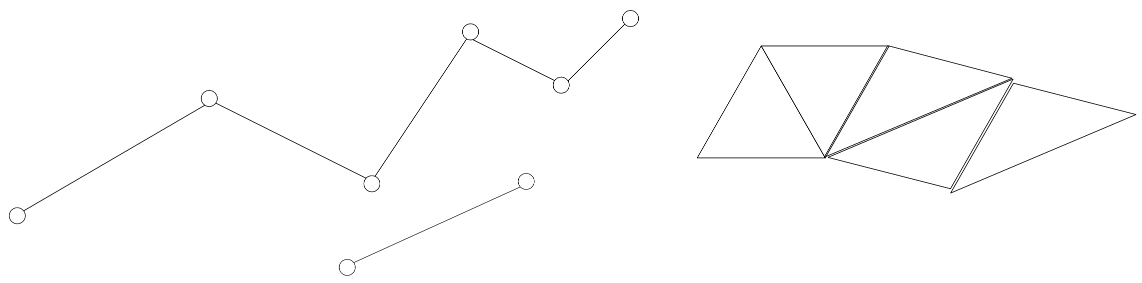
- Staggered Meshes in Space-time used in the Constrained Transport (CT) Method for Magnetohydrodynamics, implemented in ZEUS-2D.



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,



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,

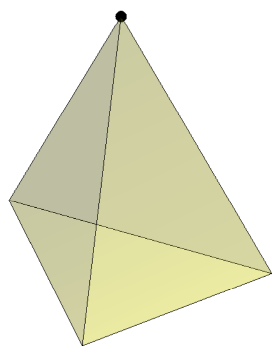
$$\star\star(\sigma^k) = (-1)^{k(n-k)}\sigma^k.$$

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

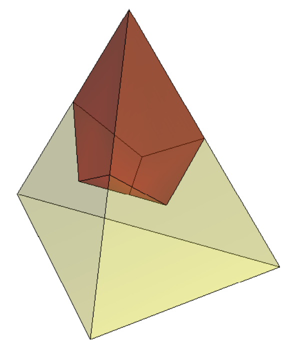
Examples of Primal Simplices and Dual Cells

- Primal Simplex
- Dual Cell

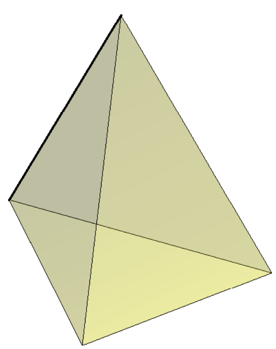
σ^0, 0-simplex



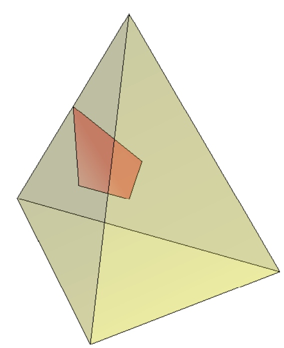
$\star\sigma^0$, 3-cell



σ^1, 1-simplex



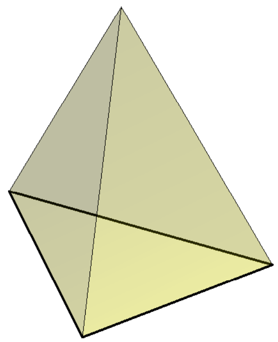
$\star\sigma^1$, 2-cell



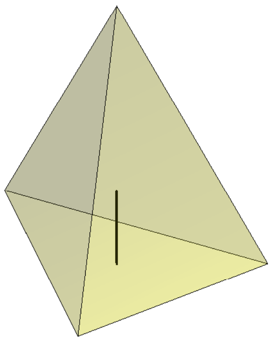
Examples of Primal Simplices and Dual Cells

- Primal Simplex
- Dual Cell

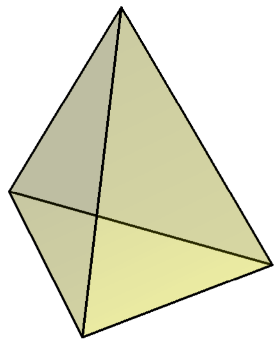
σ^2, 2-simplex



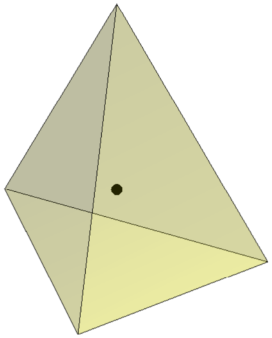
$\star\sigma^2$, 1-cell



σ^3, 3-simplex



$\star\sigma^3$, 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

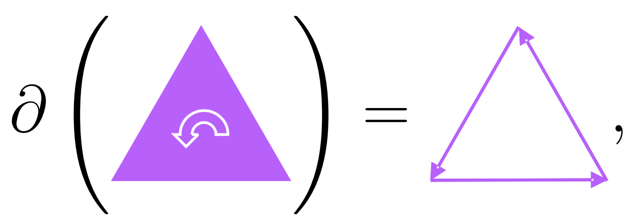
- The **Exterior Derivative** is defined by using the Generalized Stokes Theorem,

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

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



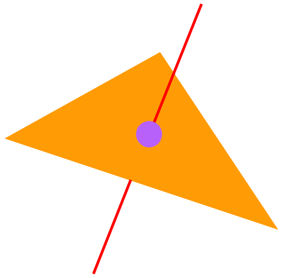
where clearly, orientation must be carefully taken into account.

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

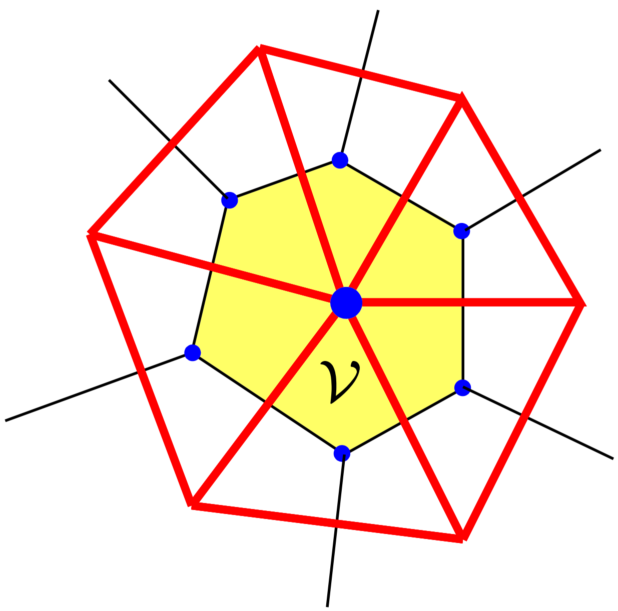
$$\delta\beta = (-1)^{nk+1} * \mathbf{d} * \beta\,.$$

Application

Laplace-Beltrami

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

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



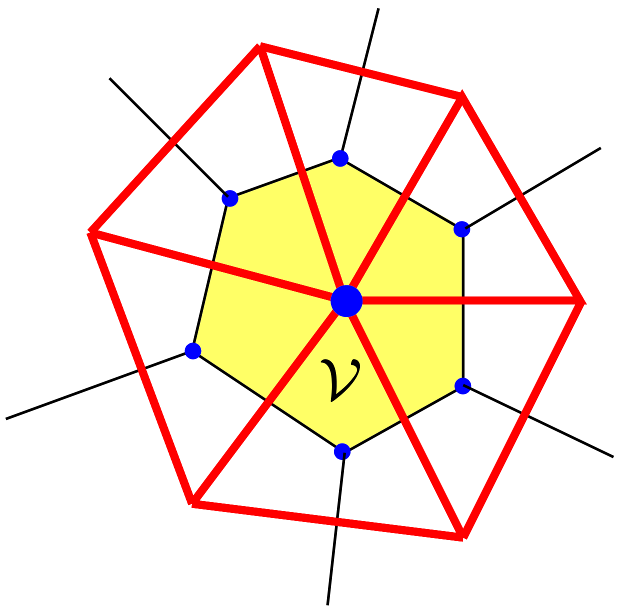
Application

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.

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,

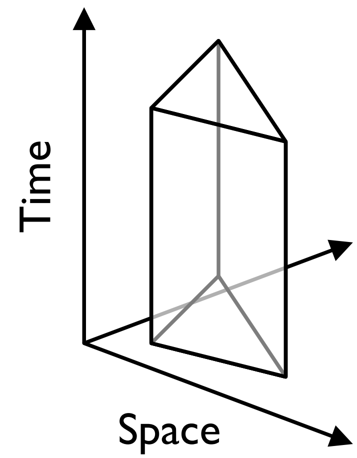
$$\sum_{\sigma^1 = [v_1, v_0] \succ v_0} \frac{2}{n} \frac{|\star \sigma^1|}{|\sigma^1|} \langle \mathbf{d} f, \sigma^1 \rangle = 0.$$

- 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.

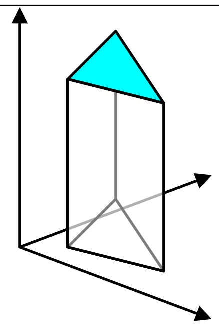
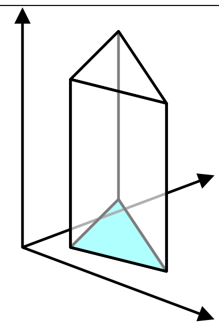
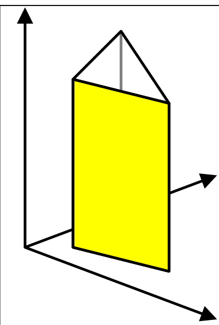
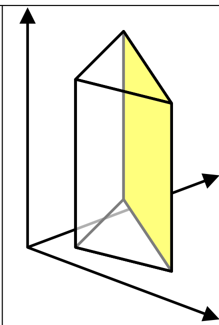
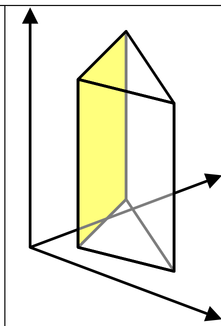
Discrete Electromagnetism

The effect of the Lorentzian metric on the Hodge Star

- The **discrete Hodge star for prismal complexes in Lorentzian space** is given by,

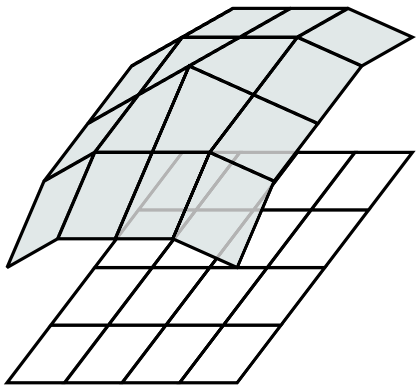
$$\frac{1}{|\star\sigma^k|}\langle *\alpha^k, \star\sigma^k\rangle = \kappa(\sigma^k)\frac{1}{|\sigma^k|}\langle \alpha^k, \sigma^k\rangle,$$

where the **causality sign** $\kappa(\sigma^k)$ is defined to be $+1$ if all the edges of σ^k are spacelike, and -1 otherwise.

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

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** $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1 q)$.
- **Hamilton's principle** $\delta\mathcal{S} = 0$.

Towards Numerical Relativity

Lagrangian Formulation of Relativity

- Introduce a **Lagrangian density** that is a 4-form on space-time, as suggested by Frank Estabrook.
- Discretize the action using **Discrete Exterior Calculus**.

Gauge Invariance and Constraints

- The invariance of the discrete Lagrangian under gauge transformations yields a discrete Noether's theorem.
- Discrete analogues of the constraint equations are automatically satisfied, thereby giving long time numerical stability.

Conclusion

Summary

- Incorporates discrete forms, vector fields, and related operators
- Construction of canonical discrete differential operators
- Applications to Laplace-Beltrami operator, Harmonic maps, and Electromagnetism
- Constraint equations are Noether quantities that arise from the gauge invariance of the Lagangian formulation of relativity.

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Slides available at,

http://www.math.lsa.umich.edu/∼mleok/ipam_dec.pdf