Cohomology Stability Criteria for Mixed Finite Element Methods

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joint work with

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Outline

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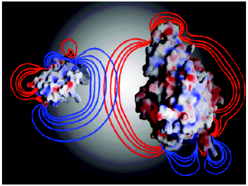
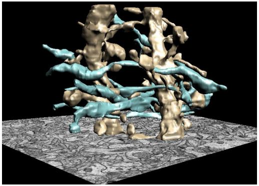
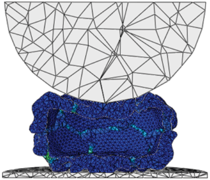
Motivation

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

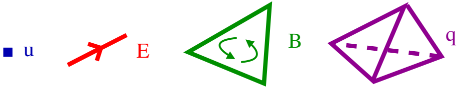
HIRANI, NAKSHATRALA, CHAUDHRY *Numerical method for Darcy Flow derived using Discrete Exterior Calculus* arXiv:0810.3434v1 [math.NA], 2008

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

Outline

(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.

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

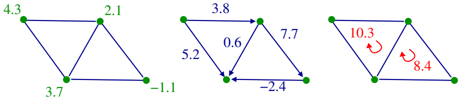
$$\Lambda^1(\Omega) \longleftarrow * \longrightarrow \Lambda^2(\Omega)$$

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

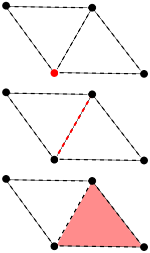
- Discrete differential k-forms are k-cochains, i.e. linear functions on k-simplices.



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

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

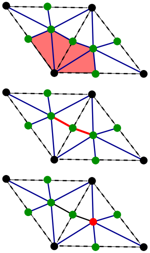
- The discrete Hodge Star $\mathbb{M}$ transfers information between complementary dimensions on **dual** meshes.



$$\mathcal{C}^0 \xrightarrow{\mathbb{M}_0} \overline{\mathcal{C}}^2$$

$$\mathcal{C}^1 \xrightarrow{\mathbb{M}_1} \overline{\mathcal{C}}^1$$

$$\mathcal{C}^2 \xrightarrow{\mathbb{M}_2} \overline{\mathcal{C}}^0$$



The Importance of Cohomology

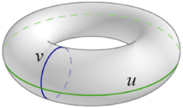
$$\Lambda^0 \xrightarrow[\text{grad}]{d_0} \Lambda^1 \xrightarrow[\text{curl}]{d_1} \Lambda^2 \xrightarrow[\text{div}]{d_2} \Lambda^3$$

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

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.



$$\begin{aligned}\text{Cohomology at } \Lambda^1 &:= \ker d_1 / \text{im } d_0 \\ &\parallel \text{(if stable)} \\ \text{Cohomology at } \mathcal{C}^1 &:= \ker \mathbb{D}_1 / \text{im } \mathbb{D}_0\end{aligned}$$

Mixed finite element methods

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

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

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

Theorem [Arnold, Falk, Winther]

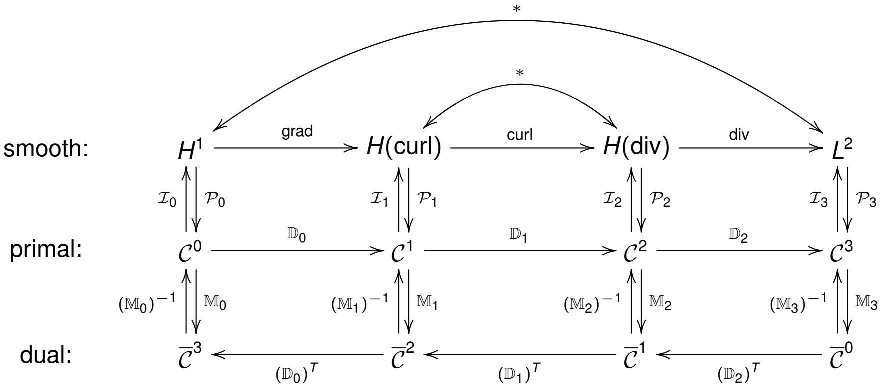
If $\mathcal{I}_k$ is Whitney interpolation and $\mathcal{P}_{k+1} d_k = \mathbb{D}_k \mathcal{P}_k$ then the top and bottom sequences have the same cohomology.

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

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.

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

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

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

Mixed (primal + dual) discretization:

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

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

Ref: Hirani, Nakshatrala, Chaudhry, 2008

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

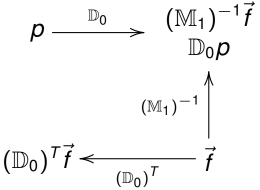
$$\begin{cases} \vec{f} + \frac{k}{\mu}\nabla p &= 0 \quad \text{in } \Omega, \\ \text{div}\vec{f} &= \phi \quad \text{in } \Omega, \\ \vec{f} &= \psi \quad \text{on } \partial\Omega, \end{cases}$$

An equally valid discretization is as follows:

- $\vec{f} \in \overline{\mathcal{C}}^2$ 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:

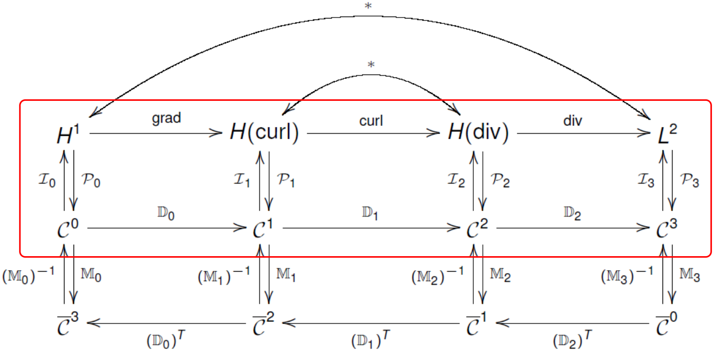
$$\begin{bmatrix} -(\mu/k)\mathbb{M}_1^{-1} & \mathbb{D}_0 \\ (\mathbb{D}_0)^T & 0 \end{bmatrix} \begin{bmatrix} \vec{f} \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ \phi \end{bmatrix}.$$



Outline

Stability Criteria for Dual Variables

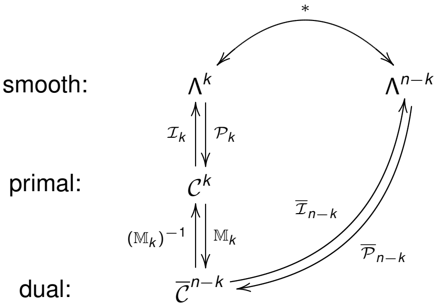
The Arnold-Falk-Winther model stability criteria only considers primal discretizations:



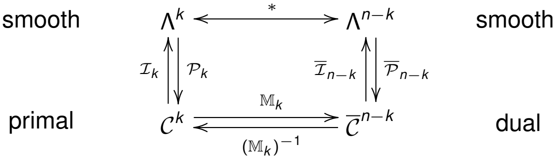
DEC-based mixed finite element methods require additional criteria for model stability.

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 commuativity of the diagram:



Stability Criteria for Dual Variables

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

We identify four “subcommutativity” conditions:

$$
\begin{array}{lrcl}
\text{Commutativity at } \Lambda^k: & \mathbb{M}_k \mathcal{P}_k & = & \overline{\mathcal{P}}_{n-k} * \\
\text{Commutativity at } \mathcal{C}^k: & * \mathcal{I}_k & = & \overline{\mathcal{I}}_{n-k} \mathbb{M}_k \\
\text{Commutativity at } \Lambda^{n-k}: & (\mathbb{M}_k)^{-1} \overline{\mathcal{P}}_{n-k} & = & \mathcal{P}_k * \\
\text{Commutativity at } \overline{\mathcal{C}}^{n-k}: & \mathcal{I}_k (\mathbb{M}_k)^{-1} & = & * \overline{\mathcal{I}}_{n-k}
\end{array}
$$

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 $* : \Lambda^k \to \Lambda^{n-k}$ 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
- μ 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

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

Whitney Interpolation

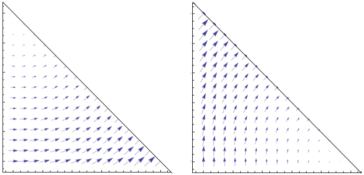
The **Whitney k-form** η_{σ^k} is associated to the k-simplex σ^k in the primal mesh.

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

where λ_i denotes the barycentric function for vertex v_i.

The **Whitney interpolant** $\mathcal{I}_k$ of a k-cochain ω, 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 $\mathcal{C}^k$

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

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

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

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

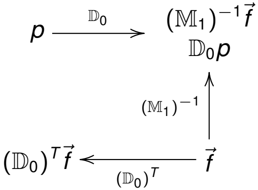
$$\alpha \wedge *\mathcal{I}_k(\omega_i^k) = \alpha \wedge \overline{\mathcal{I}}_{n-k}(\mathbb{M}_k\omega_i^k).$$

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

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

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

Criteria Applied to Darcy Flow - Dual Flux



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

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

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

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

Criteria Applied to Darcy Flow - Dual Flux

The left side:

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

The right side:

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

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 - Conclusions

Dual flux condition:

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

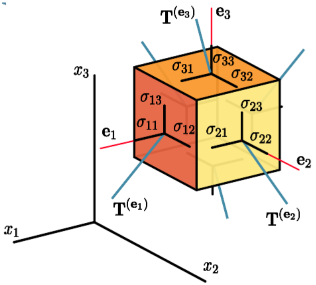
Primal flux condition:

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

- In both instances, an arbitrary test function α 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 α.
- 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.

Outline

Elasticity Basics



(image from Wikipedia)

Elasticity problems try to find the stress σ on a domain $\Omega \subset \mathbb{R}^3$ via:

$$\begin{aligned} \text{net force (known)} &= \int_\Omega \text{body forces} \\ &= \int_{\partial\Omega} \sigma \cdot \vec{n} \\ &= \int_\Omega \text{div}\sigma \end{aligned}$$

Stress is treated as a 2-tensor since it pairs with a velocity field $\vec{v}$ and $\vec{n}$

$$\begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{23} & \sigma_{33} \end{bmatrix} \begin{bmatrix} n_1 & n_2 & n_3 \end{bmatrix}^T$$

Stress is symmetric: the σ_{ii} are normal stresses while σ_{ij} are shear stresses.

Elasticity as a PDE in $\mathbb{R}^3$

Solve for stress σ and displacement u given a body force field f:

$$\begin{cases} A\sigma = {}^{\text{sym}}\vec{\nabla} u & \text{in } \Omega \\ \text{div}\sigma = f & \text{in } \Omega \end{cases}$$

where

$$u \in \mathcal{V} := \text{tangent space at } x \in \Omega \cong \mathbb{R}^3$$

$$\sigma \in \mathcal{S} := \text{symmetric second order tensors}$$

The operator ${}^{\text{sym}}\vec{\nabla}$ is the symmetric gradient:

$${}^{\text{sym}}\vec{\nabla} : \mathcal{V} \to \mathcal{S}$$

$${}^{\text{sym}}\vec{\nabla} u = \frac{1}{2} \begin{bmatrix} \partial_x \\ \partial_y \\ \partial_z \end{bmatrix} \begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \begin{bmatrix} \partial_x & \partial_y & \partial_z \end{bmatrix}$$

The operator A is called a compliance tensor:

$$A : \mathcal{S} \to \mathcal{S}$$

It describes the relation between the stress σ and strain ${}^{\text{sym}}\vec{\nabla} u$.

Elasticity Complex in $\mathbb{R}^3$

$$\begin{cases} A\sigma & = & {}^{\text{sym}}\vec{\nabla} u & \text{in } \Omega \\ \text{div}\sigma & = & f & \text{in } \Omega \end{cases}$$

$$\mathcal{V} = \text{tangent space at } x \in \Omega \cong \mathbb{R}^3$$

$$\mathcal{S} = \text{symmetric second order tensors}$$

Arnold, Falk and Winther derived the following elasticity complex:

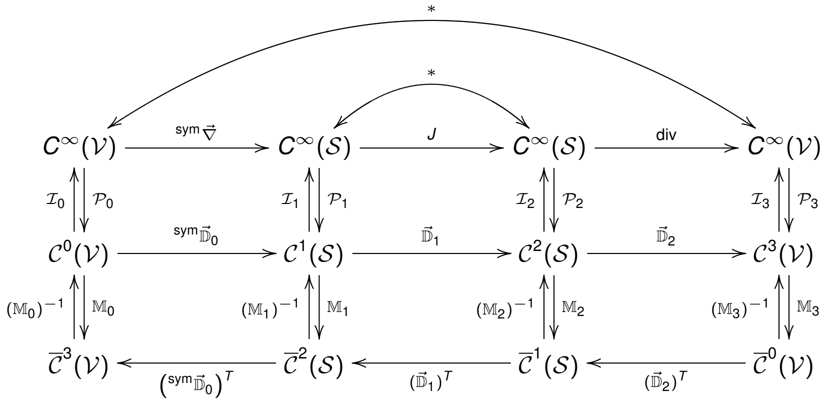
$$C^\infty(\mathcal{V}) \xrightarrow{\ {}^{\text{sym}}\vec{\nabla}\ } C^\infty(\mathcal{S}) \xrightarrow{\ J\ } C^\infty(\mathcal{S}) \xrightarrow{\ \text{div}\ } C^\infty(\mathcal{V})$$

$$u \qquad {}^{\text{sym}}\vec{\nabla} u \qquad \sigma \qquad \text{div}\sigma$$

Note that u is a V-valued 0-form while σ is a $\mathcal{S}$-valued 2-form.

DEC-deRham Elasticity Complex

Projecting to $\mathcal{V}$- and $\mathcal{S}$-valued cochain spaces yields a DEC-deRham complex for elasticity:

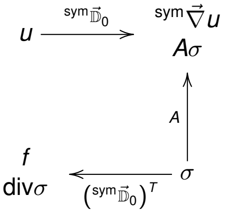


Primal-Dual Discretization

$$\begin{cases} A\sigma = {}^{\text{sym}}\vec{\nabla} u & \text{in } \Omega, \\ \text{div}\sigma = f & \text{in } \Omega, \end{cases}$$

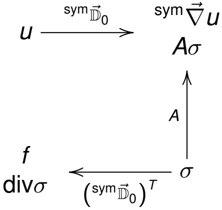
Yavari's discretization:

- $u \in \mathcal{C}^0(\mathcal{V})$ = $\mathcal{V}$-valued primal 0-cochains
- $\sigma \in \overline{\mathcal{C}}^2$ = $\mathcal{S}$-valued dual 2-cochains



This raises a number of research directions...

Additional Research Directions



- Clarify definitions of operators on vector- and matrix-valued cochains.
- Define interpolants $\mathcal{I}_k$ and projections $\mathcal{P}_k$ for these spaces.
- Derive model stability criteria for the elasticity complex.

Questions?

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