Application of algebraic topology to compatible spatial discretizations

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Motivation

Consistency and approximation are insufficient to avoid unphysical modes

Hyperbolic PDEs (conservation laws)

Failure to maintain conservation lead to **wrong** shock **locations** and **speeds.**

MHD

Failure to maintain div-free leads to significant errors for small velocity due to unphysical component in the Lorenz force *Brackbill, Barnes; JCP 35, 1980*

$$\mathbf{F} = \nabla \cdot \underbrace{\left(-\frac{1}{2}(\mathbf{B}\cdot\mathbf{B})\mathbf{I} + \mathbf{B}\mathbf{B} \right)}_{\text{Maxwell stress tensor}} \qquad \nabla \cdot \mathbf{B} \neq 0 \quad \Rightarrow \quad \mathbf{F}\cdot\mathbf{B} = (\mathbf{B}\cdot\mathbf{B})\nabla\cdot\mathbf{B} \neq 0$$

force parallel to B

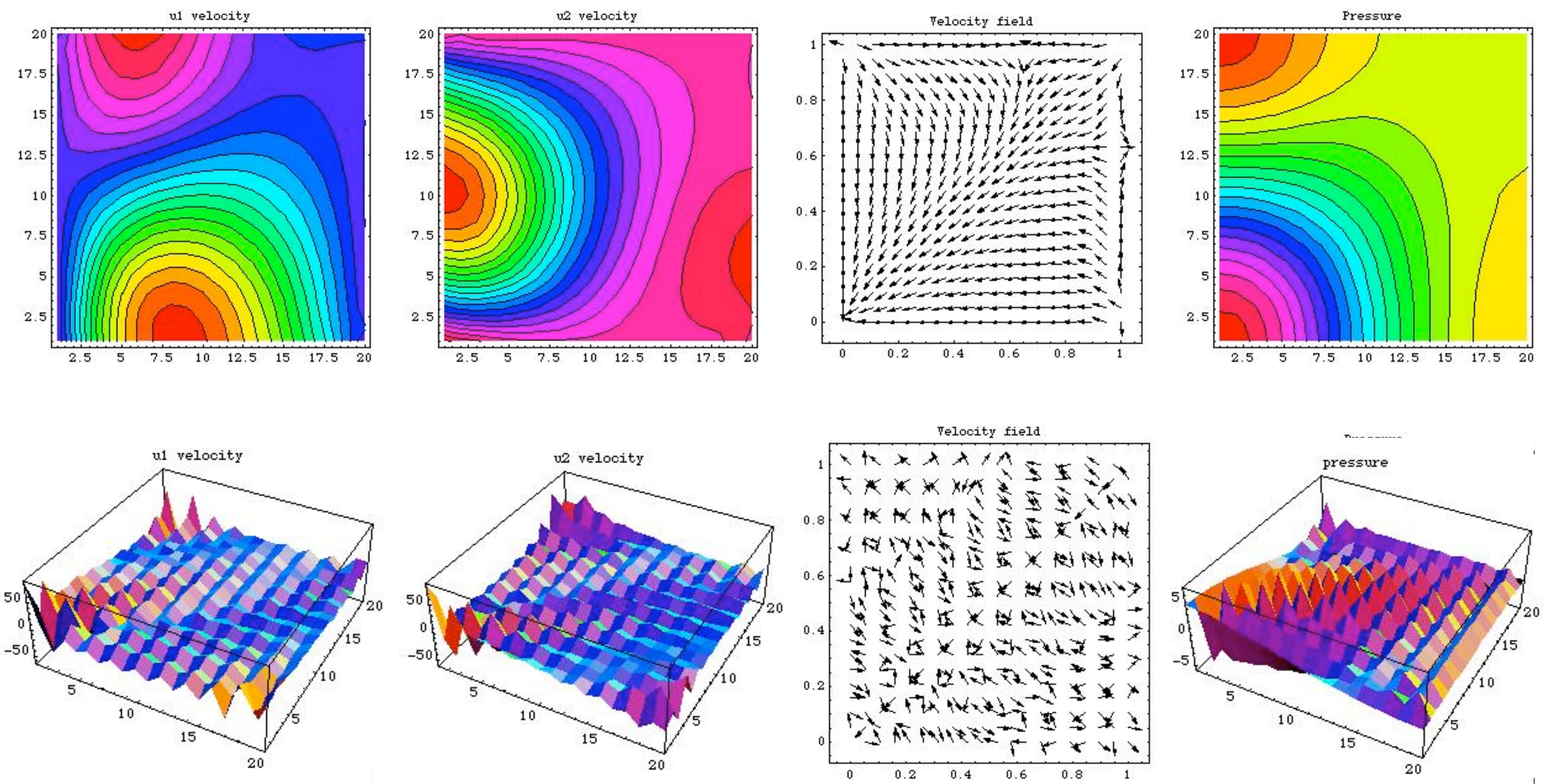
Electromagnetics

Failure to approximate ker(curl) by exact gradients gives rise to **spurious modes** and instabilities in transient simulations.

Incompressible flows

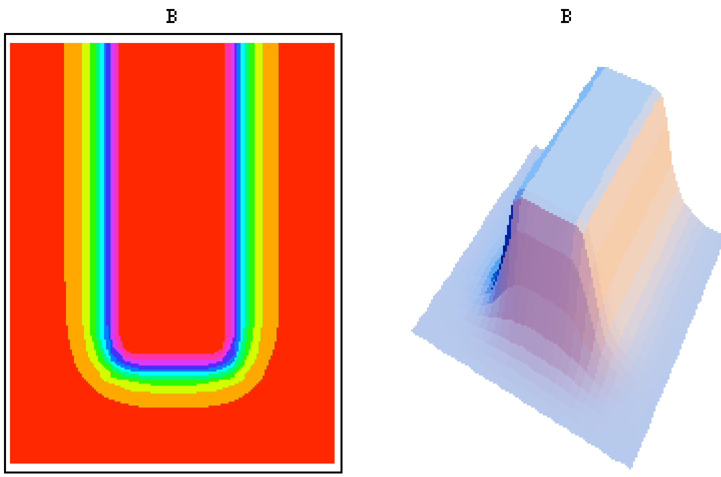
Failure to maintain discrete pressure in the range of the divergence of the **discrete velocity** leads to spurious modes and/or locking.

Examples



Collocated Mixed FEM for incompressible flow (same stencil for div and grad) and $\boldsymbol{P}^h \notin \mathrm{div}\,\boldsymbol{V}^h$

Examples

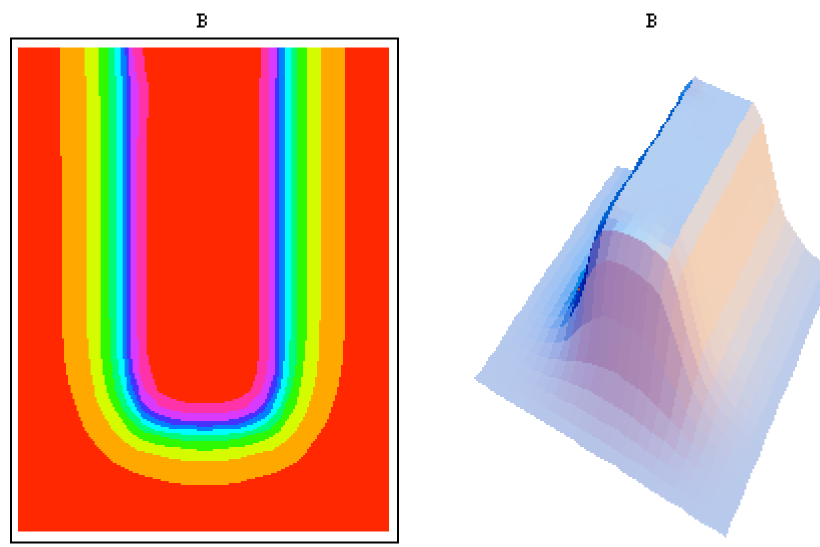


Low order edge FE solution

Ker(curl)={grad p}

Lagrange C^0 FE solution

Ker(curl)={0}



Solutions that work

Lax-Wendroff theorem:

If approximation computed by a **conservative** and **consistent** method converges, then the limit is a **weak solution** of the conservation law.

Grid decomposition property (Fix, Gunzburger, Nicolaides, 1978)

A **discrete Hodge decomposition** property is **necessary** and **sufficient** for stable and accurate mixed FE discretization of the Kelvin principle.

Staggered FD and FV (MAC, Yee's FDTD, Box integration)

Conservation requires placing **different variables** at **different grid locations** so as to achieve **discrete Stokes** theorem.

Discrete models must reflect mathematical structure of continuum models

How to achieve compatibility?

Compatible discretization requires:

- Mathematical tools to **discover** and **encode** structure of PDEs
- A discrete framework that **mimics** that structure: mutually consistent notions of
  - Discrete vector calculus, Hodge theory, entropy condition, conservation…

In most physical models

- **Fields** are observed **indirectly** by measuring **global** quantities (flux, circulation, etc)
- **Physical laws** are **relationships** between **global** quantities (conservation, equilibrium)

Differential forms provide the tools to encode such relationships

- **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*

Algebraic topology approach

Algebraic topology provides the tools to mimic the structure

- **Computational grid** is algebraic topological complex
- ***k*-forms** are encoded as *k*-cell quantities (*k*-cochains)
- **Derivative** is provided by the coboundary
- **Inner product** induces combinatorial Hodge theory
- **Singular cohomology** preserved by the complex

Framework for mimetic discretizations

- **Translation:** Fields → forms → cochains
- **Basic mappings:** **reduction** and **reconstruction**
  - **Combinatorial operations:** induced by **reduction** map
  - **Natural operations:** induced by **reconstruction** map
  - **Derived operations:** induced by **natural** operations

Branin (1966), Dodzuik (1976), Hyman & Scovel (1988-92), Nicolaides (1993), Dezin (1995), Shashkov (1990-), Mattiussi (1997), Schwalm (1999), Teixeira (2001)

Differential Forms

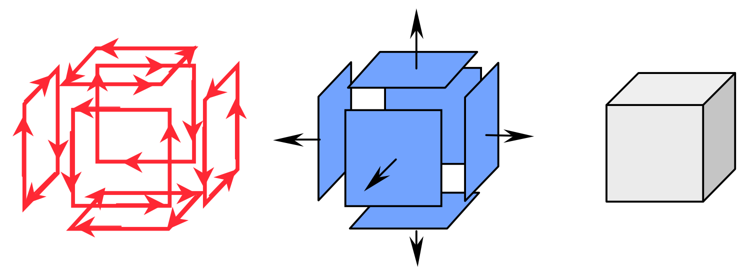
Smooth differential forms	$\Lambda^k(\Omega): \quad x \to \omega(x) \in \Lambda^k(T_x\Omega)$
DeRham complex	$\mathbf{R} \to \Lambda^0 \xrightarrow{d} \Lambda^1 \xrightarrow{d} \Lambda^2 \xrightarrow{d} \Lambda^3 \to 0$
Metric conjugation	$*: \Lambda^k(T_x\Omega) \to \Lambda^{n-k}(T_x\Omega) \;\Leftrightarrow\; \omega \wedge *\xi = (\omega,\xi)_x \omega_n$
L² inner product on Λ*k*(Ω)	$(\omega,\xi)_\Omega = \int_\Omega (\omega,\xi)_x \omega_n \quad \Rightarrow \quad (\omega,\xi)_\Omega = \int_\Omega \omega \wedge *\xi$
Codifferential	$d^*: \Lambda^{k+1}(\Omega) \to \Lambda^{k+1}(\Omega) \;\Leftrightarrow\; (d\omega,\xi)_\Omega = (\omega, d^*\xi)_\Omega$
Hodge Laplacian	$\Delta: \Lambda^k(\Omega) \to \Lambda^k(\Omega) \quad \to \quad \Delta = dd^* + d^*d$
Completion of Λ*k*(Ω)	$\Lambda^k(L^2,\Omega)$
Sobolev spaces	$\Lambda^k(d,\Omega) = \{\omega \in \Lambda^k(L^2,\Omega) \mid d\omega \in \Lambda^{k+1}(L^2,\Omega)\}$

Chains and cochains

Computational grid = Chain complex

$$\partial : C_k \to C_{k-1}$$

$$\partial\partial = 0 \qquad C_0 \xleftarrow{\partial} C_1 \xleftarrow{\partial} C_2 \xleftarrow{\partial} C_3$$



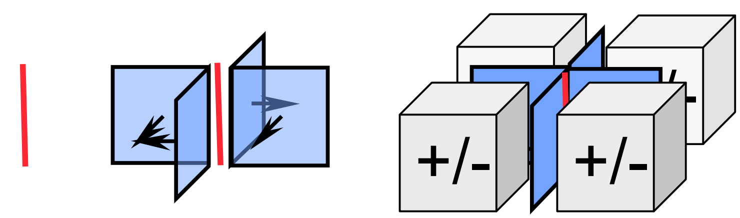
$$0 = \partial\partial K^3 \xleftarrow{\partial} \partial K^3 \xleftarrow{\partial} K^3$$

Field representation = Cochain complex

$$C^k = L(C_k, \mathbf{R}) = C_k^{\,*} \qquad \langle \sigma^i, \sigma_j \rangle = \delta_{ij}$$

$$K^1 \xrightarrow{\delta} \delta K^1 \xrightarrow{\delta} \delta\delta K^1 = 0$$

$$\delta : C^k \to C^{k+1} \qquad \langle \omega, \partial\eta \rangle = \langle \delta\omega, \eta \rangle$$



$$\delta\delta = 0 \qquad C^0 \xrightarrow{\delta} C^1 \xrightarrow{\delta} C^2 \xrightarrow{\delta} C^3$$

Basic mappings

Reduction

$$\mathcal{R} : \Lambda^k(L^2,\Omega) \to C^k$$

Natural choice

$$\langle \mathcal{R}\omega, \sigma \rangle = \int_\sigma \omega$$

DeRham map

$$\mathcal{R}d = \delta\mathcal{R}$$

Proof

$$\langle \delta\mathcal{R}\omega, c \rangle = \langle \mathcal{R}\omega, \partial c \rangle = \int_{\partial c} \omega = \int_c d\omega = \langle \mathcal{R}d\omega, c \rangle$$

$$\begin{tikzcd} \cdots \Lambda^k \arrow[r, "d"] \arrow[d] & \Lambda^{k+1} \cdots \arrow[d] \\ \cdots C^k \arrow[r, "\delta"] \arrow[d, leftrightarrow] & C^{k+1} \cdots \arrow[d, leftrightarrow] \\ \cdots C_k & C_{k+1} \cdots \arrow[l, "\partial"'] \end{tikzcd}$$

$$\begin{tikzcd} \Lambda^k \arrow[r, "d"] \arrow[d, "\mathcal{R}"'] \arrow[dr, phantom, "\textbf{CDP I}"] & \Lambda^{k+1} \arrow[d, "\mathcal{R}"] \\ C^k \arrow[r, "\delta"] & C^{k+1} \end{tikzcd}$$

natural

$$\begin{tikzcd} \Lambda^k \arrow[r, "d"] \arrow[dr, phantom, "\textbf{CDP2}"] & \Lambda^{k+1} \\ C^k \arrow[r, "\delta"] \arrow[u, "\mathcal{I}"] & C^{k+1} \arrow[u, "\mathcal{I}"'] \end{tikzcd}$$

required

$$\text{Range } \mathcal{I}\mathcal{R} = \Lambda^k(L^2,K) \subset \Lambda^k(L^2,\Omega)$$

$$\text{Range } \mathcal{I}\mathcal{R} = \Lambda^k(d,K) \subset \Lambda^k(d,\Omega)$$

Reconstruction

$$\mathcal{I} : C^k \to \Lambda^k(L^2,\Omega)$$

No natural choice

$$\mathcal{R}\mathcal{I} = id$$

$$\mathcal{I}\mathcal{R} = id + O(h^s)$$

$$\ker \mathcal{I} = 0$$

Conforming

$$\mathcal{I} : C^k \to \Lambda^k(d,\Omega)$$

$$\mathcal{I}d = \delta\mathcal{I}$$

Combinatorial operations

Discrete derivative

Forms are dual to **manifolds** $\langle d\omega, \Omega \rangle = \langle \omega, \partial\Omega \rangle$

Cochains are dual to **chains** $\langle \delta a, \sigma \rangle = \langle a, \partial\sigma \rangle$

δ approximates *d* on cochains

Discrete integral

$$\int_\sigma a = \langle a, \sigma \rangle$$

Stokes theorem

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

grad

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \end{pmatrix}$$

curl

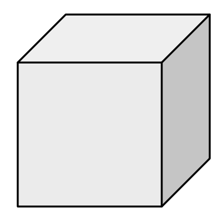
$$\begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 \end{pmatrix}$$

div

$$\begin{pmatrix} -1 & 1 & 1 & -1 & -1 & 1 \end{pmatrix}$$

$$\delta\delta = 0$$

$$\mathcal{R}d = \delta\mathcal{R}$$



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Natural and derived operations

Natural Inner product $(a,b)_x = (\mathcal{I}a, \mathcal{I}b)_x$ $\quad (a,b)_\Omega = \int_\Omega (a,b)_x \omega_n = (\mathcal{I}a, \mathcal{I}b)_\Omega$

Wedge product $\wedge : C^k \times C^l \mapsto C^{k+l}$ $\quad a \wedge b = \mathcal{R}(\mathcal{I}a \wedge \mathcal{I}b)$

Derived Adjoint derivative $\delta^* : C^{k+1} \mapsto C^k$ $\quad (\delta^* a, b)_\Omega = (a, \delta b)_\Omega$

Provides a second set of **grad**, **div** and **curl** operators. Scalars encoded as 0 or 3-forms, vectors as 1 or 2-forms, derivative choice depends on encoding.

Discrete Laplacian $D : C^k \mapsto C^k$ $\quad D = \delta^* \delta + \delta \delta^*$

Derived operations are necessary to avoid **internal inconsistencies** between the discrete operations: $\mathcal{I}$ is only **approximate inverse** of $\mathcal{R}$ and natural operations will clash

Example Natural adjoint $d^* = (-1)^k * d *$ $\longrightarrow$ $\delta^* = (-1)^k \mathcal{R} * d * \mathcal{I}$

$\mathcal{I}$ must be regular and $(\delta^* a, b)_\Omega = (a, \delta b)_\Omega + O(h^s)$ $\Rightarrow$ δ^* not true adjoint

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Mimetic properties

Discrete Poincare lemma (existence of potentials in contractible domains)

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

Discrete Stokes Theorem

$$\left\langle d\omega_{k-1}, c_k \right\rangle = \left\langle \omega_{k-1}, \partial c_k \right\rangle \qquad\qquad \left\langle \delta c^{k-1}, c_k \right\rangle = \left\langle c^{k-1}, \partial c_k \right\rangle$$

Discrete "Vector Calculus"

$$dd = 0 \qquad\qquad \delta\delta = \delta * \delta * = 0$$

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

$$d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^k \omega \wedge d\eta \qquad\qquad \delta(a \wedge b) = \delta a \wedge b + (-1)^k a \wedge \delta b$$

(Regular $\mathcal{I}$)

Any feature of the continuum system that is implied by differential forms calculus is inherited by the discrete model

Called ***mimetic*** property by Hyman and Scovel (1988)

Mimetic properties

Inner product induces combinatorial Hodge theory on cochains

$$\text{Co-cycles of } (W_0, W_1, W_2, W_3) \xrightarrow{\mathcal{R}} \text{co-cycles of } (C^0, C^1, C^2, C^3)$$

$$d\omega = 0 \quad \Rightarrow \quad \delta\mathcal{R}\omega = 0$$

Discrete Harmonic forms

$$H^k(\Omega) = \left\{\eta \in \Lambda^k(\Omega) \mid d\eta = d^*\eta = 0\right\} \qquad H^k(K) = \left\{c^k \in C^k \mid \delta c^k = \delta^* c^k = 0\right\}$$

Discrete Hodge decomposition

$$\omega = d\rho + \eta + d^*\sigma \qquad a = \delta b + h + \delta^* c$$

Theorem $\quad \operatorname{dimker}(\Delta) = \operatorname{dimker}(D)$

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

Discrete $*$ operation

Natural definition

$*_N : C^k \mapsto C^{n-k}$ $\qquad$ $*_N = \mathcal{R} * \mathcal{I}$

Derived definition

$*_D : C^k \mapsto C^{n-k}$ $\qquad$ $\int_\Omega a \wedge *_D b = (a,b)_\Omega$ mimics $(\omega,\xi)_\Omega = \int_\Omega \omega \wedge *\xi$

Theorem

$*_N \mathcal{R}\omega^h = \mathcal{R} * \omega^h \quad \forall \omega^h \in \mathrm{Range}(\mathcal{I}\mathcal{R})$ — CDP on the range

$\int_\Omega \mathcal{I}\mathcal{R}(\mathcal{I}a \wedge \mathcal{I} *_D b) = \int_\Omega (\mathcal{I}a \wedge *\mathcal{I}b)$ — Weak CDP

$\int_\Omega b \wedge *_N b = (a,b)_\Omega + O(h^s)$ $\qquad$ $*_N = *_D + O(h^s)$

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Problems with the discrete $*$

Action of $*$ must be coordinated with two other discrete operations

	$(\bullet,\bullet)$	$\wedge$	δ^*	$\mathcal{R}$	$\mathcal{I}$
$*_N$	—	—	—	✓	—
$*_D$	✓	✓	—	—	—

Analytic $*$ is a **local, invertible** operation $\Rightarrow$ **positive diagonal** matrix

$\dim C^k \neq \dim C^{n-k}$ $\Rightarrow$ $*_N : C^k \mapsto C^{n-k}$ **cannot be a square matrix!**

Construction of $*$ is nontrivial task unless primal-dual grid is used!

Implications

A consistent discrete framework requires a choice of a primary operation

either $*$ or $(\cdot,\cdot)$ but not both

A **discrete** $*$ is the primary concept in Hiptmair (2000), Bossavit (1999)

- Inner product derived from discrete $*$
- Used in explicit discretization of material laws

The **natural inner product** is the primary operation in our approach

- **Sufficient** to give rise to combinatorial Hodge theory on cochains
- **Easier** to define than a discrete $*$ operation
- **Incorporate** material laws in the natural inner product, or
- **Enforce** material laws **weakly** (justified by their approximate nature)

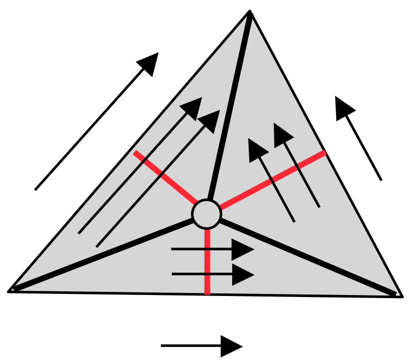
Algebraic equivalents

Operation	Matrix form	type
δ	$\mathbf{D}_k$	{-1,0,1}
$(\cdot,\cdot)$	$\mathbf{M}_k$	SPD
$a_1 \wedge b_1$	$\sum \mathbf{W}_{11}$	Skew symm.
$a_1 \wedge b_2$	$\sum \mathbf{W}_{12}$	$\mathbf{W}_{12}{}^T = \mathbf{W}_{21}$
$b_2 \wedge a_1$	$\sum \mathbf{W}_{21}$	
δ^*	$\mathbf{M}_k{}^{-1}\,\mathbf{D}_k{}^T\mathbf{M}_{k+1}$	rectangular
$\mathcal{D}$	$\mathbf{M}_k{}^{-1}\,\mathbf{D}_k{}^T\mathbf{M}_{k+1}\mathbf{D}_k + \mathbf{D}_{k-1}\mathbf{M}_{k-1}{}^{-1}\,\mathbf{D}_{k-1}{}^T\mathbf{M}_k$	square
$*_D$	$\mathbf{W}_{12}(*_D\mathbf{a}) = \mathbf{M}_3\mathbf{a}$	pair

Reconstruction and natural inner products

Co-volume

$\mathcal{I}$



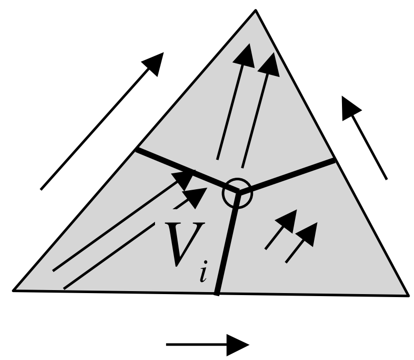
Nicolaides, Trapp (1992-04)

$\mathbf{M}$

$$\begin{pmatrix} h_1 h_1^{\perp} & & \\ & h_2 h_2^{\perp} & \\ & & h_3 h_3^{\perp} \end{pmatrix}$$

δ^* **local**

Mimetic

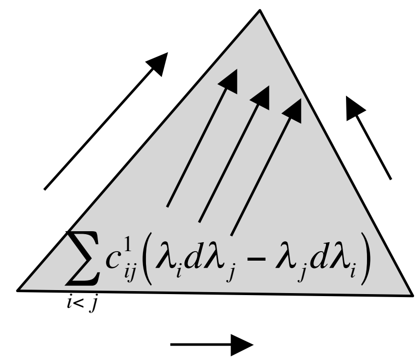


Hyman, Shashkov, Steinberg (1985-04)

$$\begin{pmatrix} \frac{V_2}{\sin^2\phi_2}+\frac{V_3}{\sin^2\phi_3} & \frac{V_3\cos\phi_3}{\sin^2\phi_3} & \frac{V_2\cos\phi_2}{\sin^2\phi_2} \\ \frac{V_3\cos\phi_3}{\sin^2\phi_3} & \frac{V_1}{\sin^2\phi_1}+\frac{V_3}{\sin^2\phi_3} & \frac{V_1\cos\phi_1}{\sin^2\phi_1} \\ \frac{V_2\cos\phi_2}{\sin^2\phi_2} & \frac{V_1\cos\phi_1}{\sin^2\phi_1} & \frac{V_1}{\sin^2\phi_1}+\frac{V_2}{\sin^2\phi_2} \end{pmatrix}$$

non-local

Whitney



Dodzuik (1976)
Hyman, Scovel (1988)

$$\omega_{ij}^1 = \lambda_i d\lambda_j - \lambda_j d\lambda_i$$

$$\begin{pmatrix} \cdots & \cdots & \cdots \\ \cdots & \left(w_{ij}, w_{kl}\right) & \\ \cdots & \cdots & \cdots \end{pmatrix}$$

non-local

Mimetic discretization: translation to forms

1st order PDE with material laws

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \mathbf{J} = \sigma \mathbf{E}$$
$$\nabla \times \mathbf{H} = \mathbf{J} \qquad \mathbf{B} = \mu \mathbf{H}$$

$\Rightarrow$

$$de = -d_t b \qquad *_{\sigma^{-1}}\, j = e$$
$$dh = j \qquad *_{\mu^{-1}}\, b = h$$

1st order PDE with codifferentials

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\frac{1}{\sigma}\nabla \times \frac{1}{\mu}\mathbf{B} = \mathbf{E}$$

$\Rightarrow$

$$de = -d_t b$$
$$e = *_{\sigma^{-1}}\, d *_{\mu^{-1}}\, b$$

2nd order PDE

$$\nabla \times \frac{1}{\sigma}\nabla \times \frac{1}{\mu}\mathbf{B} = -\frac{\partial \mathbf{B}}{\partial t}$$

$\Rightarrow$

$$d *_{\sigma^{-1}}\, d *_{\mu^{-1}}\, b = -d_t b$$

Direct and conforming mimetic models

$$\delta\delta^* b^2 = -\delta_t b^2$$

$$e^1 \in C^2; \quad b^2 \in C^2$$

$$\delta e^1 = -\delta_t b^2$$
$$e^1 = \delta^* b^2$$

$$d *_{\sigma^{-1}} d *_{\mu^{-1}} b = -d_t b$$

Direct

Conforming

$$de = -d_t b$$
$$e = *_{\sigma^{-1}} d *_{\mu^{-1}} b$$

$$\left(db_h^2, d\hat{b}_h^2\right)_\Omega = \left(-d_t b_h^2, \hat{b}_h^2\right)_\Omega$$

$$e_h^1 \in \Lambda^1(d,K); \quad b_h^2 \in \Lambda^2(d,K)$$

$$de_h^1 = -d_t b_h^2$$
$$\left(e_h^1, \hat{e}_h^1\right)_\Omega = \left(b_h^2, d\hat{e}_h^1\right)_\Omega$$

Theorem (Bochev & Hyman)

Assume that $\mathcal{I}$ is **regular** reconstruction operator. Then, the **direct** and the **conforming** mimetic methods are completely equivalent.

Mimetic models with weak material laws

Translate to an equivalent constrained optimization problem

$$de = -d_t b \qquad *_{\sigma^{-1}}\, j = e$$
$$dh = j \qquad *_{\mu^{-1}}\, b = h$$

$$\min \frac{1}{2}\left(\left\| j - *_\sigma e \right\|^2 + \left\| b - *_\mu h \right\|^2 \right)$$

subject to $de = -d_t b$ and $dh = j$

Conforming **Mimetic discretization** **Direct**

$$\min \frac{1}{2}\left(\left\| j_h^2 - e_h^1 \right\|^2 + \left\| b_h^2 - h_h^1 \right\|^2 \right)$$

subject to $de_h^1 = -d_t b_h^2$ and $dh_h^1 = j_h^2$

$$\min \frac{1}{2}\left(\left\| j^2 - e^1 \right\|^2 + \left\| b^2 - h^1 \right\|^2 \right)$$

subject to $\delta e^1 = -\delta_t b^2$ and $\delta h^1 = j^2$

Advantages

– Does not require a primal-dual grid complex

– Explicit discretization of material laws is avoided

– Construction of a discrete $*$ operation not required

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Conclusions

- **Algebraic topology** provides powerful tools for mimetic discretizations
- We presented a **mimetic framework** where:
  - All operations defined by **two mappings**: reduction $\mathcal{R}$ and reconstruction $\mathcal{I}$
  - The central concept is the natural inner product
- The framework consists of three operation types
  - **Combinatorial** integral and derivative
  - **Natural** inner product and wedge product
  - **Derived** adjoint derivative, Hodge Laplacian
- Choice of **natural** and **derived** operations governed by **internal consistency**
- Operations provide **discrete vector calculus** and **combinatorial Hodge theory**
- Instead of explicit discretization of material laws they are
  - **incorporated** in the inner product or
  - **imposed weakly** through equivalent constrained optimization problem
- **Direct** and **conforming** mimetic methods are **identical** for regular $\mathcal{I}$
  - Differences between FV, FD and FE are largely **superficial**
  - Distinctions arise primarily from the **choice** of reconstruction operators