A Generalization for Stable Mixed Finite Elements

Andrew Gillette

joint work with

Chandrajit Bajaj

Department of Mathematics
Institute of Computational Engineering and Sciences
University of Texas at Austin, USA

http://www.math.utexas.edu/users/agillette
Motivation

Biological modeling requires **robust** computational methods to solve integral and differential equations over spatially realistic domains.

Electrostatics  Electromagnetics/ Electrodiffusion  Elasticity

These methods must accommodate

- complicated domain geometry and topology
- multiple variables and operators
Notions of Robustness

A robust computational method for solving PDEs should exhibit

- **Model Conformity**: Computed solutions are found in a subspace of the solution space for the continuous problem
  
  *Criterion*: Discrete solution spaces replicate the the deRham sequence.

- **Discretization Stability**: The true error between the discrete and continuous solutions is bounded by a multiple of the best approximation error
  
  *Criterion*: The discrete inf-sup condition is satisfied.

- **Bounded Roundoff Error**: Accumulated numerical errors due to machine precision do not compromise the computed solution
  
  *Criterion*: Matrices inverted by the linear solver are well-conditioned.

**Problem Statement**

Use the theory of Discrete Exterior Calculus to evaluate the robustness of existing computational methods for PDEs arising in biology and create novel methods with improved robustness.
Outline

1. Basics of Discrete Exterior Calculus
2. Alternative Discretization Pathways
3. Stability Criteria from Discrete Hodge Stars
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1. Basics of Discrete Exterior Calculus
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3. Stability Criteria from Discrete Hodge Stars
Differential $k$-forms model $k$-dimensional physical phenomena.

The exterior derivative $d$ generalizes common differential operators.

\[ H^1 \xrightarrow{d_0 \text{ grad}} \ H(\text{curl}) \xrightarrow{d_1 \text{ curl}} \ H(\text{div}) \xrightarrow{d_2 \text{ div}} \ L^2 \]

The Hodge Star transfers information between complementary dimensions of primal and dual spaces.

\[ H^1 \leftrightarrow * \xrightarrow{\text{curl}} L^2 \]

\[ H(\text{curl}) \leftrightarrow * \xrightarrow{\text{div}} H(\text{div}) \]

**Fundamental “Theorem” of Discrete Exterior Calculus**

Conforming computational methods must recreate the essential properties of (continuous) exterior calculus on the discrete level.
Discrete Exterior Calculus

- Discrete differential $k$-forms are $k$-cochains, i.e. linear functions on $k$-simplices.

- The discrete exterior derivative $\nabla$ is the transpose of the boundary operator.

- This creates a discrete analogue of the deRham sequence.

\[
\begin{align*}
C^0 & \xrightarrow{\nabla_0} C^1 \xrightarrow{\nabla_1} C^2 \xrightarrow{\nabla_2} C^3 \\
(\text{grad}) & \quad (\text{curl}) & \quad (\text{div})
\end{align*}
\]
Discrete Exterior Calculus

- The discrete Hodge Star $\mathbb{M}$ transfers information between complementary dimensions on dual meshes. In this example, we use the identity matrix for $\mathbb{M}_1$.

\[
\begin{bmatrix}
1 \\
-3 \\
2 \\
5 \\
3
\end{bmatrix}
\xrightarrow{M_1}
\begin{bmatrix}
1 \\
-3 \\
2 \\
5 \\
3
\end{bmatrix}
\]

- The discrete exterior derivative on the dual mesh is $\nabla^T$

\[
\begin{bmatrix}
4 \\
6 \\
-2 \\
-8
\end{bmatrix}
\xrightarrow{\nabla^T_1}
\begin{bmatrix}
1+3 \\
5+2-1 \\
-3-5 \\
-3-2+3
\end{bmatrix}
\]

- This creates a dual discrete analogue of the deRham sequence.

\[
\overline{C}^3 \xleftarrow{\nabla^T_2} \overline{C}^2 \xleftarrow{\nabla^T_1} \overline{C}^1 \xleftarrow{\nabla^T_0} \overline{C}^0
\]
The DEC-deRham Diagram for $\mathbb{R}^3$

We combine the Discrete Exterior Calculus maps with the $L^2$ deRham sequence.

The combined diagram elucidates alternative discretization pathways for finite element methods.
Outline

1. Basics of Discrete Exterior Calculus
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3. Stability Criteria from Discrete Hodge Stars
Linear Poisson-Boltzmann Equation

\[
\text{div} \left( \epsilon(\vec{x}) \nabla \phi(\vec{x}) \right) = \rho_c(\vec{x}) + \bar{\kappa}(\vec{x}) \phi(\vec{x}) \text{ in } \mathbb{R}^3
\]

\[
\phi(\vec{x}) = \text{electrostatic potential}
\]

\[
\epsilon(\vec{x}) = \text{dielectric coefficient} = \begin{cases} 
\epsilon_I, & \vec{x} \in \Omega \\
\epsilon_E, & \vec{x} \in \mathbb{R}^3 - \Omega 
\end{cases}
\]

\[
\rho_c(\vec{x}) = \text{charge density from atomic charges}
\]

\[
\bar{\kappa}(\vec{x}) = \text{modified Debye-Huckel parameter}
\]

Exterior calculus formulation: \( d \ast \epsilon d\phi = f, \quad \phi \in H^1, f \in L^2 \)

**Primal discretization:** \( D_0^T M_1 \epsilon D_0 \phi = f \)

**Dual discretization:** \( D_2 \epsilon(M_2)^{-1}(D_2)^T \phi = f \)
The two discretizations inside the DEC-deRham diagram:

\[ H^1 \xrightarrow{\text{grad}} H(\text{curl}) \xrightarrow{\text{curl}} H(\text{div}) \xrightarrow{\text{div}} L^2 \]

\[ I_0 \xrightarrow{\phi} P_0 \quad I_1 \xrightarrow{\epsilon D_0 \phi} D_0 \quad I_2 \xrightarrow{I_3} \]

\[ (D_0)^T M_1 \epsilon D_0 \phi \xleftarrow{M_1 \epsilon D_0 \phi} (D_0)^T \phi \]

\[ \epsilon (M_2)^{-1} (D_2)^T \phi \xrightarrow{D_2} D_2 \epsilon (M_2)^{-1} (D_2)^T \phi \]

The definition of the discrete Hodge star matrix $M_k$ and its inverse are essential in ensuring the robustness of a primal or dual discretization.
Further Examples

- **Maxwell’s Curl Equations**

  \[
  \nabla \frac{1}{\mu} \times \nabla \times \vec{E} = \omega^2 \epsilon \vec{E} \\
  \nabla \frac{1}{\epsilon} \times \nabla \times \vec{h} = \omega^2 \vec{H}
  \]

- **Darcy Flow**

  \[
  \begin{aligned}
  \vec{f} + \frac{k}{\mu} \nabla p &= 0 \quad \text{in } \Omega, \\
  \text{div } \vec{f} &= \phi \quad \text{in } \Omega, \\
  \vec{f} \cdot \hat{n} &= \psi \quad \text{on } \partial \Omega,
  \end{aligned}
  \]

- **Diagram**

  \[
  \begin{array}{ccc}
  \text{primal:} & \vec{E} & \xrightarrow{\mathbb{D}_1} & C^2 \\
  \text{dual:} & C^2 & \xleftarrow{\mathbb{D}_1^T} & \vec{H}
  \end{array}
  \]

  \[
  \begin{array}{ccc}
  \text{primal:} & p & \xrightarrow{\mathbb{D}_0} & \mathbb{D}_0 p \\
  \text{dual:} & (\mathbb{D}_0)^T \vec{f} & \xleftarrow{(\mathbb{D}_0)^T} & \vec{f}
  \end{array}
  \]

  \[
  \begin{array}{ccc}
  \text{dual:} & \vec{f} & \xrightarrow{\mathbb{D}_2} & \mathbb{D}_2 \vec{f} \\
  \text{primal:} & \mathbb{M}_2 \mathbb{D}_2 p & \xleftarrow{\mathbb{M}_2} & p
  \end{array}
  \]
Outline

1. Basics of Discrete Exterior Calculus
2. Alternative Discretization Pathways
3. Stability Criteria from Discrete Hodge Stars
Discrete Hodge Star Criteria

A discrete Hodge star transfers information between primal and dual meshes:

**primal mesh simplex** \( \sigma^k \) \iff **dual mesh cell** \( \star \sigma^k \)

\[ \text{DIAGONAL} \quad [\text{Desbrun et al.}] \quad (M^\text{Diag}_k)_{ij} := \frac{|\star \sigma^k_i|}{|\sigma^k_j|} \delta_{ij} \]

\[ \text{WHITNEY} \quad [\text{Dodziuk}, [\text{Bell}]] \quad (M^\text{Whit}_k)_{ij} := \left( \eta_{\sigma^k_i}, \eta_{\sigma^k_j} \right)_{c_k} \quad (\eta_{\sigma^k} = \text{Whitney } k\text{-form for } \sigma^k) \]

A robust definition of a discrete Hodge star matrix \( M_k \) and its inverse should provide for:

1. Commutativity of discrete dual operators
2. Local structure of \( M_k \) and \( M_k^{-1} \)
3. Well-conditioned matrices
Commutativity of Discrete Dual Operators

Given projection to ($\overline{P}$) or interpolation from ($\overline{I}$) a dual mesh, we have the maps:

\[
\begin{align*}
\text{deRham:} & \quad \Lambda^k \downarrow \quad \overline{\Lambda}^{n-k} \\
\text{primal:} & \quad C^k \downarrow \quad M_k \downarrow \quad \overline{C}^{n-k} \\
\text{dual:} & \quad (M_k)^{-1} \downarrow \quad \overline{\Lambda}^{n-k} \downarrow \quad \overline{C}^{n-k}
\end{align*}
\]

Thus, we expect some commutativity of the diagram:

\[
\begin{align*}
\text{deRham} & \quad \Lambda^k \quad \downarrow \quad \overline{\Lambda}^{n-k} \\
\text{primal} & \quad C^k \quad \downarrow \quad \overline{C}^{n-k} \\
\text{dual} & \quad (M_k)^{-1} \quad \downarrow \quad \overline{\Lambda}^{n-k} \quad \downarrow \quad \overline{C}^{n-k}
\end{align*}
\]
Commutativity of Discrete Dual Operators

\[
\begin{array}{ccc}
\text{deRham} & \Lambda^k & \text{deRham} \\
\uparrow i_k & \star & \uparrow i_{n-k} \\
\mathcal{P}_k & \Lambda^n & \mathcal{P}_{n-k} \\
\downarrow & & \downarrow \\
\text{primal} & C^k & \text{dual} \\
\downarrow M_k & \rightarrow & \downarrow (M_k)^{-1} \\
C^n & \leftarrow & C^{n-k} \\
\end{array}
\]

Strong commutativity at \( C^k \):
\[
\star i_k = i_{n-k} M_k
\]

Weak commutativity at \( C^k \):
\[
\int_T \alpha \wedge \star i_k = \int_T \alpha \wedge i_{n-k} M_k, \quad \forall \alpha \in \Lambda^k
\]

**Example:** Discrete Hodge star definitions can be evaluated by this criteria:

Using \( M_0^{Diag} \):
\[
|T| (\alpha, \lambda_i)_{H^1} = |\star \sigma_i^0| \int_{\star \sigma_i^0} \alpha \mu, \quad \forall \alpha \in H^1
\]

Using \( M_0^{Whit} \):
\[
|T| (\alpha, \lambda_i)_{H^1} = \sum_{\text{vertex } j} (\lambda_i, \lambda_j)_{H^1} \int_{\star \sigma_i^0} \alpha \mu, \quad \forall \alpha \in H^1
\]
Local Structure of $M_k$ and $M_k^{-1}$

- Existing inverse discrete Hodge stars are either too full or too empty for use in discretizations on dual meshes.
- We present a novel **dual** discrete Hodge star for this purpose using generalized barycentric coordinate functions (details in the paper).

<table>
<thead>
<tr>
<th>type</th>
<th>definition</th>
<th>$M_k$</th>
<th>$M_k^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DIAGONAL</strong></td>
<td>$(M_k^{Diag})_{ij} = \frac{</td>
<td>\star \sigma_i^k</td>
<td>}{</td>
</tr>
<tr>
<td><strong>WHITNEY</strong></td>
<td>$(M_k^{Whit})<em>{ij} = \left(\eta</em>{\sigma_i^k}, \eta_{\sigma_j^k}\right)_{C^k}$</td>
<td>sparse</td>
<td>(full)</td>
</tr>
<tr>
<td><strong>DUAL</strong></td>
<td>($(M_k^{Dual})^{-1})<em>{ij} = \left(\eta</em>{\star \sigma_i^k}, \eta_{\star \sigma_j^k}\right)_{C^k}$</td>
<td>(full)</td>
<td>sparse</td>
</tr>
</tbody>
</table>
Well-Conditioned Matrices

The condition number of a discrete Hodge star matrix depends on the size of both primal and dual mesh elements.

1. Primal simplices $\sigma^k$ satisfy geometric quality measures.
2. Dual cells $\star\sigma^k$ satisfy geometric quality measures.
3. The value of $|\star\sigma^k|/|\sigma^k|$ is bounded above and below.
4. The primal and dual meshes do not have large gradation of elements.

We identify which geometric criteria are required to provide bounded condition numbers on the various discrete Hodge star matrices.

<table>
<thead>
<tr>
<th></th>
<th>$i$</th>
<th>$ii$</th>
<th>$iii$</th>
<th>$iv$</th>
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<tr>
<td><strong>Diagonal</strong></td>
<td>$M_k^{Diag}$</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Whitney</strong></td>
<td>$M_k^{Whit}$</td>
<td>✓</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td><strong>Dual</strong></td>
<td>$(M_k^{Dual})^{-1}$</td>
<td>✓</td>
<td>✓</td>
<td></td>
</tr>
</tbody>
</table>

Computational Visualization Center, I C E S (Department of Mathematics Institute of Computational Engineering and Sciences University of Texas at Austin, USA)

The University of Texas at Austin

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