Conforming Vector Interpolation Functions for Polyhedral Meshes

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joint work with

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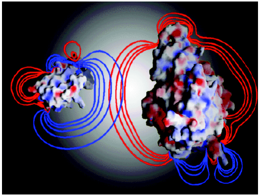
Interpolation in Graphics vs. Simulation

- Interpolation of vector fields required for geometric design.
- No natural constraints on interpolation properties.
- Some exploration of scalar interpolation over polyhedra.

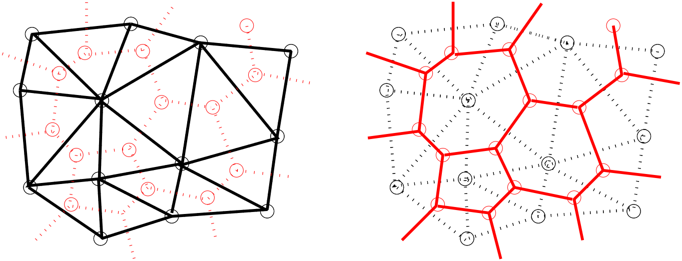


- Coupled vector fields related by integral and differential equations.
- Physical nature of problem offers natural discretizations of variables and boundary conditions.
- Discrete Exterior Calculus suggests a need for vector interpolation over polyhedra.

Goal: Develop a theory of vector interpolation over polyhedra conforming to physical requirements with provable error estimates.

Motivation

Many authors (Bossavit, Hiptmair, Shashkov, . . .) have recognized the natural interplay between **primal** and **dual** domain meshes for discretization of physical equations.



Potential benefits of a theory based on interpolation over dual meshes:

1. Accuracy vs. speed tradeoffs available between primal and dual methods.
2. Error estimates for dual interpolation methods analogous to standard estimates.
3. Validation of primal-based results with dual-based discretization methods.

Outline

Outline

$H(Curl)$ versus $H(Div)$

Throughout, we will consider a model problem from **magnetostatics**:

- **Domain**: Contractible 3-manifold $\Omega \subset \mathbb{R}^3$ with boundary Γ
- **Variables**:

  b (magnetic field / magnetic induction)

  h (magnetizing field / auxiliary magnetic field)
- **Input**:

  j (current density field)
- **Equations**:

$$\text{div } b = 0, \quad *b = h, \quad \text{curl } h = j$$

- **Boundary Conditions:** Γ written as a disjoint union $\Gamma^e \cup \Gamma^h$ such that

  $\hat{n} \cdot b = 0$ on Γ^e, $\quad \hat{n} \times h = 0$ on Γ^h.

While b and h are both discretized as vector fields, they lie in different function spaces:

$$h \in H(\text{curl }) := \left\{ \vec{v} \in \left(L^2(\Omega)\right)^3 \quad \text{s.t.} \quad \nabla \times \vec{v} \in \left(L^2(\Omega)\right)^3 \right\}$$

$$b \in H(\text{div }) := \left\{ \vec{v} \in \left(L^2(\Omega)\right)^3 \quad \text{s.t.} \quad \nabla \cdot \vec{v} \in L^2(\Omega) \right\}$$

Local Conformity Constraints

- Functional continuity can be enforced on a mesh $\mathcal{T}$ by imposing certain constraints at each face $F = T_1 \cap T_2$, involving the normals to the mesh elements T_1, T_2:

$$H(\text{curl}\ ) := \left\{ \vec{v} \in \left(L^2(\Omega)\right)^3 \quad \text{s.t.} \quad \nabla \times \vec{v} \in \left(L^2(\Omega)\right)^3 \right\}$$

$$h \in H(\text{curl}\ ) \Longleftrightarrow h|_{T_1} \times \hat{n}_1 + h|_{T_2} \times \hat{n}_2 = 0, \quad \forall F \in \mathcal{T}$$

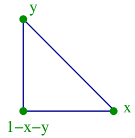
$$H(\text{div}\ ) := \left\{ \vec{v} \in \left(L^2(\Omega)\right)^3 \quad \text{s.t.} \quad \nabla \cdot \vec{v} \in L^2(\Omega) \right\}$$

$$b \in H(\text{div}\ ) \Longleftrightarrow b|_{T_1} \cdot \hat{n}_1 + b|_{T_2} \cdot \hat{n}_2 = 0, \quad \forall F \in \mathcal{T}$$

- These constraints hold for primal meshes (T_i=tetrahedra) **and** dual meshes (T_i=polyhedra).
- **Goal**: Solve for h and b as functions defined piecewise over $\mathcal{T}$, guaranteed to satisfy the applicable conformity constraints.

Whitney Elements for Primal Meshes

- The **Whitney elements** provide a simple and canonical way to construct piecewise functions over a **primal** mesh $\mathcal{T}$ in $H(\text{curl})$ or $H(\text{div})$:



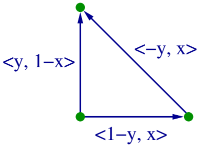
$\lambda_i \rightarrow$ 1 d.o.f. per vertex

0. Start with linear barycentric coordinates:

$$\lambda_i(\mathbf{v}_j) = \delta_{ij}$$

1. Define for each edge $\mathbf{v}_i\mathbf{v}_j$::

$$\eta_{ij} := \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i$$



$\eta_{ij} \rightarrow$ 1 d.o.f. per edge

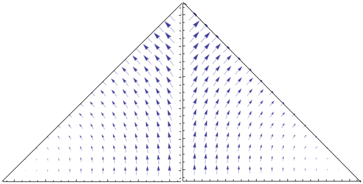
2. Define for each face $\mathbf{v}_i\mathbf{v}_j\mathbf{v}_k$:

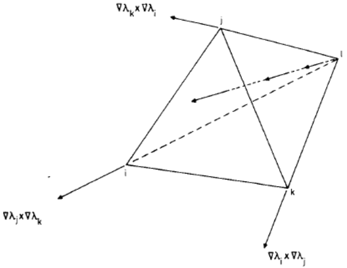
$$\eta_{ijk} := \lambda_i \nabla \lambda_j \times \nabla \lambda_k + \lambda_j \nabla \lambda_k \times \nabla \lambda_i$$
$$+ \lambda_k \nabla \lambda_i \times \nabla \lambda_j$$

$< -x, -y, 1-z >, < x, y-1, z >$
$< 1-x, -y, -z >, < x, y, z >$
$\eta_{ijk} \rightarrow$ 1 d.o.f. per face

Whitney Elements for Primal Meshes

In 3D, it can be shown that the η_{ij} satisfy the $H(\text{curl})$ constraints and the η_{ijk} satisfy the $H(\text{div})$ constraints.





See, e.g. Bossavit *Computational Electromagnetism*, 1998.

Discrete deRham Diagrams

- We now have a basis for finite dimensional subspaces of the deRham Diagram:

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

$$\{\lambda_i\} \xrightarrow[\text{(grad)}]{\mathbb{D}_0} \{\eta_{ij}\} \xrightarrow[\text{(curl)}]{\mathbb{D}_1} \{\eta_{ijk}\} \xrightarrow[\text{(div)}]{\mathbb{D}_2} \{\chi_T\}$$

- These are called the **primal cochain spaces** in Discrete Exterior Calculus:

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

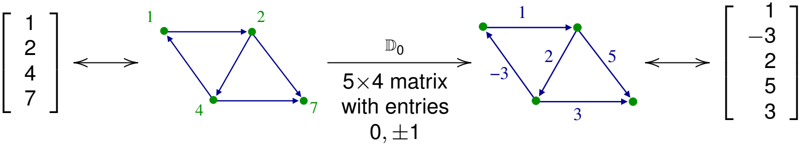
- Supposing for a moment we can construct conforming interpolation functions on the dual mesh, we also have a sequence of **dual cochain spaces**:

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

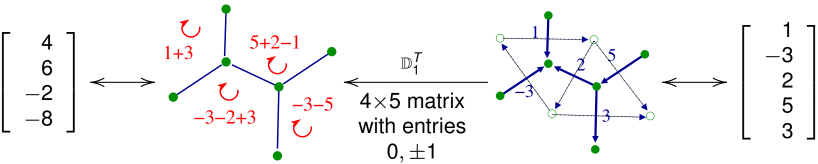
DESBRUN, HIRANI, LEOK, MARSDEN *Discrete Exterior Calculus*,
arXiv:math/0508341v2 [math.DG], 2005

Discrete Exterior Derivative

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



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



These cochain vectors and derivative matrices are the building blocks for equation discretization.

Outline

Discrete Magnetostatics - Primal

Returning to the magnetostatics problem, we can discretize the equations in two ways:

- **Continuous Equations**:

$$\text{div } b = 0, \quad *b = h, \quad \text{curl } h = j$$

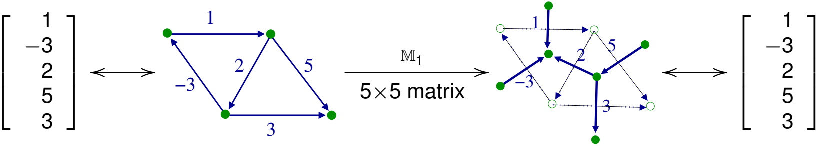
- **'Primal' Discrete Equations**, with b as a primal 2-cochain:

$$\mathbb{D}_2 \mathsf{B} = 0, \quad \mathbb{M}_2 \mathsf{B} = \overline{\mathsf{H}}, \quad \mathbb{D}_1^T \overline{\mathsf{H}} = \overline{\mathsf{J}}.$$

- **'Dual' Discrete Equations**, with b as a dual 2-cochain:

$$\mathbb{D}_0^T \overline{\mathsf{B}} = 0, \quad \mathbb{M}_1^{-1} \overline{\mathsf{B}} = \mathsf{H}, \quad \mathbb{D}_1 \mathsf{H} = \mathsf{J}.$$

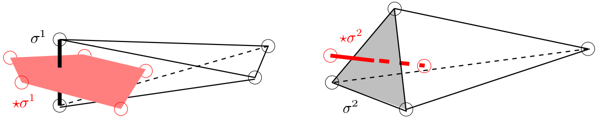
The discrete Hodge Star $\mathbb{M}$ transfers information between complementary dimensions on **dual** meshes. In this example, we use the identity matrix for $\mathbb{M}_1$.



Discrete Hodge Stars

- Discretization of the Hodge star operator is non-canonical.
- 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 polyhedral vector interpolation functions

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

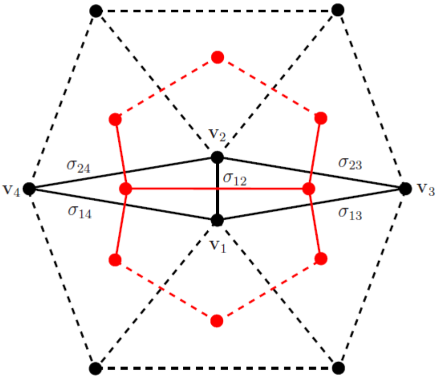


type	reference	definition	$\mathbb{M}_k$	$\mathbb{M}_k^{-1}$
DIAGONAL	[Desbrun et al.]	$(\mathbb{M}_k^{Diag})_{ij} := \frac{\lvert\star\,\sigma_i^k\rvert}{\lvert\sigma_j^k\rvert}\delta_{ij}$	diagonal	diagonal
WHITNEY	[Dodziuk],[Bell]	$(\mathbb{M}_k^{Whit})_{ij} := \int_{\mathcal{T}} \eta_{\sigma_i^k} \cdot \eta_{\sigma_j^k}$	sparse	(full)
DUAL	[G, Bajaj]	$((\mathbb{M}_k^{Dual})^{-1})_{ij} := \int_{\mathcal{T}} \eta_{\star\sigma_i^k} \cdot \eta_{\star\sigma_j^k}$	(full)	sparse

Condition Number of Discrete Hodge Stars

Theorem [G, Bajaj]

The condition number of $\left(\mathbb{M}_k^{Dual}\right)^{-1}$ is governed by different mesh criteria than the condition number of $\mathbb{M}_k^{Diag}$ and $\mathbb{M}_k^{Whit}$.



$\mathbf{v}_1 = (0,0) \qquad \mathbf{v}_3 = (P, \frac{1}{2})$
$\mathbf{v}_2 = (0,1) \qquad \mathbf{v}_4 = (-P, \frac{1}{2})$

Condition numbers as functions of P:

P	$\mathbb{M}_1^{Diag}$	$\mathbb{M}_1^{Whit}$	$\left(\mathbb{M}_1^{Dual}\right)^{-1}$
2	6.3	3.2	1.5
5	17.2	9.9	1.3
10	34.6	21.6	1.4
order	$O(P)$	$O(P)$	$O(1)$

Dual Formulations of Mixed Finite Element Methods. Submitted, 2010.

Dual-based Linear Systems

Independence of primal and dual discrete Hodge stars implies **accuracy vs. speed** tradeoffs are possible between primal and dual methods.
Ex: Fewer elements in dual mesh → smaller system → faster.
Ex: Better condition number in dual system → more accurate.

- **'Primal' Linear System**, with b as a primal 2-cochain:

$$\mathbb{D}_2 \mathrm{B} = 0, \quad \mathbb{M}_2 \mathrm{B} = \overline{\mathrm{H}}, \quad \mathbb{D}_1^T \overline{\mathrm{H}} = \overline{\mathrm{J}}.$$

$$\begin{pmatrix} -\mathbb{M}_2 & \mathbb{D}_2^T \\ \mathbb{D}_2 & 0 \end{pmatrix} \begin{pmatrix} \mathrm{B} \\ \overline{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} -\overline{\mathrm{H}}_0 \\ 0 \end{pmatrix}.$$

  Here, $\overline{\mathrm{H}}_0 \in \overline{\mathcal{C}}^1$ satisfies $\mathbb{D}_1^T \overline{\mathrm{H}}_0 = \overline{\mathrm{J}}$ and $\overline{\mathrm{H}}$ is defined by $\overline{\mathrm{H}} := \overline{\mathrm{H}}_0 + \mathbb{D}_2^T \overline{\mathrm{P}}$.
  Thus $\mathbb{D}_1^T \overline{\mathrm{H}} = \mathbb{D}_1^T (\overline{\mathrm{H}}_0 + \mathbb{D}_2^T \overline{\mathrm{P}}) = \overline{\mathrm{J}}$ is assured.

- **'Dual' Linear System**, with b as a dual 2-cochain:

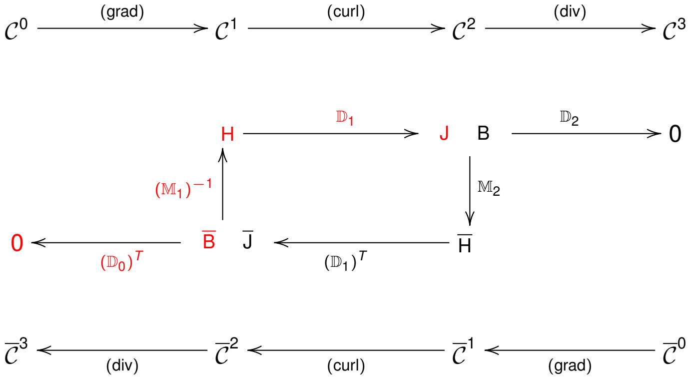
$$\mathbb{D}_0^T \overline{\mathrm{B}} = 0, \quad \mathbb{M}_1^{-1} \overline{\mathrm{B}} = \mathrm{H}, \quad \mathbb{D}_1 \mathrm{H} = \mathrm{J}.$$

$$\begin{pmatrix} -\mathbb{M}_1^{-1} & \mathbb{D}_0 \\ \mathbb{D}_0^T & 0 \end{pmatrix} \begin{pmatrix} \overline{\mathrm{B}} \\ \mathrm{P} \end{pmatrix} = \begin{pmatrix} -\mathrm{H}_0 \\ 0 \end{pmatrix}.$$

  Here, $\mathrm{H}_0 \in \mathcal{C}^1$ satisfies $\mathbb{D}_1 \mathrm{H}_0 = \mathrm{J}$ and H is defined by $\mathrm{H} := \mathbb{M}_1^{-1} \overline{\mathrm{B}}$.
  Thus $\mathbb{D}_1 \mathrm{H} = \mathbb{D}_1 (\mathrm{H}_0 + \mathbb{D}_0 \mathrm{P}) = \mathrm{J}$ is assured.

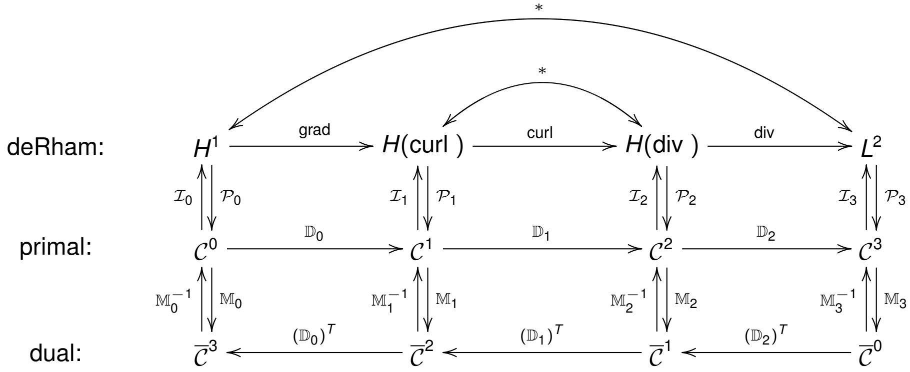
Dual-based Linear Systems

The duality of the systems is easily visualized via the cochain sequences:



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

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



The combined diagram can be used to formulate dual-based discretizations for many problems including electromagnetics, Darcy flow, and electrodiffusion.

The question remains: How do we construct polyhedral vector interpolation functions?

Outline

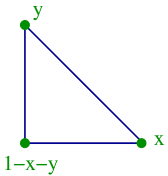
Scalar Interpolation: Generalized Barycentric Functions

Let Ω be a convex polygon in $\mathbb{R}^2$ with vertices $\mathbf{v}_1, \ldots, \mathbf{v}_n$. Functions $\lambda_i : \Omega \to \mathbb{R}$, $i = 1, \ldots, n$ are called **barycentric coordinates** on Ω if they satisfy two properties:

1. **Non-negative**: $\lambda_i \geq 0$ on Ω.
2. **Linear Completeness**: For any linear function $L : \Omega \to \mathbb{R}$, $L = \sum_{i=1}^{n} L(\mathbf{v}_i)\lambda_i$.

It can be shown that any set of barycentric coordinates under this definition also satisfy:

3. **Partition of unity:** $\sum_{i=1}^{n} \lambda_i \equiv 1$.
4. **Linear precision:** $\sum_{i=1}^{n} \mathbf{v}_i \lambda_i(\mathbf{x}) = \mathbf{x}$.
5. **Interpolation:** $\lambda_i(\mathbf{v}_j) = \delta_{ij}$.



Theorem [Warren, 2003]

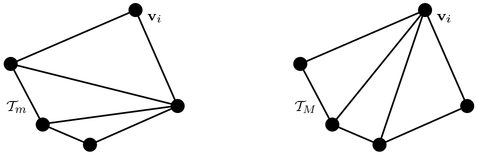
If the λ_i are rational functions of degree $n - 2$, then they are unique.

Triangulation Coordinates

Let $\mathcal{T}$ be a triangulation of Ω formed by adding edges between the $\mathbf{v}_j$ in some fashion. Define

$$\lambda_{i,\mathcal{T}}^{\mathrm{Tri}} : \Omega \to \mathbb{R}$$

to be the barycentric function associated to $\mathbf{v}_i$ on triangles in $\mathcal{T}$ containing $\mathbf{v}_i$ and identically 0 otherwise. Trivially, these are barycentric coordinates on Ω.



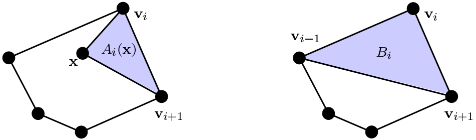
Theorem [Floater, Hormann, Kós, 2006]

For a fixed i, let $\mathcal{T}_m$ denote any triangulation with an edge between $\mathbf{v}_{i-1}$ and $\mathbf{v}_{i+1}$. Let $\mathcal{T}_M$ denote the triangulation formed by connecting $\mathbf{v}_i$ to all the other $\mathbf{v}_j$. Any barycentric coordinate function λ_i satisfies the bounds

$$0 \leq \lambda_{i,\mathcal{T}_m}^{\mathrm{Tri}}(\mathbf{x}) \leq \lambda_i(\mathbf{x}) \leq \lambda_{i,\mathcal{T}_M}^{\mathrm{Tri}}(\mathbf{x}) \leq 1, \quad \forall \mathbf{x} \in \Omega. \tag{1}$$

Wachspress Coordinates

Let $\mathbf{x} \in \Omega$ and define $A_i(\mathbf{x})$ and B_i as the areas shown.



Define the Wachspress weight function as

$$w_i^{\text{Wach}}(\mathbf{x}) = B_i \prod_{j \neq i, i-1} A_j(\mathbf{x}).$$

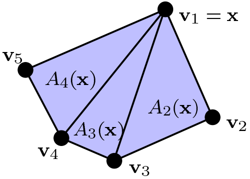
The Wachspress coordinates are then given by the *rational* functions

$$\lambda_i^{\text{Wach}}(\mathbf{x}) = \frac{w_i^{\text{Wach}}(\mathbf{x})}{\sum_{j=1}^{n} w_j^{\text{Wach}}(\mathbf{x})} \quad (2)$$

Wachspress Coordinates Example

Let $\mathbf{x} = \mathbf{v}_1$.

Note $A_1(\mathbf{x})$ = area of $(\mathbf{v}_1, \mathbf{v}_1, \mathbf{v}_2) = 0$. Similarly $A_5(\mathbf{x}) = 0$



$$w_1^{\text{Wach}}(\mathbf{x}) = B_1 A_2(\mathbf{x}) A_3(\mathbf{x}) A_4(\mathbf{x}) = W$$
$$w_2^{\text{Wach}}(\mathbf{x}) = B_2 A_3(\mathbf{x}) A_4(\mathbf{x}) A_5(\mathbf{x}) = 0$$
$$w_3^{\text{Wach}}(\mathbf{x}) = B_3 A_4(\mathbf{x}) A_5(\mathbf{x}) A_1(\mathbf{x}) = 0$$
$$w_4^{\text{Wach}}(\mathbf{x}) = B_4 A_5(\mathbf{x}) A_1(\mathbf{x}) A_2(\mathbf{x}) = 0$$
$$w_5^{\text{Wach}}(\mathbf{x}) = B_5 A_1(\mathbf{x}) A_2(\mathbf{x}) A_3(\mathbf{x}) = 0$$

$$\lambda_1^{\text{Wach}}(\mathbf{x}) = \frac{w_1^{\text{Wach}}(\mathbf{x})}{\sum w_i^{\text{Wach}}(\mathbf{x})} = \frac{W}{W} = 1$$

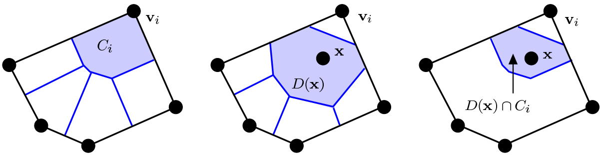
$$\lambda_2^{\text{Wach}}(\mathbf{x}) = \frac{w_2^{\text{Wach}}(\mathbf{x})}{\sum w_1^{\text{Wach}}(\mathbf{x})} = 0$$

Similarly $\lambda_3^{\text{Wach}}(\mathbf{x}) = \lambda_4^{\text{Wach}}(\mathbf{x}) = \lambda_5^{\text{Wach}}(\mathbf{x}) = 0$.

This is an illustration of the property $\lambda_i^{\text{Wach}}(\mathbf{v}_j) = \delta_{ij}$

Sibson (Natural Neighbor) Coordinates

Let P denote the set of vertices $\{\mathbf{v}_i\}$ and define $P' = P \cup \{\mathbf{x}\}$.



$$\begin{aligned} C_i &:= |V_P(\mathbf{v}_i)| = |\{\mathbf{y} \in \Omega : |\mathbf{y} - \mathbf{v}_i| < |\mathbf{y} - \mathbf{v}_j| \ , \forall j \neq i\}| \\ &= \text{area of cell for } \mathbf{v}_i \text{ in Voronoi diagram on the points of } P, \end{aligned}$$

$$\begin{aligned} D(\mathbf{x}) &:= |V_{P'}(\mathbf{x})| = |\{\mathbf{y} \in \Omega : |\mathbf{y} - \mathbf{x}| < |\mathbf{y} - \mathbf{v}_i| \ , \forall i\}| \\ &= \text{area of cell for } \mathbf{x} \text{ in Voronoi diagram on the points of } P'. \end{aligned}$$

By a slight abuse of notation, we also define

$$D(\mathbf{x}) \cap C_i := |V_{P'}(\mathbf{x}) \cap V_P(\mathbf{v}_i)|.$$

The Sibson coordinates are defined to be

$$\lambda_i^{\text{Sibs}}(\mathbf{x}) := \frac{D(\mathbf{x}) \cap C_i}{D(\mathbf{x})} \qquad \text{or, equivalently,} \qquad \lambda_i^{\text{Sibs}}(\mathbf{x}) = \frac{D(\mathbf{x}) \cap C_i}{\sum_{j=1}^{n} D_j(\mathbf{x}) \cap C_j}.$$

Optimal Coordinates

Let $g_i : \partial\Omega \to \mathbb{R}$ be the piecewise linear function satisfying

$$g_i(\mathbf{v}_j) = \delta_{ij}, \quad g_i \text{ linear on each edge of } \Omega.$$

The optimal coordinate function λ_i^{Opt} is defined to be the solution of Laplace's equations with g_i as boundary data,

$$\begin{cases} \Delta\left(\lambda_i^{\mathrm{Opt}}\right) = 0, & \text{on } \Omega, \\ \lambda_i^{\mathrm{Opt}} = g_i. & \text{on } \partial\Omega. \end{cases} \tag{3}$$

These coordinates are optimal in the sense that they minimize the norm of the gradient over all functions satisfying the boundary conditions,

$$\lambda_i^{\mathrm{Opt}} = \operatorname{argmin}\left\{|\lambda|_{H^1(\Omega)} \,:\, \lambda = g_i \text{ on } \partial\Omega\right\}.$$

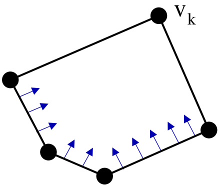
Polyhedral $H(Curl)$ Vector Interpolantion

- Let $\{\overline{\lambda}_i\}$ denote a set of generalized barycentric coordinates for a polygon (2D) or polyhedra (3D).
- Define for each edge $\mathbf{v}_i\mathbf{v}_j$::

$$\overline{\eta}_{ij} := \overline{\lambda}_i \nabla \overline{\lambda}_j - \overline{\lambda}_j \nabla \overline{\lambda}_i$$

Theorem [G,Bajaj]

Constructing **Whitney-like 1-forms** analogously to the triangular case produces globally H(curl)-conforming **vector fields**.



PROOF: Consider edge $\mathbf{v}_i\mathbf{v}_j$ and λ_k associated to a different vertex $\mathbf{v}_k$. Then the edge is part of the zero level set of λ_k. Hence $\nabla\lambda_k$ must be perpendicular to the edge at all points along it and any summand $\lambda_l \nabla \lambda_k$ has no tangential component on the edge. Therefore, the tangential components only depend on λ_i and λ_j. Hence the H(curl) conformity constraints are satisfied. □

To decide which definition of $\{\overline{\lambda}_i\}$ is suitable, we need error estimates.

Error Estimates: 2D Scalar Case

The **optimal convergence estimate** for a finite element method bounds the interpolation error in H^1-norm of an unknown function u by a constant multiple of the mesh size times the H^2 semi-norm of u:

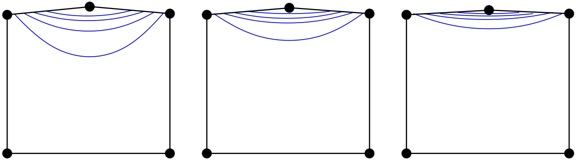
$$\left|\left|u - \overline{\mathcal{I}}_0 u\right|\right|_{H^1(\Omega)} \leq C \,\mathrm{diam}(\Omega)\, |u|_{H^2(\Omega)}, \quad \forall u \in H^2(\Omega). \tag{4}$$

(Note that $\overline{\mathcal{I}}_0 u$ assumes u is known or computed at vertices of the dual mesh.)

Theorem [G, Rand, Bajaj]

Assume certain standard geometric quality conditions on the dual mesh can be guaranteed. Then a **dual formulation** of a finite element method using any of the coordinate systems has the **optimal convergence estimate** on the mesh.

Error Estimates for Generalized Barycentric Interpolation. Submitted, 2010.



Example showing necessity of geometric criteria for Wachspress coordinates.

Future Work

- Efficient computation of $\overline{\lambda}_i$ basis functions
- Error estimates for polyhedral vector functions
- $H(\text{div}\ )$-conforming vector elements for polyhedral meshes

Questions?

- Thank you for inviting me to visit.
- Slides and pre-prints available at http://www.math.utexas.edu/users/agillette