

# New Model Stability Criteria for Mixed Finite Elements

Andrew Gillette

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

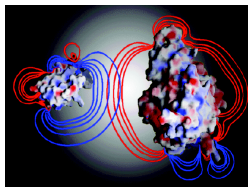
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- 1 Introduction and Prior Work
- 2 Motivation: The DEC-deRham diagram
- 3 Application: Mixed Finite Element Problems
- 4 New Stability Criteria for Dual Variables

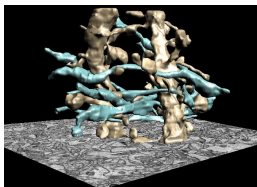
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# Motivation

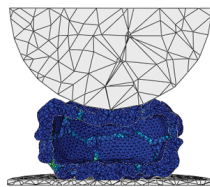
Biological modeling requires **stable** computational methods to solve PDEs



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:

**ARNOLD, FALK, WINTHER** *Finite element exterior calculus, homological techniques, and applications* Acta Numerica, 15:1-155, 2006.

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

**HE, TEIXEIRA** *Geometric finite element discretization of Maxwell equations in primal and dual spaces* Physics Letters A, 349(1-4):1–14, 2006

**HIRANI, NAKSHATRALA, CHAUDHRY** *Numerical method for Darcy Flow derived using Discrete Exterior Calculus* arXiv:0810.3434v1 [math.NA], 2008

**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.

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

- The Hodge Star transfers information between complementary dimensions.

$$\Lambda^0(\Omega) \longleftarrow * \longrightarrow \Lambda^3(\Omega)$$

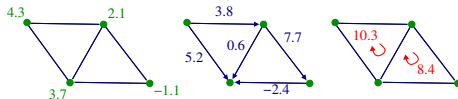
$$\Lambda^1(\Omega) \longleftarrow * \longrightarrow \Lambda^2(\Omega)$$

## 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

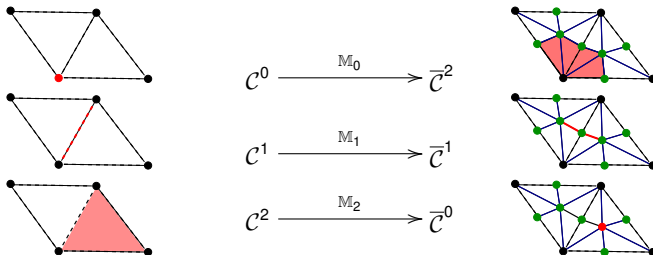
- Discrete differential  $k$ -forms are  $k$ -cochains, i.e. linear functions on  $k$ -simplices.



- The discrete exterior derivative is  $\mathbb{D} = (\partial)^T$ , the transpose of the boundary operator.

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

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



# The Importance of Cohomology

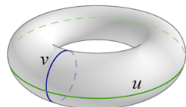
$$\Lambda^0 \xrightarrow[\text{grad}]{d_0} \Lambda^1 \xrightarrow[\text{curl}]{d_1} \Lambda^2 \xrightarrow[\text{div}]{d_2} \Lambda^3$$

$$\mathcal{C}^0 \xrightarrow{\mathbb{D}_0} \mathcal{C}^1 \xrightarrow{\mathbb{D}_1} \mathcal{C}^2 \xrightarrow{\mathbb{D}_2} \mathcal{C}^3$$

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.



$$\text{Cohomology at } \Lambda^1 := \ker d_1 / \text{im } d_0$$

|| (if stable)

$$\text{Cohomology at } \mathcal{C}^1 := \ker \mathbb{D}_1 / \text{im } \mathbb{D}_0$$

# Mixed finite element methods

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

$$\begin{array}{ccccccc} H^1 & \xrightarrow[\text{grad}]{d_0} & H(\text{curl}) & \xrightarrow[\text{curl}]{d_1} & H(\text{div}) & \xrightarrow[\text{div}]{d_2} & L^2 \\ \mathcal{I}_0 \updownarrow \mathcal{P}_0 & & \mathcal{I}_1 \updownarrow \mathcal{P}_1 & & \mathcal{I}_2 \updownarrow \mathcal{P}_2 & & \mathcal{I}_3 \updownarrow \mathcal{P}_3 \\ C^0 & \xrightarrow{\mathbb{D}_0} & C^1 & \xrightarrow{\mathbb{D}_1} & C^2 & \xrightarrow{\mathbb{D}_2} & C^3 \end{array}$$

where  $\mathcal{I}$  is an interpolation map and  $\mathcal{P}$  is a projection map.

## Theorem [Arnold, Falk, Winther]

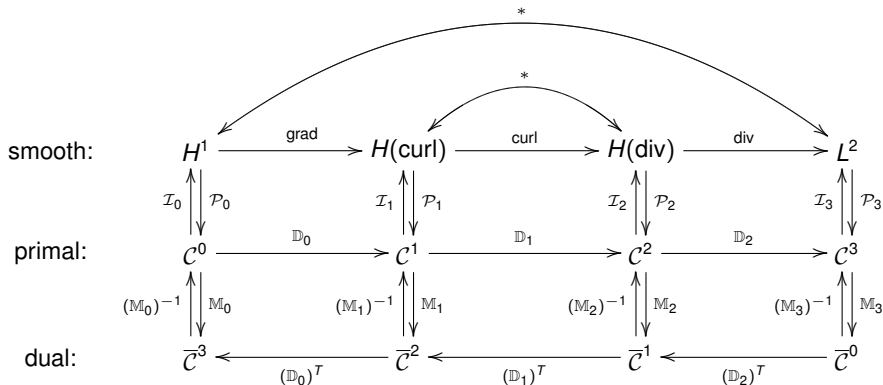
If  $\mathcal{I}_k$  is Whitney interpolation and  $\mathcal{P}_{k+1}d_k = \mathbb{D}_k\mathcal{P}_k$  then the top and bottom sequences have the same cohomology.

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

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.

# Outline

- 1 Introduction and Prior Work
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- 4 New Stability Criteria for Dual Variables

# Poisson Problem - Primal

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

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

Typical primal discretization:

$$\mathbb{D}_0^T \mathbb{M}_1 \mathbb{D}_0 u = f$$

Portion of DEC-deRham diagram:

$$\begin{array}{ccc} u & \xrightarrow{\mathbb{D}_0} & \mathbb{D}_0 u \\ & & \downarrow \mathbb{M}_1 \\ (\mathbb{D}_0)^T \mathbb{M}_1 \mathbb{D}_0 u & \xleftarrow{(\mathbb{D}_0)^T} & \mathbb{M}_1 \mathbb{D}_0 u \end{array}$$

Ref: W.N. Bell, Dissertation, 2008.

# 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:

$$\mathbb{D}_0^T \mathbb{M}_1 \mathbb{D}_0 u = f$$

$$\begin{array}{ccc} u & \xrightarrow{\mathbb{D}_0} & \mathbb{D}_0 u \\ & & \downarrow \mathbb{M}_1 \\ (\mathbb{D}_0)^T \mathbb{M}_1 \mathbb{D}_0 u & \xleftarrow{(\mathbb{D}_0)^T} & \mathbb{M}_1 \mathbb{D}_0 u \end{array}$$

Dual discretization:

$$\mathbb{D}_2 (\mathbb{M}_2)^{-1} (\mathbb{D}_2)^T u = f.$$

$$\begin{array}{ccc} (\mathbb{M}_2)^{-1} (\mathbb{D}_2)^T u & \xrightarrow{\mathbb{D}_2} & \mathbb{D}_2 (\mathbb{M}_2)^{-1} (\mathbb{D}_2)^T u \\ \uparrow (\mathbb{M}_2)^{-1} & & \\ (\mathbb{D}_2)^T u & \xleftarrow{(\mathbb{D}_2)^T} & u \end{array}$$

- The dual discretization may offer improved stability (model, discretization, or numerical).

# Darcy Flow in $\mathbb{R}^3$ - Primal Flux

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

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

Mixed (primal + dual) discretization:

$$\begin{bmatrix} -(\mu/k)\mathbb{M}_2 & \mathbb{D}_2^T \\ \mathbb{D}_2 & 0 \end{bmatrix} \begin{bmatrix} \vec{f} \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ \phi \end{bmatrix}.$$

$$\begin{array}{ccc} \vec{f} & \xrightarrow{\mathbb{D}_2} & \mathbb{D}_2 \vec{f} \\ \downarrow \mathbb{M}_2 & & \\ \mathbb{M}_2 \vec{f} & & \\ (\mathbb{D}_2)^T p & \xleftarrow{(\mathbb{D}_2)^T} & p \end{array}$$

Ref: Hirani, Nakshatrala, Chaudhry, 2008

# Darcy Flow in $\mathbb{R}^3$ - Dual Flux

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

An equally valid discretization is as follows:

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

New mixed discretization:

$$\begin{bmatrix} -(\mu/k)\mathbb{M}_1^{-1} & \mathbb{D}_0 \\ (\mathbb{D}_0)^T & 0 \end{bmatrix} \begin{bmatrix} \vec{f} \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ \phi \end{bmatrix}.$$

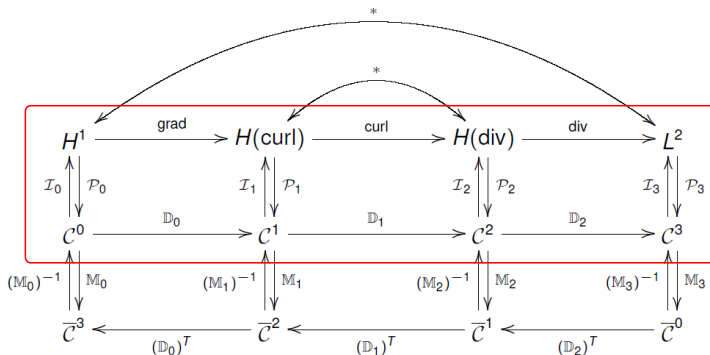
$$\begin{array}{ccc} p & \xrightarrow{\mathbb{D}_0} & (\mathbb{M}_1)^{-1} \vec{f} \\ & & \mathbb{D}_0 p \\ & & \uparrow \\ & & (\mathbb{M}_1)^{-1} \\ (\mathbb{D}_0)^T \vec{f} & \xleftarrow{(\mathbb{D}_0)^T} & \vec{f} \end{array}$$

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# Stability Criteria for Dual Variables

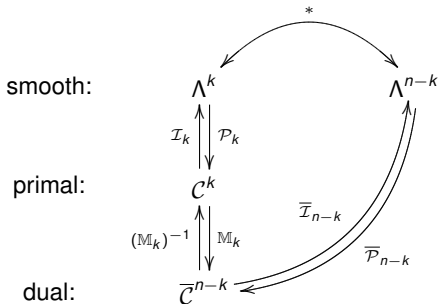
The Arnold-Falk-Winther model stability criteria only considers primal discretizations:



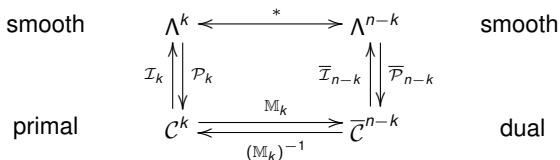
DEC-based mixed finite element methods require additional criteria for model stability.

# Stability Criteria for Dual Variables

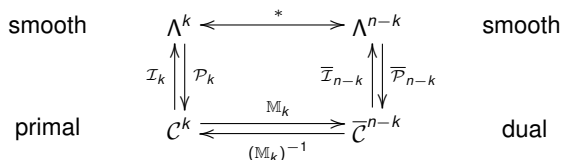
If we have projection to or interpolation from a dual mesh, we have the maps:



More concisely, we expect some commutativity of the diagram:



# Stability Criteria for Dual Variables



We identify four “subcommutativity” conditions:

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

To evaluate these conditions, we must now define the various maps involved.

# Smooth Hodge Star

The **smooth Hodge star** is defined as the unique map  $*$  :  $\Lambda^k \rightarrow \Lambda^{n-k}$  satisfying the property

$$\alpha \wedge * \beta = (\alpha, \beta)_{\Lambda^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k$$

- $\wedge$  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

$$\alpha \wedge * \beta = dx \wedge * dx = dx \wedge dydz = \mu = (dx, dx)_{\Lambda^k} \mu = (\alpha, \beta)_{\Lambda^k} \mu$$

**Example 2:** In  $\mathbb{R}^3$ , let  $\alpha = dx, \beta = dy$ . Then

$$\alpha \wedge * \beta = dx \wedge * dy = dx \wedge (-dx dz) = 0 = (dx, dy)_{\Lambda^k} \mu = (\alpha, \beta)_{\Lambda^k} \mu$$

# Whitney Interpolation

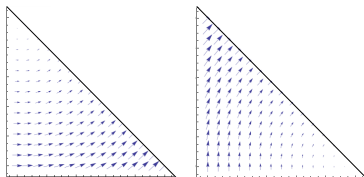
The **Whitney  $k$ -form**  $\eta_{\sigma^k}$  is associated to the  $k$ -simplex  $\sigma^k$  in the primal mesh.

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

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

The **Whitney interpolant**  $\mathcal{I}_k$  of a  $k$ -cochain  $\omega$ , is

$$\mathcal{I}_k(\omega) := \sum_{\sigma^k \in \mathcal{C}_k} \omega(\sigma^k) \eta_{\sigma^k}.$$



Examples of Whitney 1-forms associated to horizontal and vertical edges, respectively

# Commutativity at $\mathcal{C}^k$

$$\begin{aligned}\text{Commutativity at } \mathcal{C}^k: \quad * \mathcal{I}_k &= \bar{\mathcal{I}}_{n-k} \mathbb{M}_k \\ \text{Smooth Hodge star:} \quad \alpha \wedge * \beta &= (\alpha, \beta)_{\Lambda^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k \\ \text{Whitney interpolant:} \quad \mathcal{I}_k(\omega) &= \sum_{\sigma^k \in \mathcal{C}_k} \omega(\sigma^k) \eta_{\sigma^k}\end{aligned}$$

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

$$\alpha \wedge * \mathcal{I}_k = \alpha \wedge \bar{\mathcal{I}}_{n-k} \mathbb{M}_k.$$

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

$$\alpha \wedge * \mathcal{I}_k(\omega_i^k) = \alpha \wedge \bar{\mathcal{I}}_{n-k}(\mathbb{M}_k \omega_i^k).$$

Use the definitions of  $\mathcal{I}_k$  and  $*$  to derive the condition:

$$(\alpha, \eta_{\sigma_i^k})_{\Lambda^k} \mu = \alpha \wedge \bar{\mathcal{I}}_{n-k}(\mathbb{M}_k \omega_i^k).$$

This condition motivates definitions of the dual interpolant  $\bar{\mathcal{I}}_{n-k}$  and the discrete Hodge star  $\mathbb{M}_k$  that ensure model stability.

# Commutativity at $\bar{\mathcal{C}}^{n-k}$

$$\begin{aligned} \text{Commutativity at } \bar{\mathcal{C}}^{n-k}: \quad \mathcal{I}_k(\mathbb{M}_k)^{-1} &= *\bar{\mathcal{I}}_{n-k} \\ \text{Smooth Hodge star:} \quad \alpha \wedge *\beta &= (\alpha, \beta)_{\Lambda^k} \mu, \quad \forall \alpha, \beta \in \Lambda^k \\ \text{Whitney interpolant:} \quad \mathcal{I}_k(\omega) &= \sum_{\sigma^k \in \mathcal{C}_k} \omega(\sigma^k) \eta_{\sigma^k} \end{aligned}$$

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

$$\alpha \wedge *\bar{\mathcal{I}}_{n-k} = \alpha \wedge \mathcal{I}_k(\mathbb{M}_k)^{-1}.$$

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

$$\alpha \wedge *\bar{\mathcal{I}}_{n-k}(\bar{\omega}_i^{n-k}) = \alpha \wedge \mathcal{I}_k(\mathbb{M}_k)^{-1}(\bar{\omega}_i^{n-k}).$$

Supposing that  $\bar{\mathcal{I}}_{n-k}(\bar{\omega}_i^{n-k}) = \eta_{\star\sigma_i^k}$ , we have

$$(\alpha, \eta_{\star\sigma_i^k})_{\Lambda^{n-k}} \mu = \alpha \wedge \mathcal{I}_k(\mathbb{M}_k)^{-1}(\bar{\omega}_i^{n-k}).$$

This complementary condition also motivates definitions of the dual interpolant  $\bar{\mathcal{I}}_{n-k}$  and the discrete Hodge star  $\mathbb{M}_k$ .

# Criteria Applied to Darcy Flow - Dual Flux

$$\begin{array}{ccc} \rho & \xrightarrow{\mathbb{D}_0} & (\mathbb{M}_1)^{-1} \vec{f} \\ & & \mathbb{D}_0 \rho \\ & & \uparrow \\ & & (\mathbb{M}_1)^{-1} \\ (\mathbb{D}_0)^T \vec{f} & \xleftarrow{(\mathbb{D}_0)^T} & \vec{f} \end{array}$$

We check for commutativity of the pressure data, i.e. at  $\mathcal{C}^0$  with  $n = 3$ ,  $k = 0$ :

$$\left( \alpha, \eta_{\sigma_i^0} \right)_{H^1} \mu = \alpha \wedge \bar{\mathcal{I}}_3(\mathbb{M}_0 \omega_i^0) \quad \forall \alpha \in H^1$$

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  $\bar{\mathcal{I}}_3$  mimicking Whitney forms, i.e.

$$\bar{\mathcal{I}}_3(\bar{\omega}) := \sum_{\star \sigma^0 \in \bar{\mathcal{C}}_3} \bar{\omega}(\star \sigma^0) \chi_{\star \sigma^0}$$

# Criteria Applied to Darcy Flow - Dual Flux

The left side:

$$\begin{aligned}(\alpha, \eta_{\sigma_i^0})_{H^1} \mu &= (\alpha, \lambda_i)_{H^1} \mu \\ &= \left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu\end{aligned}$$

The right side:

$$\begin{aligned}\alpha \wedge \bar{\mathcal{I}}_3(\mathbb{M}_0 \omega_i^0) &= \alpha \wedge \sum_{\star \sigma^0 \in \bar{\mathcal{C}}_3} (\mathbb{M}_0^{Diag} \omega_i)(\star \sigma^0) \chi_{\star \sigma^0} \mu \\ &= \alpha \wedge | \star \sigma_i^0 | \chi_{\star \sigma_i^0} \mu \\ &= \alpha | \star \sigma_i^0 | \chi_{\star \sigma_i^0} \mu\end{aligned}$$

The condition:

$$\left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu = \alpha | \star \sigma_i^0 | \chi_{\star \sigma_i^0} \mu \quad \forall \alpha \in H^1$$

# Criteria Applied to Darcy Flow - Primal Flux

$$\begin{array}{ccc} \vec{f} & \xrightarrow{\mathbb{D}_2} & \mathbb{D}_2 \vec{f} \\ \downarrow \mathbb{M}_2 & & \\ \mathbb{M}_2 \vec{f} & & \\ (\mathbb{D}_2)^T \rho & \xleftarrow{(\mathbb{D}_2)^T} & \rho \end{array}$$

Similarly, we can check for commutativity at  $\bar{C}^0$  for the primal flux version.

$$\left( \int_K \alpha(x) \bar{\lambda}_i(x) dx \right) \mu = \alpha |\sigma_i^3| \chi_{\sigma_i^3} \mu \quad \forall \alpha \in L^2$$

# Criteria Applied to Darcy Flow - Conclusions

Dual flux condition:

$$\left( \int_K \alpha \lambda_i + \nabla \alpha \cdot \nabla \lambda_i \right) \mu = \alpha \left| \star \sigma_i^0 \right| \chi_{\star \sigma_i^0} \mu \quad \forall \alpha \in H^1$$

Primal flux condition:

$$\left( \int_K \alpha(x) \bar{\lambda}_i(x) dx \right) \mu = \alpha \left| \sigma_i^3 \right| \chi_{\sigma_i^3} \mu \quad \forall \alpha \in L^2$$

- 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  $\bar{\mathcal{I}}_k$  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/>