A Generalization for Stable Mixed Finite Elements

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joint work with

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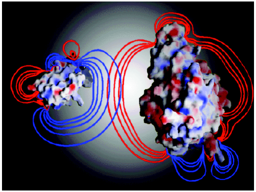
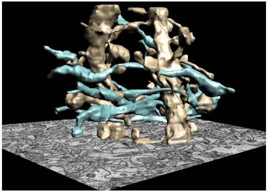
Motivation

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

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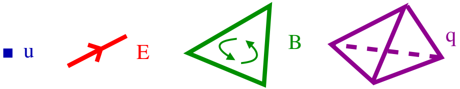
1. Basics of Discrete Exterior Calculus
2. Alternative Discretization Pathways
3. Stability Criteria from Discrete Hodge Stars

(Continuous) Exterior Calculus

- Differential *k*-forms model *k*-dimensional physical phenomena.



- The exterior derivative d generalizes common differential operators.

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

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

$$H^1 \longleftarrow * \longrightarrow L^2$$

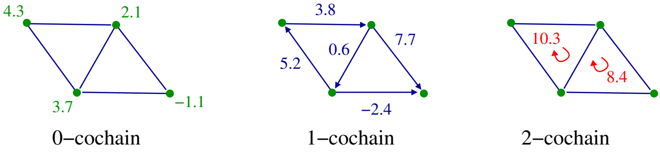
$$H(\text{curl}) \longleftarrow * \longrightarrow H(\text{div})$$

Fundamental "Theorem" of Discrete Exterior Calculus

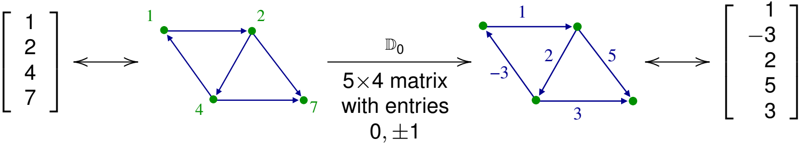
Conforming computational methods must recreate the essential properties of (continuous) exterior calculus on the discrete level.

Discrete Exterior Calculus

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



- The discrete exterior derivative $\mathbb{D}$ is the transpose of the boundary operator.



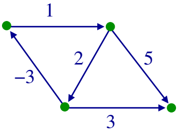
- This creates a discrete analogue of the deRham sequence.

$$\mathcal{C}^0 \xrightarrow[\text{(grad)}]{\mathbb{D}_0} \mathcal{C}^1 \xrightarrow[\text{(curl)}]{\mathbb{D}_1} \mathcal{C}^2 \xrightarrow[\text{(div)}]{\mathbb{D}_2} \mathcal{C}^3$$

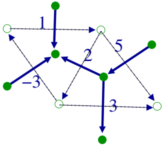
Discrete Exterior Calculus

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

$$\begin{bmatrix} 1 \\ -3 \\ 2 \\ 5 \\ 3 \end{bmatrix} \longleftrightarrow$$



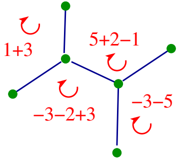
$$\xrightarrow[5\times 5 \text{ matrix}]{\mathbb{M}_1}$$



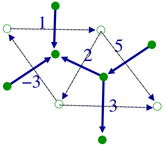
$$\longleftrightarrow \begin{bmatrix} 1 \\ -3 \\ 2 \\ 5 \\ 3 \end{bmatrix}$$

- The discrete exterior derivative on the **dual** mesh is $\mathbb{D}^T$

$$\begin{bmatrix} 4 \\ 6 \\ -2 \\ -8 \end{bmatrix} \longleftrightarrow$$



$$\xleftarrow[4\times 5 \text{ matrix with entries } 0, \pm 1]{\mathbb{D}_1^T}$$



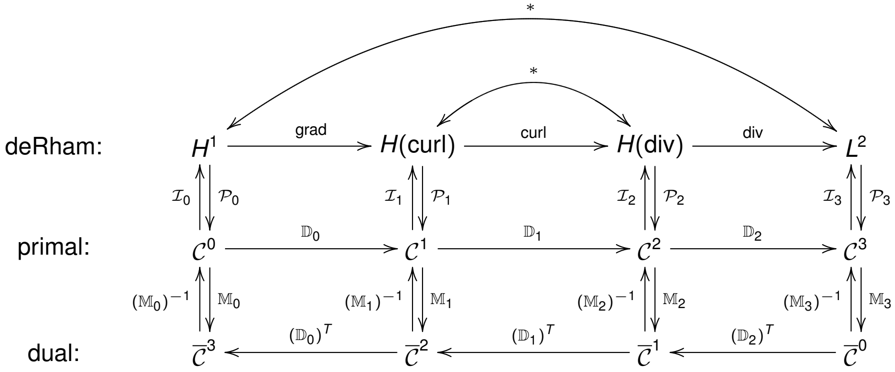
$$\longleftrightarrow \begin{bmatrix} 1 \\ -3 \\ 2 \\ 5 \\ 3 \end{bmatrix}$$

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

$$\overline{\mathcal{C}}^3 \xleftarrow[\text{(div)}]{\mathbb{D}_2^T} \overline{\mathcal{C}}^2 \xleftarrow[\text{(curl)}]{\mathbb{D}_1^T} \overline{\mathcal{C}}^1 \xleftarrow[\text{(grad)}]{\mathbb{D}_0^T} \overline{\mathcal{C}}^0$$

The DEC-deRham Diagram for $\mathbb{R}^3$

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

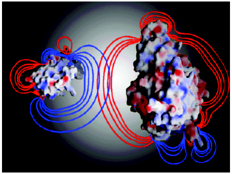


The combined diagram elucidates alternative discretization pathways for finite element methods.

Outline

Linear Poisson-Boltzmann Equation

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



$$\begin{aligned}
\phi(\vec{x}) &= \text{electrostatic potential} \\
\epsilon(\vec{x}) &= \text{dielectric coefficient} = \begin{cases} \epsilon_I, & \vec{x} \in \Omega \\ \epsilon_E, & \vec{x} \in \mathbb{R}^3 - \Omega \end{cases} \\
\rho_c(\vec{x}) &= \text{charge density from atomic charges} \\
\bar{\kappa}(\vec{x}) &= \text{modified Debye-Huckel parameter}
\end{aligned}$$

Exterior calculus formulation: $d * \epsilon d\phi = f, \qquad \phi \in H^1, f \in L^2$

Primal discretization: $\mathbb{D}_0^T \mathbb{M}_1 \epsilon \mathbb{D}_0 \phi = f$

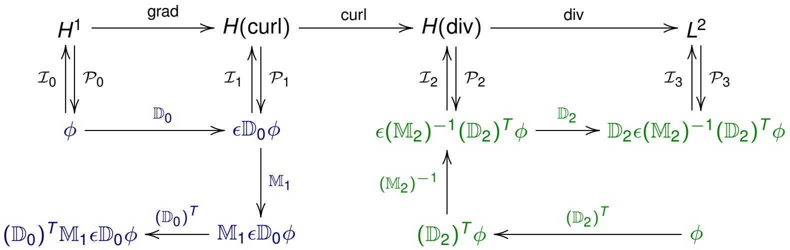
Dual discretization: $\mathbb{D}_2 \epsilon (\mathbb{M}_2)^{-1} (\mathbb{D}_2)^T \phi = f$

$$\phi \xrightarrow{\mathbb{D}_0} \epsilon\mathbb{D}_0\phi \xrightarrow{\mathbb{M}_1} \mathbb{M}_1\epsilon\mathbb{D}_0\phi \xrightarrow{(\mathbb{D}_0)^T} (\mathbb{D}_0)^T\mathbb{M}_1\epsilon\mathbb{D}_0\phi$$

$$\phi \xrightarrow{(\mathbb{D}_2)^T} (\mathbb{D}_2)^T\phi \xrightarrow{(\mathbb{M}_2)^{-1}} \epsilon(\mathbb{M}_2)^{-1}(\mathbb{D}_2)^T\phi \xrightarrow{\mathbb{D}_2} \mathbb{D}_2\epsilon(\mathbb{M}_2)^{-1}(\mathbb{D}_2)^T\phi$$

DEC for LPBE

The two discretizations inside the DEC-deRham diagram:



The definition of the discrete Hodge star matrix $\mathbb{M}_k$ and its inverse are essential in ensuring the robustness of a primal or dual discretization.

Further Examples

- **Maxwell's Curl Equations**

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

$$\begin{array}{lccc}
\text{primal:} & \vec{E} & \xrightarrow{\mathbb{D}_1} & \mathcal{C}^2 \\
 & (\mathbb{M}_1)^{-1} \uparrow \downarrow \mathbb{M}_1 & & (\mathbb{M}_2)^{-1} \uparrow \downarrow \mathbb{M}_2 \\
\text{dual:} & \overline{\mathcal{C}}^2 & \xleftarrow[(\mathbb{D}_1)^T]{} & \vec{H}
\end{array}$$

- **Darcy Flow**

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

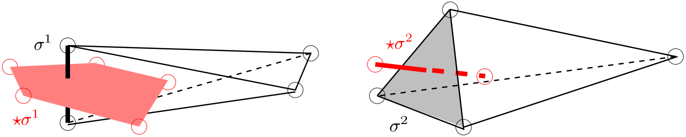
$$\begin{array}{lccc}
\text{primal:} & p & \xrightarrow{\mathbb{D}_0} & \begin{array}{c} \mathbb{D}_0 p \\ (\mathbb{M}_1^{Dual})^{-1} \vec{f} \end{array} \\
 & & & \uparrow (\mathbb{M}_1^{Dual})^{-1} \\
\text{dual:} & (\mathbb{D}_0)^T \vec{f} & \xleftarrow[(\mathbb{D}_0)^T]{} & \vec{f}
\end{array}
\qquad
\begin{array}{ccc}
\vec{f} & \xrightarrow{\mathbb{D}_2} & \mathbb{D}_2 \vec{f} \\
\downarrow \mathbb{M}_2^{Diag} & & \\
\begin{array}{c} \mathbb{M}_2^{Diag} \vec{f} \\ (\mathbb{D}_2)^T p \end{array} & \xleftarrow[(\mathbb{D}_2)^T]{} & p
\end{array}$$

Outline

Discrete Hodge Star Criteria

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

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



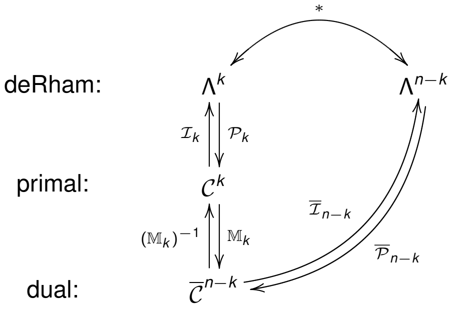
DIAGONAL	[Desbrun et al.]	$(\mathbb{M}_k^{Diag})_{ij}$	$:=$	$\frac{\lvert \star\sigma_i^k \rvert}{\lvert \sigma_j^k \rvert}\delta_{ij}$
WHITNEY	[Dodziuk],[Bell]	$(\mathbb{M}_k^{Whit})_{ij}$	$:=$	$\left(\eta_{\sigma_i^k}, \eta_{\sigma_j^k}\right)_{\mathcal{C}^k}$ $\quad (\eta_{\sigma^k} =$ Whitney k-form for $\sigma^k)$

A **robust** definition of a discrete Hodge star matrix $\mathbb{M}_k$ and its inverse should provide for:

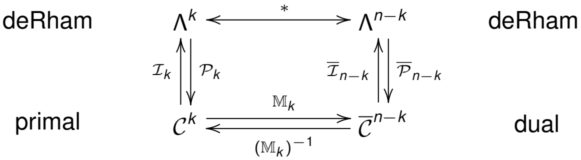
1. Commutativity of discrete dual operators
2. Local structure of $\mathbb{M}_k$ and $\mathbb{M}_k^{-1}$
3. Well-conditioned matrices

Commutativity of Discrete Dual Operators

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



Thus, we expect some commutativity of the diagram:



Commutativity of Discrete Dual Operators

$$
\begin{array}{ccccc}
\text{deRham} & \Lambda^k & \xleftrightarrow{\;*\;} & \Lambda^{n-k} & \text{deRham} \\
 & \mathcal{I}_k \uparrow \downarrow \mathcal{P}_k & & \overline{\mathcal{I}}_{n-k} \uparrow \downarrow \overline{\mathcal{P}}_{n-k} & \\
\text{primal} & \mathcal{C}^k & \underset{(\mathbb{M}_k)^{-1}}{\overset{\mathbb{M}_k}{\rightleftarrows}} & \overline{\mathcal{C}}^{n-k} & \text{dual}
\end{array}
$$

Strong commutativity at $\mathcal{C}^k$: $\quad *\mathcal{I}_k = \overline{\mathcal{I}}_{n-k}\mathbb{M}_k$

Weak commutativity at $\mathcal{C}^k$: $\quad \int_{\mathcal{T}} \alpha \wedge *\mathcal{I}_k = \int_{\mathcal{T}} \alpha \wedge \overline{\mathcal{I}}_{n-k}\mathbb{M}_k, \quad \forall \alpha \in \Lambda^k$

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

Using $\mathbb{M}_0^{Diag}$: $\quad |\mathcal{T}|\,(\alpha, \lambda_i)_{H^1} = |\star\sigma_i^0| \int_{\star\sigma_i^0} \alpha\mu, \quad \forall \alpha \in H^1$

Using $\mathbb{M}_0^{Whit}$: $\quad |\mathcal{T}|\,(\alpha, \lambda_i)_{H^1} = \sum_{\text{vertex } j} (\lambda_i, \lambda_j)_{H^1} \int_{\star\sigma_i^0} \alpha\mu, \quad \forall \alpha \in H^1$

Local Structure of $\mathbb{M}_k$ and $\mathbb{M}_k^{-1}$

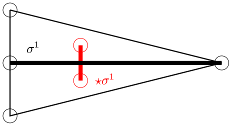
- Existing inverse discrete Hodge stars are either too full or too empty for use in discretizations on dual meshes
- We present a novel **dual** discrete Hodge star for this purpose using generalized barycentric coordinate functions (details in the paper)

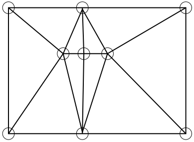
type	definition	$\mathbb{M}_k$	$\mathbb{M}_k^{-1}$
DIAGONAL	$(\mathbb{M}_k^{Diag})_{ij} = \frac{\lvert \star\, \sigma_i^k \rvert}{\lvert \sigma_j^k \rvert} \delta_{ij}$	diagonal	diagonal
WHITNEY	$(\mathbb{M}_k^{Whit})_{ij} = \left(\eta_{\sigma_i^k}, \eta_{\sigma_j^k} \right)_{\mathcal{C}^k}$	sparse	(full)
DUAL	$((\mathbb{M}_k^{Dual})^{-1})_{ij} = \left(\eta_{\star\sigma_i^k}, \eta_{\star\sigma_j^k} \right)_{\overline{\mathcal{C}}^k}$	(full)	sparse

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 σ^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.

		i	*ii*	*iii*	*iv*
DIAGONAL	$\mathbb{M}_k^{Diag}$	✓	✓	✓	✓
WHITNEY	$\mathbb{M}_k^{Whit}$	✓			✓
DUAL	$(\mathbb{M}_k^{Dual})^{-1}$		✓		✓

Questions?

- Slides available at http://www.ma.utexas.edu/users/agillette
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