Mimetic Discretizations
and what they can do for you

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Supported in part by

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- Jonathan Hu
- Rich Lehoucq
- Denis Ridzal
- Allen Robinson
- John Shadid
- Chris Siefert
- Ray Tuminaro
- Max Gunzburger, Florida State
- Mac Hyman, Los Alamos
- Misha Shashkov, Los Alamos
- Pavel Solin, UTEP
- Kate Trapp, U. Richmond

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
Research Drivers

Discretization
\[ Lu = f \rightarrow Ax = b \]

model reduction, accompanied by loss of information that can be:

- ☺ Acceptable ➔ physically meaningful, accurate and stable solutions.
- ⚔ Trivial ➔ spectacular failure that is easy to detect.
- ⚔ Malicious ➔ subtle failure, imperceptible in the “eye ball” norm.

Research goals:

- Develop “compatible” discretizations to manage information loss
- Use these discretizations and their properties to
  - a) Formulate and analyze new numerical methods for PDEs
  - b) Support the development of better iterative solvers
  - c) Guide the design of better software tools for PDEs

Focus of this talk is on b) and c)
Impact

Project inception: FY03

External

- **2 short courses**: Von Karman Institute (2003), VA Tech (2005)
- **2 book chapters**
- **14 papers** in peer reviewed journals
- **15 talks** (invited and plenary)
- **14 colloquium** talks

**Originator and organizer:**
- 2007 SIAM CS/E (with M. Shashkov)
- 2007 FE Fluids (with M. Gunzburger)
- 2006 CSRI PDE workshop (with R. Lehoucq and M. Gunzburger)
- 2004 IMA Workshop on compatible discretizations (Arnold, Lehoucq, Nicolaides, Shashkov)
- 2003 SIAM CS/E (with R. Tuminaro)

Internal

- **Compatible methods for x-MHD** - with J. Shadid, L. Chacon (LANL)
- **z-pinch modeling and simulation in Alegra** - with A. Robinson
- **Device modeling and simulation in CHARON** - with J. Shadid, R. Pawlovski
- **ML solvers for Maxwell’s** - with R. Tuminaro, J. Hu, C. Siefert
Research Approach

- **Use homological ideas** to identify formal mathematical structures ("analytic home") that allow to encode a representative set of PDEs.

- **Translate analytic structures** into "compatible" discrete structures ("discrete home") that inherit their key properties.

- **Manage loss of information** by translating PDEs into compatible discrete models that live in the "discrete home".

**Overview of my talk:**

- **A compendium of failed discretizations**

- **Analytic → discrete translation**
  - Based on two fundamental operators: **Reduction and reconstruction**

- **Mimetic properties:**
  - Vector calculus and discrete cohomology

- **Payback:**
  - New infrastructure for interoperable software tools for FEM, FV, and FD discretizations
  - More efficient AMG solvers via reformulation of the discrete Maxwell’s equations
Deal or No Deal?

**Trivial failure:** Mixed Galerkin and nodal (collocated) FEM

\[ \nabla \cdot \mathbf{u} = f \text{ in } \Omega \]
\[ \nabla \phi + \mathbf{u} = 0 \text{ in } \Omega \]
\[ \phi = 0 \text{ on } \Gamma \]

**Malicious failure:** Ritz-Galerkin and nodal (collocated) FEM

\[ \sigma \mathbf{E} + \nabla \times \nabla \mu^{-1} \times \mathbf{E} = 0 \text{ in } \Omega \]
\[ \mathbf{n} \times \mathbf{E} = 0 \text{ on } \Gamma \]
Deal or No Deal?

Another malicious failure: false transient (spatially regularized nodal FE)

\[
-\Delta u + \nabla p = f \quad \text{in } \Omega \\
\nabla \cdot u = 0 \quad \text{in } \Omega \\
u = 0 \quad \text{on } \Gamma
\]

Common wisdom: \( \Delta t \to 0 \quad \Rightarrow \quad \text{more accurate results} \)

True solution is time independent!

Bochev, Gunzburger, Lehoucq, IJNMF, 2007
Why Homological Ideas?

In the examples, there was nothing wrong with the approximation properties of the FEMs or the formal consistency of the methods.

However, key relationships between differential operators and function spaces, necessary for the well-being of the PDE, were “lost in translation”.

We seek a discrete framework that mimics these relationships and provides mutually consistent notions of derivative, integral, inner product, Hodge theory, etc.

Cohomology: Describes structural relationships relevant to PDEs
Differential forms: Provide tools for abstraction of physical models leading to PDEs:

Integration: → an abstraction of the measurement process
Differentiation: → gives rise to local invariants
Poincare Lemma: → expresses local geometric relations
Stokes Theorem: → gives rise to global relations
An (incomplete) Historical Survey

In finite elements

1977 - Fix, Gunzburger and Nicolaides: GDP (a discrete Hodge decomposition) is necessary and sufficient for stable and optimally accurate mixed Galerkin discretization of the Poisson equation
⇒ first (!) example of application of homological ideas in FEMs.

1989 - Bossavit: reveals connection between Whitney forms and stable elements for mixed methods for diffusion and eddy currents

1997 - Hiptmair: uses exterior calculus to develop uniform definitions of FEM spaces

1999 - Demkowicz, Ainsworth, et al: develop hp-DeRham polynomial spaces

2002 - Arnold et al.: uses homological ideas to find stable FEMs for mixed elasticity

2003 - White et al.: FEMSTER, a software realization of polynomial differential forms

Elsewhere: Discrete vector calculus structures

1980s - Shashkov, Samarskii - Support operator method

1992 - Nicolaides - direct covolume discretization for div-curl and incompressible flows

1990s - Hyman, Scovel, Shashkov, Steinberg - Mimetic finite difference methods

1997 - Mattiussi - connection between FV and FEM

2004 - Bochev and Hyman - Algebraic topology approach: includes FV, FD and FEM
Framework for mimetic discretizations (IMA Proceedings, 2006)

- Exterior Derivative
- Metric structure
- Adjoint derivative
- Natural operations
- Discrete inner product
- Derived operations

induced by 2 basic operations

\[
\Omega \rightarrow \Lambda^k \text{ Forms} \rightarrow \{C_0, C_1, C_2, C_3\} \text{ Chains} \\
\Lambda^k \text{ d} \rightarrow \Lambda^{k+1} \\
\{C^k\} \rightarrow \{C^l\} \text{ Pullback - FEM} \\
\Lambda^k \text{ d} \rightarrow \Lambda^{k+1} \\
\{C^k\} \rightarrow \{C^{k+1}\} \text{ Direct - FVD} \\
\{C_0, C_1, C_2, C_3\} \text{ Cochains} \\
\{C^i\} \rightarrow \{C^l\} \\
\omega = \int_{\Omega} \omega \zeta, dx \\
\{C^k\} \rightarrow \{C^{k+1}\} \\
\{C_0, C_1, C_2, C_3\} \\
\Omega \rightarrow \text{Domain} \\
\{C_0, C_1, C_2, C_3\} \text{ Chains} \\
\{C^k\} \rightarrow \{C^{k+1}\} \\
\text{Reduction} \\
\text{Joint work with M. Hyman}
Discrete Operations for $R: \Lambda^k \mapsto C^k$

Natural derivative

$\delta: C^k \mapsto C^{k+1}$

$\langle \delta a, \sigma \rangle = \langle a, \partial \sigma \rangle$

Natural inner product

$(\cdot, \cdot)_k: C^k \times C^k \to \mathbb{R}$

$(a, b)_k = (Ia, Ib)_k$

Adjoint derivative

$\delta^*: C^{k+1} \mapsto C^k$

$\langle \delta^* a, b \rangle_k = \langle a, \delta b \rangle_{k+1}$

Provides a second set of $\text{grad}$, $\text{div}$ and $\text{curl}$ operators.

Derivative choice depends on encoding:

- **Scalars** $\mapsto 0$ or $3$-forms
- **Vectors** $\mapsto 1$ or $2$-forms.

Discrete Laplacian

$D: C^k \mapsto C^k$

$D = \delta^* \delta + \delta \delta^*$

Natural wedge product

$\wedge: C^k \times C^l \mapsto C^{k+l}$

$a \wedge b = R (Ia \wedge Ib)$

**Flat** and **sharp** can be defined using the inner product

Derived operations help to avoid **internal inconsistencies** between the discrete operations:

- $I$ is only **approximate inverse** of $R$ and natural definitions will clash.
Discrete Vector Calculus

**Poincare lemma** (existence of potentials in contractible domains)

\[ d\omega_k = 0 \quad \Rightarrow \quad \omega_k = d\omega_{k+1} \quad \Rightarrow \quad \delta c^k = 0 \quad \Rightarrow \quad c^k = \delta c^{k+1} \]

**Stokes Theorem**

\[ \langle d\omega_{k-1}, c_k \rangle = \langle \omega_{k-1}, \delta c_k \rangle \quad \Rightarrow \quad \langle \delta c^{k-1}, c_k \rangle = \langle c^{k-1}, \delta c_k \rangle \]

**Vector Calculus**

\[ dd = 0 \quad \Rightarrow \quad \delta\delta = \delta^* \delta^* = 0 \]

\[ \omega \wedge \eta = (-1)^{kl} \eta \wedge \omega \quad \Rightarrow \quad a \wedge b = (-1)^{kl} b \wedge a \]

\[ d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^k \omega \wedge d\eta \quad \Rightarrow \quad \delta(a \wedge b) = \delta a \wedge b + (-1)^k a \wedge \delta b \]

**Mimetic** = Key properties of the analytic structures inherited by the discrete structures. First used by Hyman and Scovel (1988)
Discrete Cohomology

\( R \) is a chain map: preserves co-boundaries and co-cycles

\[
d\omega = 0 \quad \Rightarrow \quad \delta R \omega = 0
\]

Co-cycles of \((\Lambda^0, \Lambda^1, \Lambda^2, \Lambda^3)\) \(\xrightarrow{R}\) co-cycles of \((C^0, C^1, C^2, C^3)\)

Natural inner product induces combinatorial Hodge theory on cochains:

**Discrete Harmonic forms**

\[
H^k(\Omega) = \{\eta \in \Lambda^k(\Omega) | d\eta = d^*\eta = 0\} \quad \xrightarrow{\quad} \quad H^k(K) = \{c^k \in C^k | \delta c^k = \delta^* c^k = 0\}
\]

**Discrete Hodge decomposition**

\[
\omega = d\rho + \eta + d^*\sigma \quad \xrightarrow{\quad} \quad a = \delta b + h + \delta^* c
\]

**Theorem** *(IMA Proc., 2006)*

\( \text{dimker}(\Delta) = \text{dimker}(D) \)

Remarkable property of the mimetic \( D \) - kernel size is a **topological invariant**!
\[
\omega = df + h + d^* g
\]

\[
\Lambda^k(\Omega) = \text{Range}(d_{k-1}) \oplus H^k \oplus \text{Range}(d_{k+1})
\]

\[
H^k = \{\omega \in \Lambda^k | d\omega = d^*\omega = 0\}
\]

\[
\ker(\Delta_k) = H^k
\]

\[
H^k = \ker(d_k)/\text{Range}(d_{k-1})
\]

\[
d : \Lambda^k(\Omega) \rightarrow \Lambda^{k+1}(\Omega)
\]

exterior derivative

\[
\langle \cdot, \cdot \rangle_k : \Lambda^k(\Omega) \times \Lambda^k(\Omega) \rightarrow \mathbb{R}
\]

inner product

\[
\int : \Lambda^k(\Omega) \rightarrow \mathbb{R}
\]

integral

\[
\wedge : \Lambda^k(\Omega) \times \Lambda^l(\Omega) \rightarrow \Lambda^{k+l}(\Omega)
\]

wedge product

\[
\Delta : \Lambda^k(\Omega) \rightarrow \Lambda^k(\Omega)
\]

Hodge Laplacian

\[
\Lambda^k(\Omega) : x \rightarrow \omega(x) \in \text{Alt}^k(T_x\Omega)
\]

Smooth differential forms
The Tenants

“Laplacians”

\[
\min_{\Lambda^k} \frac{1}{2} \left( \|du\|^2 + \|d^* u\|^2 \right) - (f, u) \rightarrow \quad d^* du + dd^* u = f \rightarrow \quad \left\{ \begin{array}{l}
-\Delta u = f \\
\n\end{array} \right.
\]

“Incomplete Laplacians”

\[
\min_{\Lambda^k} \frac{1}{2} \left( \|u\|^2 + \|du\|^2 \right) - (f, u) \rightarrow \quad \left\{ \begin{array}{l}
 dd^* u + u = f \\
 d^* du + u = f \\
\n\end{array} \right. \rightarrow \quad \left\{ \begin{array}{l}
-\Delta u + u = f \\
\n\end{array} \right.
\]

“Div-curl systems”

\[
\min_{\Lambda^k} \frac{1}{2} \left( \|du\|^2 + \|d^* u\|^2 \right) - (f, u) \rightarrow \quad \left\{ \begin{array}{l}
 du + d^* p = f \\
 d^* u = 0 \\
 d^* u + dp = f \\
 du = 0 \\
\n\end{array} \right. \rightarrow \quad \left\{ \begin{array}{l}
\n\end{array} \right.
\]

Div of a vector field

\[
d^* (u) = (\ast d^*) (u) \rightarrow \quad \nabla \cdot u
\]
Placing a PDE in the Discrete Home

**Analytic problem**
\[ \tilde{\mathbf{E}} + \sigma^{-1} \nabla \times \mu^{-1} \nabla \times \mathbf{E} = 0 \]

**Form translation**
\[ d_i e^1 + \delta^* \delta e^1 = 0 \]

**Discrete problem**
\[ M_i e^1 + D_i^* D_i e^1 = f \]

**Theorem** (*IMA Proc.*, 2006)

Let \( R : \Lambda^k \rightarrow C^k \). **Direct** and **pullback** reconstructions yield equivalent methods.

\[ \Rightarrow \text{There’s only “one” low-order compatible method} \]
This prompts a fresh look at software design for compatible discretizations:

- Different methods are defined by choosing a specific reconstruction operator \( I \):
  - **Direct:** \( I \) is **low order** but more easily extendable to arbitrary cells
  - **Pullback:** \( I \) is **high order** but not easy to extend beyond standard cells

- There’s no fundamental reason not to have simultaneous access to both…
**Intrepid**

**INteroperable Tools for Rapid dEveloPment of compatIble Discretizations**

- **Global_kForm**
- **ChainComplex** (MOAB/TSTT)
- **MultiCell**
- **Local_kForm**
- **DiscreteOperator** (Epetra/Trilinos)
- **LocalOperator**
  - **Order**
  - **Flavor**
  - **Type** (FEM ↔ FVD)

Joint work with D. Ridzal, D. Day
Anticipated Applications

CHARON - X-MHD

**Intrepid** will enable side by side comparisons of FV and mimetic div free methods and FEM using vector potential and B-projection, and discretization tools for extended MHD modeling and simulation (Shadid, Banks, Chacon).

CHARON - DEVICE

**Intrepid** will be used to test compatible discretizations for device modeling, prototype optimization and control problems, and as a discretization library (Pawlovski, Shadid, Bartlet).

ALEGRA

**Intrepid** will provide discretization tools for multimaterial ALE modeling and simulation on general polyhedral cells (Robinson, Shashkov, Lipnikov).

Org.1641 (HEDP Theory)

**Intrepid** will provide discretization tools for Sandia’s Pulsed Power modeling and simulation effort (Hanshaw, Brunner, Robinson)

External:

- LANL Theoretical Division T-7 (Shashkov)
- Center for computation & technology, Louisiana State University
- HERMES project, UT El Paso (Solin)
Reformulation of Maxwell’s equations

Recall the mimetic discretization of the primal equation

\[ \sigma \dot{E} + \nabla \times \mu^{-1} \nabla \times E = 0 \]

PDE

\[ \sigma e + d^* de = f \]

Forms

\[ M_1 e^1 + D_1^* D_1 e^1 = f \]

Matrix equation

Relevant operators acting on 1-cochains:

\[ D_1^* D_1 = D_1^T M_2 D_1 \]

A curl-curl operator

\[ D_0 D_0^* = M_1 D_0 M_0^{-1} D_0^T M_1 \]

A grad-div operator

\[ D_1^* D_1 \begin{cases} D_1^T M_2 D_1 \\ + \\ D_0^* D_0 \end{cases} = \begin{cases} D_1^T M_2 D_1 \\ + \\ M_1 D_0 M_0^{-1} D_0^T M_1 \end{cases} \]

A Hodge Laplacian

\[ e^1 = D_0 p^0 + D_1^* b^2 \]

A Hodge decomposition
Why Reformulate?

ML methods work well for Laplacians $\Rightarrow$ make curl-curl more “Laplace”-like

- **Reformulate and then discretize**: first add grad div and then discretize
  - Misconception: reformulation allows to use collocated methods, e.g., nodal FE
  - Major issue: scaling of the Laplacian when $\sigma$ varies orders of magnitude

\[
\nabla \times \mu^{-1} \nabla \times - \sigma \nabla \nabla \cdot \sigma \approx C_h + G_h
\]

- **Discretize and then reformulate**: our approach - add discrete grad div
  - Key idea: use different inner product for the Hodge decomposition of 1-cochains

\[
e^1 = D_0 P^0 + \tilde{D}_1^* b^2 = D_0 P^0 + \tilde{M}_1^{-1} D_1^T M_2 b^2
\]

\[
D_1^T M_2 D_1 + \tilde{M}_1 D_0 M_0^{-1} D_0^T \tilde{M}_1 \approx \nabla \times \mu^{-1} \nabla \times - \nabla \gamma^{-1} \nabla.
\]

- **Issue**: does this “mismatched” Laplacian have the same null-space as the true one?
Why not Reformulate and Then Discretize?

Assume a general unstructured grid without a topologically dual

Reformulated problem

$\left( \nabla \times \mathbf{E}, \nabla \times \hat{\mathbf{E}} \right)_{\mu^{-1}} + \left( \nabla \cdot \sigma \mathbf{E}, \nabla \cdot \sigma \mathbf{E} \right)_{\gamma^{-1}} = 0 \quad \forall \hat{\mathbf{E}} \in H(\Omega, \text{div}) \cap H(\Omega, \text{curl})$

Conforming discretization

\[
\begin{align*}
V_h \subset H(\Omega, \text{curl}) & \Rightarrow [E_h \times n] = 0 \\
H(\Omega, \text{div}) \cap H(\Omega, \text{curl}) & \supset V_h \\
V_h \subset H(\Omega, \text{div}) & \Rightarrow [E_h \cdot n] = 0 \\
\end{align*}
\]

The problem: in 3D $H^1$ can have infinite co-dimension in $H(\text{div}) \cap H(\text{curl})$

Reformulate and discretize approaches that work need additional structure:

- **Single mesh**: Manteuffel et. al. - using potentials for $E, J, B, H$ (potentials are more regular)
- **Primal-dual**: Haber et al. - using Yee scheme (curl on primal, div on dual)
**Theorem**

Assume that $e^1$ solves the discrete Maxwell’s equation and let $e^1 = D_0p^0 + \tilde{D}_1^* b^2$. The pair $(a^1, p^0)$, where $a^1 = \tilde{D}_1^* b^2$, solves the reformulated Maxwell’s equation

$$
\begin{bmatrix}
M_1 + D_1^T M_2 D_1 + \tilde{M}_1 D_0 M_0^{-1} D_0^T \tilde{M}_1 & M_1 D_0 \\
D_0^T M_1 & D_0^T M_1 D_0
\end{bmatrix}
\begin{bmatrix}
a^1 \\
p^0
\end{bmatrix}
= \begin{bmatrix}
f \\
g
\end{bmatrix}
$$

**Theorem**

Kernels of the mismatched and standard Laplacian have the same dimension

$$\dim \ker (D_1^T M_2 D_1 + \tilde{M}_1 D_0 M_0^{-1} D_0^T \tilde{M}_1) = \dim \ker (D_1^T M_2 D_1 + M_1 D_0 M_0^{-1} D_0^T M_1) = 0$$

Proof uses that mimetic spaces *inherit the cohomology* of the analytic spaces and so: $\dim \ker (\Delta) = \dim \ker (D)$ for contractible domains.

**Exercise:** try proving this directly using only linear algebra!

**Related approaches:**

- Hiptmair, Xu, Kolev, Vassilevski: *auxiliary space preconditioners* use the so-called *regular decomposition* of $H(\text{curl})$ instead of the Hodge decomposition;
- Bossavit: same edge inner product, uses lumped mass over dual volumes.
Solver Performance

Because the blocks of the reformulated system are the edge Laplacian and node Laplacian, we can apply a standard AMG for the Laplace eq. to solve the problem (after applying edge to node interpolant to 1-1 block).

A-slot regression test problem: ALEGRA (C. Siefert)

- mesh refinement 1, 4, 8 times
- conductivity: $\sigma = 1$ (void); $\sigma = 6 \times 10^6$ (material)

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<th>ML-edge elements</th>
<th>Reformulated</th>
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- ML = specialized, highly tuned AMG for edge elements (Trilinos)
- Reformulated = off the shelf AMG for Poisson equation, few tricks!
Solver Performance

**σ sensitivity:**

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**μ sensitivity:**

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**ML trivia**

The new solver has been run in parallel to ~2000 processors with about a 65% (weak scaling) efficiency on a model problem.

**Under the hood**

- The edge Laplacian has the right null-space but lives on the edges - needs to be transferred to a nodal Laplacian before we apply OTS AMG.

- **Trick 1:** piecewise edge constants on first fine level only (theory “says” that’s OK) are used to define a cheap grid transfer to nodes to avoid complexity.

- **Trick 2:** the fine grid smoother ignores the discrete gauge term! Hence we never need to form it explicitly, effectively it gauges the coarse grid operator.
Conclusions

- **Compatible** discretizations inherit key structural properties of analytic spaces & operators
  - discrete models are physical ⇒ have intrinsic control over information loss

- We presented a framework for compatible discretizations where:
  - All operations are defined by **two mappings**: reduction \( R \) and reconstruction \( I \)
  - The central concept is the natural inner product

- The framework has two basic operation types
  - **Natural** derivative, inner product, wedge product,…
  - **Derived** adjoint derivative, Hodge Laplacian,…

- The framework has important mimetic properties:
  - discrete vector calculus
  - combinatorial Hodge theory

- The framework helped us to
  - Recognize that differences between FV, FD and FE are largely **superficial**
  - Derive a powerful **abstraction of the discretization process** and use it to develop new software design for interoperable discretization tools
  - Reformulate the discrete Maxwell’s equations so as to make them better suited for ML solvers