New Model Stability Criteria for Mixed Finite Elements

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Outline

1. Introduction and Prior Work
2. Motivation: The DEC-deRham diagram
3. Application: Mixed Finite Element Problems
4. New Stability Criteria for Dual Variables
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Motivation

Biological modeling requires **stable** computational methods to solve PDEs.

Electromagnetics  Electrodiffusion  Elasticity

These methods must accommodate:

- multiple variables
- large meshes
- multi-scale phenomena

What does **stability** mean in such contexts?
Problem Statement

A computational method for solving PDEs should exhibit

- **Model Stability**: Computed solutions are found in a subspace of the solution space for the smooth problem
  
  *Criterion*: Solution spaces for variables respect the deRham sequence.

- **Discretization Stability**: Computed solutions converge as mesh size $h$ decreases and/or polynomial degree of approximation $p$ increases
  
  *Criterion*: The LBB inf-sup condition is satisfied.

- **Numerical Stability**: Calculation of the numerical solution has controlled computational complexity.
  
  *Criterion*: Matrices inverted by the linear solver are well-conditioned.

**Problem Statement**

Use the theory of Discrete Exterior Calculus to evaluate the stability of existing computational methods for PDEs arising in biology and create novel methods with improved stability. **This talk’s focus: model stability.**
Selected Prior Work

- Importance of differential geometry in computational methods for electromagnetics:
  
  **BOSSAVIT** *Computational Electromagnetism* Academic Press Inc. 1998

- Primer on DEC theory and program of work:
  
  **DESBRUN, HIRANI, LEOK, MARSDEN** *Discrete Exterior Calculus* arXiv:math/0508341v2 [math.DG], 2005

- Generalization of deRham diagram criteria for model stability:
  

- Applications of DEC to electromagnetics, Darcy flow, and elasticity problems:
  


  **YAVARI** *On geometric discretization of elasticity* Journal of Mathematical Physics, 49(2):022901-1–36, 2008
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(Smooth) Exterior Calculus

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

- The exterior derivative $d$ generalizes common differential operators.

\[
\Lambda^0(\Omega) \xrightarrow{d_0 \text{ grad}} \Lambda^1(\Omega) \xrightarrow{d_1 \text{ curl}} \Lambda^2(\Omega) \xrightarrow{d_2 \text{ div}} \Lambda^3(\Omega)
\]

- The Hodge Star transfers information between complementary dimensions.

\[
\Lambda^0(\Omega) \leftrightarrow * \rightarrow \Lambda^3(\Omega) \\
\Lambda^1(\Omega) \leftrightarrow * \rightarrow \Lambda^2(\Omega)
\]

Fundamental “Theorem” of Discrete Exterior Calculus

Stable computational methods must recreate the essential properties of smooth 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 is $\mathbb{D} = (\partial)^T$, the transpose of the boundary operator.

- The discrete Hodge Star $\mathbb{M}$ transfers information between complementary dimensions on dual meshes.
The Importance of Cohomology

Cohomology classes represent the different types of solutions permitted by the topology of the space.

The solution spaces for a discrete method should include representatives from all cohomology classes. Hence model stability requires that the top and bottom sequences have the same cohomology.

Example: The torus has two non-zero cohomology classes in dimension 1.

\[
\begin{align*}
\Lambda^0 & \xrightarrow{d_0} \Lambda^1 \xrightarrow{d_1} \Lambda^2 \xrightarrow{d_2} \Lambda^3 \\
C^0 & \xrightarrow{D_0} C^1 \xrightarrow{D_1} C^2 \xrightarrow{D_2} C^3
\end{align*}
\]

Cohomology at \( \Lambda^1 \) := \( \ker d_1 / \im d_0 \)

\( \parallel \) (if stable)

Cohomology at \( C^1 \) := \( \ker D_1 / \im D_0 \)
Mixed finite element methods

Mixed finite element methods seek solutions in subspaces of the $L^2$ deRham sequence.

$$
\begin{align*}
H^1 & \xrightarrow{d_0 \text{ grad}} H(\text{curl}) & H(\text{curl}) & \xrightarrow{d_1 \text{ curl}} H(\text{div}) & H(\text{div}) & \xrightarrow{d_2 \text{ div}} L^2 \\
I_0 & \downarrow P_0 & I_1 & \downarrow P_1 & I_2 & \downarrow P_2 & I_3 & \downarrow P_3 \\
C^0 & \xrightarrow{D_0} C^1 & C^1 & \xrightarrow{D_1} C^2 & C^2 & \xrightarrow{D_2} C^3
\end{align*}
$$

where $I$ is an interpolation map and $P$ is a projection map.

**Theorem [Arnold, Falk, Winther]**

If $I_k$ is Whitney interpolation and $P_{k+1} d_k = D_k P_k$ then the top and bottom sequences have the same cohomology.

**Proof:** The cohomology induced by Whitney interpolation is the simplicial cohomology [Whitney 1957] which is isomorphic to the deRham cohomology [deRham]. □

Whitney interpolation provides for model stability in simple cases.
The DEC-deRham Diagram for $\mathbb{R}^3$

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

The combined diagram helps elucidate primal and dual formulations of finite element methods.
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Poisson Problem - Primal

The smooth Poisson problem on a domain \( \Omega \subset \mathbb{R}^3 \) is

\[
\begin{aligned}
\Delta u &= f \quad \text{in} \ \Omega \\
\frac{\partial u}{\partial n} &= 0 \quad \text{on} \ \partial \Omega
\end{aligned}
\]

Typical primal discretization:

\[
\mathcal{D}_0^T M_1 \mathcal{D}_0 u = f
\]

Portion of DEC-deRham diagram:

Poisson Problem - Dual

\[ \begin{cases} \Delta u = f & \text{in } \Omega \\ \frac{\partial u}{\partial n} = 0 & \text{on } \partial \Omega \end{cases} \]

- \( u \) is a 0-form but it need not be discretized on a primal mesh.
- From the DEC-deRham diagram, we can derive a dual discretization.

**Primal discretization:**

\[
D_0^T M_1 D_0 u = f
\]

**Dual discretization:**

\[
D_2 (M_2)^{-1} (D_2)^T u = f.
\]

The dual discretization may offer improved stability (model, discretization, or numerical).
Darcy Flow in $\mathbb{R}^3$ - Primal Flux

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

- $\vec{f} \in C^2$ is the volumetric flux through faces of the \textbf{primal} mesh
- $p \in \overline{C}^0$ is the pressure at vertices of the \textbf{dual} mesh
- $k$ and $\mu$ are constants

Mixed (primal + dual) discretization:

\[
\begin{bmatrix}
-(\mu/k)M_2 & D_2^T \\
D_2 & 0
\end{bmatrix}
\begin{bmatrix}
\vec{f} \\
p
\end{bmatrix} =
\begin{bmatrix}
0 \\
\phi
\end{bmatrix}.
\]

Ref: Hirani, Nakshatrala, Chaudhry, 2008
Darcy Flow in $\mathbb{R}^3$ - Dual Flux

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

An equally valid discretization is as follows:

- $\vec{f} \in \mathcal{C}^2$ is the volumetric flux through faces of the dual mesh
- $p \in \mathcal{C}^0$ is the pressure at vertices of the primal mesh

New mixed discretization:

\[
\begin{bmatrix}
-(\mu/k)M^{-1}_1 & D_0 \\
(D_0)^T & 0
\end{bmatrix}
\begin{bmatrix}
\vec{f} \\
p
\end{bmatrix}
= \begin{bmatrix}
0 \\
\phi
\end{bmatrix}.
\]

\[
p \xrightarrow{D_0} (M_1)^{-1}\vec{f} \xleftarrow{(D_0)^T} (D_0)p
\]
Stability Criteria for Dual Variables

The Arnold-Falk-Winhther model stability criteria only considers primal discretizations:

DEC-based mixed finite element methods require additional criteria for model stability.
If we have projection to or interpolation from a dual mesh, we have the maps:

**smooth:**

\[ \Lambda^k \xrightarrow{\mathcal{I}_k} \mathcal{P}_k \xleftarrow{} \Lambda^{n-k} \]

\[ \Lambda^k \xleftarrow{\mathcal{P}_k} \mathcal{I}_k \xrightarrow{} \Lambda^{n-k} \]

**primal:**

\[ C^k \xrightarrow{\mathcal{M}_k} \mathcal{I}_{n-k} \xleftarrow{} C^{n-k} \]

\[ C^k \xleftarrow{\mathcal{I}_{n-k}} \mathcal{M}_k \xrightarrow{} C^{n-k} \]

**dual:**

\[ \mathcal{C}^{n-k} \xrightarrow{\mathcal{P}_{n-k}} \mathcal{I}_{n-k} \xleftarrow{} \mathcal{C}^k \]

\[ \mathcal{C}^{n-k} \xleftarrow{\mathcal{I}_{n-k}} \mathcal{P}_{n-k} \xrightarrow{} \mathcal{C}^k \]

More concisely, we expect some commutativity of the diagram:
Stability Criteria for Dual Variables

We identify four “subcommutativity” conditions:

Commutativity at $\Lambda^k$:
$$\mathcal{M}_k \mathcal{P}_k = \overline{\mathcal{P}}_{n-k}^*$$

Commutativity at $\mathcal{C}^k$:
$$*\mathcal{I}_k = \overline{\mathcal{I}}_{n-k} \mathcal{M}_k$$

Commutativity at $\Lambda^{n-k}$:
$$(\mathcal{M}_k)^{-1} \overline{\mathcal{P}}_{n-k} = \mathcal{P}_k^*$$

Commutativity at $\overline{\mathcal{C}}^{n-k}$:
$$\mathcal{I}_k (\mathcal{M}_k)^{-1} = *\overline{\mathcal{I}}_{n-k}$$

To evaluate these conditions, we must now define the various maps involved.
The **smooth Hodge star** is defined as the unique map $\star : \Lambda^k \to \Lambda^{n-k}$ satisfying the property
\[ \alpha \wedge \star \beta = (\alpha, \beta)_{\Lambda^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k \]

- $\wedge$ denotes the wedge product
- $(\cdot, \cdot)_{\Lambda^k}$ denotes the inner product on $k$-forms
- $\mu$ is the volume $n$-form on the domain

**Example 1:** In $\mathbb{R}^3$, let $\alpha = \beta = dx$. Then
\[ \alpha \wedge \star \beta = dx \wedge \star dx = dx \wedge dydz = \mu = (dx, dx)_{\Lambda^k} \mu = (\alpha, \beta)_{\Lambda^k} \mu \]

**Example 2:** In $\mathbb{R}^3$, let $\alpha = dx, \beta = dy$. Then
\[ \alpha \wedge \star \beta = dx \wedge \star dy = dx \wedge (-dxdz) = 0 = (dx, dy)_{\Lambda^k} \mu = (\alpha, \beta)_{\Lambda^k} \mu \]
Whitney Interpolation

The **Whitney k-form** $\eta_{\sigma^k}$ is associated to the $k$-simplex $\sigma^k$ in the primal mesh.

\[
\begin{align*}
\sigma^0 & := [v_i] & \eta_{\sigma^0} & := \lambda_i \\
\sigma^1 & := [v_i, v_j] & \eta_{\sigma^1} & := \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i \\
\sigma^2 & := [v_i, v_j, v_k] & \eta_{\sigma^2} & := 2 \left( \lambda_i \nabla \lambda_j \times \nabla \lambda_k + \lambda_j \nabla \lambda_k \times \nabla \lambda_i + \lambda_k \nabla \lambda_i \times \nabla \lambda_j \right) \\
\sigma^3 & := [v_i, v_j, v_k, v_l] & \eta_{\sigma^3} & := \chi_{\sigma^3} = \begin{cases} 
1 & \text{on } \sigma^3 \\
0 & \text{otherwise}
\end{cases}
\end{align*}
\]

where $\lambda_i$ denotes the barycentric function for vertex $v_i$.

The **Whitney interpolant** $I_k$ of a $k$-cochain $\omega$, is

\[
I_k(\omega) := \sum_{\sigma^k \in C_k} \omega(\sigma^k) \eta_{\sigma^k}.
\]

Examples of Whitney 1-forms associated to horizontal and vertical edges, respectively.
Commutativity at $C^k$

Commutativity at $C^k$:  
\[ \star I_k = \overline{I}_{n-k}M_k \]

Smooth Hodge star:  
\[ \alpha \wedge \star \beta = (\alpha, \beta)_{\wedge^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k \]

Whitney interpolant:  
\[ I_k(\omega) = \sum_{\sigma^k \in C_k} \omega(\sigma^k)\eta_{\sigma^k} \]

It suffices to show that for any test function $\alpha \in \Lambda^k$

\[ \alpha \wedge \star I_k = \alpha \wedge \overline{I}_{n-k}M_k. \]

Check on a basis \( \{\omega_i^k\} \) where $\omega_i^k$ is 1 on $\sigma_i^k$ and 0 on all other $k$-simplices:

\[ \alpha \wedge \star I_k(\omega_i^k) = \alpha \wedge \overline{I}_{n-k}(M_k\omega_i^k). \]

Use the definitions of $I_k$ and $\star$ to derive the condition:

\[ (\alpha, \eta_{\sigma_i^k})_{\wedge^k} \mu = \alpha \wedge \overline{I}_{n-k}(M_k\omega_i^k). \]

This condition motivates definitions of the dual interpolant $\overline{I}_{n-k}$ and the discrete Hodge star $M_k$ that ensure model stability.
Commutativity at $\bar{C}^{n-k}$

Commutativity at $\bar{C}^{n-k}$:  \[ I_k(M_k)^{-1} = *I_{n-k} \]

Smooth Hodge star:  \[ \alpha \wedge *\beta = (\alpha, \beta)_{\Lambda^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k \]

Whitney interpolant:  \[ I_k(\omega) = \sum_{\sigma^k \in C_k} \omega(\sigma^k)\eta_{\sigma^k} \]

It suffices to show that for any test function $\alpha \in \Lambda^{n-k}$

\[ \alpha \wedge *I_{n-k} = \alpha \wedge I_k(M_k)^{-1}. \]

Check on a basis $\{\bar{\omega}_i^{n-k}\}$ where $\bar{\omega}_i^{n-k}$ is 1 on $*\sigma_i^k$ and 0 on all other duals of $k$-simplices:

\[ \alpha \wedge *I_{n-k}(\bar{\omega}_i^{n-k}) = \alpha \wedge I_k(M_k)^{-1}(\bar{\omega}_i^{n-k}). \]

Supposing that $I_{n-k}(\bar{\omega}_i^{n-k}) = \eta_{*\sigma_i^k}$, we have

\[ (\alpha, \eta_{*\sigma_i^k})_{\Lambda^{n-k}} \mu = \alpha \wedge I_k(M_k)^{-1}(\bar{\omega}_i^{n-k}). \]

This complementary condition also motivates definitions of the dual interpolant $I_{n-k}$ and the discrete Hodge star $M_k$. 
We check for commutativity of the pressure data, i.e. at $C^0$ with $n = 3$, $k = 0$:

$$\begin{pmatrix} \alpha, \eta_{\sigma^0} \end{pmatrix}_{H^1} \mu = \alpha \wedge \overline{I}_3(\mathbb{M}_0 \omega^0_i) \quad \forall \alpha \in H^1$$

We use the Hodge star proposed by the authors of the paper

$$(\mathbb{M}_0)_{ii} := \frac{|\star \sigma_i^k|}{|\sigma_i^k|}$$

We use any dual interpolant $\overline{I}_3$ mimicking Whitney forms, i.e.

$$\overline{I}_3(\omega) := \sum_{\star \sigma^0 \in \mathcal{C}_3} \omega(\star \sigma^0) \chi_{\star \sigma^0}$$
Criteria Applied to Darcy Flow - Dual Flux

The left side:

\[ \left( \alpha, \eta_{\sigma_i^0} \right)_{H^1} \mu = (\alpha, \lambda_i)_{H^1} \mu \]
\[ = \left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu \]

The right side:

\[ \alpha \wedge \overline{I}_3(\mathbb{M}_0 \omega_i^0) = \alpha \wedge \sum_{\star \sigma^0 \in \mathcal{C}_3} (\mathbb{M}_0^{\text{Diag}} \omega_i)(\star \sigma^0) \chi_{\star \sigma^0} \mu \]
\[ = \alpha \wedge |\star \sigma_i^0| \chi_{\star \sigma^0} \mu \]
\[ = \alpha |\star \sigma_i^0| \chi_{\star \sigma^0} \mu \]

The condition:

\[ \left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu = \alpha |\star \sigma_i^0| \chi_{\star \sigma^0} \mu \quad \forall \alpha \in H^1 \]
Similarly, we can check for commutativity at $\overline{C}^0$ for the primal flux version.

$$\left( \int_K \alpha(x) \overline{\lambda}_i(x) \, dx \right) \mu = \alpha \sigma_i^3 \chi_{\sigma_i^3} \mu \quad \forall \alpha \in L^2$$
Dual flux condition:

\[
\left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu = \alpha \left| \star \sigma^0_i \right| \chi \star \sigma^0_i \mu \quad \forall \alpha \in H^1
\]

Primal flux condition:

\[
\left( \int_K \alpha(x) \lambda_i(x) dx \right) \mu = \alpha \left| \sigma^3_i \right| \chi \sigma^3_i \mu \quad \forall \alpha \in L^2
\]

- In both instances, an arbitrary test function \( \alpha \) must be approximately constant on a neighborhood of vertex \( i \) and this constant is a multiple of a measure of the region and an integral involving \( \alpha \).
- This is certainly false in general, as \( L^2 \) or \( H^1 \) functions need not be locally constant.
- Hence, the diagonal Hodge star espoused by the authors does not provide a stable method in the general setting, in either of the possible mixed finite element methods.
Additional Research Directions

- Evaluate alternate definitions of $\mathbb{M}_k$ for our model stability commutativity conditions.
- Define dual interpolants $\overline{I}_k$ mimicking Whitney primal interpolants.
- Define $\mathbb{M}_k^{-1}$ using dual interpolants to avoid inverting sparse matrices.
- Compare discretization and numerical stability for these definitions to existing methods.
- Derive model stability criteria for the elasticity complex which involves vector-valued and tensor-valued forms.
Questions?

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