Mimetic Discretizations and what they can do for you

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- David Day
- 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



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- ☺ Acceptable physically meaningful, accurate and stable solutions.
 - **spectacular failure** that is easy to detect.
 - **Malicious** subtle failure, imperceptible in the "eye ball" norm.

Research goals:

Trivial

×

- 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
 - Guide the design of better software tools for PDEs C)

Focus of this talk is on b) and c)



Impact

External

- □ 2 short courses: Von Karman Institute (2003), VA Tech (2005)
- 1 book: Proceedings IMA workshop, Springer IMA series 142. (Arnold, Bochev,Lehoucq, Nicolaides, Shashkov, eds.)
- **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



Project inception: FY03

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
- $\label{eq:analytic} \square \ \ \text{Analytic} \rightarrow \text{discrete translation}$
 - 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



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Deal or No Deal?

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 $\nabla \cdot \mathbf{u} = 0$ in Ω

 $-\Delta \mathbf{u} + \nabla p = \mathbf{f}$ in Ω

 $\mathbf{u} = 0$ on Γ

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



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Common wisdom:



 $\rightarrow 0 \Rightarrow$ 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 PDEsDifferential forms:Provide tools for abstraction of physical models leading to PDEs:

- **Integration:** \rightarrow an abstraction of the *measurement* process
- **Differentiation:** \rightarrow gives rise to *local invariants*
- **Poincare Lemma:** \rightarrow expresses *local geometric* relations
- **Stokes Theorem:** \rightarrow 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



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Joint work with M. Hyman

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Analytic -> Discrete

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



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Discrete Operations for $R: \Lambda^k \rightarrow C^k$

Natural derivative	$\delta\!:\!C^k\mapsto C^{k+1}$	$\langle \delta a, \sigma \rangle = \langle a, \partial \sigma \rangle$
Natural inner product	$(\cdot,\cdot)_k: C^k \times C^k \to \mathbf{R}$	$(a,b)_k = (Ia,Ib)_k$
Adjoint derivative	$\delta^*: C^{k+1} \mapsto C^k$	$\left(\delta^*a,b\right)_k = \left(a,\delta b\right)_{k+1}$

Provides a second set of grad, div and curl operators.

Derivative choice depends on encoding: **scalars** \rightarrow 0 or 3-forms **vectors** \rightarrow 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. p://www.cs.sandia.gov/~pbboche/

Discrete Vector Calculus

Poincare lemma (existence of potentials in contractible domains)

 $d\omega_{k} = 0 \implies \omega_{k} = d\omega_{k+1} \qquad \qquad \delta c^{k} = 0 \implies c^{k} = \delta c^{k+1}$ Stokes Theorem $\langle d\omega_{k-1}, c_{k} \rangle = \langle \omega_{k-1}, \partial c_{k} \rangle \qquad \qquad \langle \delta c^{k-1}, c_{k} \rangle = \langle c^{k-1}, \partial c_{k} \rangle$

Vector Calculus

 $\omega \wedge \eta = (-1)^{kl} \eta \wedge \omega$

dd = 0

 $d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^k \omega \wedge d\eta$

 $\delta\delta = \delta^* \,\delta^* = 0$ $a \wedge b = (-1)^{kl} b \wedge a$ $\delta(a \wedge b) = \delta a \wedge b + (-1)^k a \wedge \delta b$

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

$$d\omega = 0 \implies \delta R \ \omega = 0$$

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

Discrete Hodge decomposition

Theorem (IMA Proc., 2006)

 $\dim \ker(\Delta) = \dim \ker(D)$

Remarkable property of the mimetic D - kernel size is a topological invariant!



w.cs.sandia.qov/~pbboche/ The Tenants "Laplacians" $\begin{cases} -\Delta u = f \\ \nabla \times \nabla \times u - \nabla \nabla \cdot u = f \end{cases}$ "Incomplete Laplacians" "Div-curl systems" $du + d^*p = f$ $d^*u=0$ $\min_{A^{k}} \frac{1}{2} \left(\left\| du \right\|^{2} + \left\| d^{*}u \right\|^{2} \right) - (f, u)$ $\begin{cases} \nabla \times u + \nabla p = f \\ \nabla \cdot u = f \end{cases}$ $d^*u + dp = f$ subject to du = 0 or $d^*u = 0$ du = 0 $d^*(\overline{u}) = (\star d \star)(\overline{u})$ Div of a vector field $\nabla \cdot u$ National

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Placing a PDE in the Discrete Home



Theorem (IMA Proc., 2006)

Let $R : \Lambda^k \to C^k$. Direct and pullback reconstructions yield equivalent methods.

 \Rightarrow There's only "one" low-order compatible method





Abstraction for OO Software Design

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This prompts a fresh look at software design for compatible discretizations:

 \Rightarrow Different **methods** are defined by choosing a specific **reconstruction** operator *I*:

- Direct:/ is low order but more easily extendable to arbitrary cellsPullback:/ is high order but not easy to extend beyond standard cells
- ⇒ There's no fundamental reason not to have simultaneous access to both...





Joint work with D. Ridzal, D. Day

INteroperable Tools for Rapid dEveloPment of compatI ble Discretizations



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)



Joint work with R. Tuminaro, J. Hu, C. Siefert

Reformulation of Maxwell's equations

Recall the mimetic discretization of the primal equation



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 σ varies orders of magnitude

$$\nabla \times \mu^{-1} \nabla \times - \sigma \nabla \nabla \cdot \sigma \approx \mathbf{C}_h + \mathbf{G}_h$$

curl curl completely dominates grad div when $\sigma \approx 0$

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

$$-e^{1} = \mathbf{D}_{0}p^{0} + \tilde{\mathbf{D}}_{1}^{*}b^{2} = \mathbf{D}_{0}p^{0} + \tilde{\mathbf{M}}_{1}^{-1}\mathbf{D}_{1}^{T}\mathbf{M}_{2}b^{2}$$

$$\mathbf{\tilde{M}}_{1} \text{ is scaled by 1!}$$

$$\mathbf{M}_{0} \text{ is scaled by } \gamma = \mu$$

$$\mathbf{M}_{0} \text{ is scaled by } \gamma = \mu$$

□ **Issue:** does this "mismatched" Laplacian have the same null-space as the true one?

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Why not Reformulate and Then Discretize?

Assume a general unstructured grid without a topologically dual

Reformulated problem

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

Conforming discretization



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

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

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Assume that e^1 solves the discrete Maxwell's equation and let $e^1 = \mathbf{D}_0 p^0 + \tilde{\mathbf{D}}_1^* b^2$. The pair (a^1, p^0) , where $a^1 = \tilde{\mathbf{D}}_1^* b^2$, solves the *reformulated* Maxwell's equation

$$\mathbf{M}_{1} + \mathbf{D}_{1}^{T}\mathbf{M}_{2}\mathbf{D}_{1} + \tilde{\mathbf{M}}_{1}\mathbf{D}_{0}\mathbf{M}_{0}^{-1}\mathbf{D}_{0}^{T}\tilde{\mathbf{M}}_{1} \qquad \mathbf{M}_{1}\mathbf{D}_{0} \qquad a^{1} \\ \mathbf{D}_{0}^{T}\mathbf{M}_{1} \qquad \mathbf{D}_{0}^{T}\mathbf{M}_{1}\mathbf{D}_{0} \qquad p^{0} \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

Theorem

Kernels of the mismatched and standard Laplacian have the same dimension

dimker
$$\left(\mathbf{D}_{1}^{T}\mathbf{M}_{2}\mathbf{D}_{1}+\tilde{\mathbf{M}}_{1}\mathbf{D}_{0}\mathbf{M}_{0}^{-1}\mathbf{D}_{0}^{T}\tilde{\mathbf{M}}_{1}\right) = \operatorname{dimker}\left(\mathbf{D}_{1}^{T}\mathbf{M}_{2}\mathbf{D}_{1}+\mathbf{M}_{1}\mathbf{D}_{0}\mathbf{M}_{0}^{-1}\mathbf{D}_{0}^{T}\mathbf{M}_{1}\right) = 0$$

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

Exercise: try proving this directly using only linear algebra!

Related approaches:

- Hiptmair, Xu, Kolev, Vassilevski: auxiliary space preconditioners use the socalled regular decomposition of H(curl) instead of the Hodge decomposition;
- ⇒ Bossavit: same edge inner product, uses lumped mass over dual volumes



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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).

QuickTime[™] and a TIFF (LZW) decompressor are needed to see this picture.

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

- mesh refinement 1,4,8 times
- → conductivity: σ =1 (void); σ =6*10⁶ (material))

METH	ML-edge	e elements	Reformulated			
DOF	2 Cheb.	3 Cheb.	2 Cheb.	3 Cheb.		
2,300	28	18	21(15%)	17(6%)		
140,528	43	35	33(28%)	26(28%)		
1,123,696	66	53	54(12%)	41(23%)		

QuickTime[™] and a TIFF (LZW) decompressor are needed to see this pictur

➡ ML = specialized, highly tuned AMG for edge elements (Trilinos)

Reformulated = off the shelf AMG for Poisson equation, few tricks!



Solver Performance

 σ sensitivity:

 μ sensitivity:

				σ_2								μ_2			
Grid	cmplx	100	10^{-2}	10^{-4}	10^{-6}	10^{-8}	Grid	cmplx	100	10^{-1}	10^{-2}	10^{-3}	101	10^{2}	10^{3}
9^{2}	1.07	7	7	7	7	7	9^{2}	1.07	7	7	7	7	7	8	9
27^{2}	1.20	12	12	12	12	12	27^{2}	1.34	12	12	13	12	12	13	13
81 ²	1.25	15	16	16	16	16	81^{2}	1.24	15	18	19	20	19	21	21
243^{2}	1.27	17	18	18	18	18	243^{2}	1.27	17	22	25	26	24	29	31

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 \Rightarrow 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 /
- 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

