Conforming Vector Interpolation Functions for Polyhedral Meshes

Andrew Gillette

joint work with

Chandrajit Bajaj and Alexander Rand

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

http://www.math.utexas.edu/users/agillette
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.
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

1. Background on Vector Interpolation
2. Novel Discretizations Using Polyhedral Vector Interpolation
3. Error Estimates for Polyhedral Vector Interpolation
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**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 $\Gamma$
- **Variables**:
  - $b$ (magnetic field / magnetic induction)
  - $h$ (magnetizing field / auxiliary magnetic field)
- **Input**:
  - $j$ (current density field)
- **Equations**:
  - $\text{div } b = 0$, $\star b = h$, $\text{curl } h = j$
- **Boundary Conditions**: $\Gamma$ written as a disjoint union $\Gamma^e \cup \Gamma^h$ such that
  - $\hat{n} \cdot b = 0$ on $\Gamma^e$
  - $\hat{n} \times h = 0$ on $\Gamma^h$.

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

- $h \in H(\text{curl }):= \left\{ \mathbf{v} \in \left(L^2(\Omega)\right)^3 \text{ s.t. } \nabla \times \mathbf{v} \in \left(L^2(\Omega)\right)^3 \right\}$
- $b \in H(\text{div }):= \left\{ \mathbf{v} \in \left(L^2(\Omega)\right)^3 \text{ s.t. } \nabla \cdot \mathbf{v} \in L^2(\Omega) \right\}$
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 $T_1, T_2$:

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

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

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

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

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

0. Start with linear barycentric coordinates:

\[ \lambda_i(v_j) = \delta_{ij} \]

1. Define for each edge $v_i v_j$:

\[ \eta_{ij} := \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i \]

2. Define for each face $v_i v_j v_k$:

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

\[ \lambda_i \rightarrow 1 \text{ d.o.f. per vertex} \]

\[ \eta_{ij} \rightarrow 1 \text{ d.o.f. per edge} \]

\[ \eta_{ijk} \rightarrow 1 \text{ d.o.f. per face} \]
In 3D, it can be shown that the $\eta_{ij}$ satisfy the $H(\text{curl})$ constraints and the $\eta_{ijk}$ satisfy the $H(\text{div})$ constraints.

Discrete deRham Diagrams

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

\[
\begin{align*}
H^1 & \xrightarrow{d_0} \text{grad } H = \text{curl } H & \xrightarrow{d_1} \text{curl } H = \text{div } H & \xrightarrow{d_2} L^2 \\
\{\lambda_i\} & \xrightarrow{\mathbb{D}_0} \{\eta_{ij}\} & \xrightarrow{\mathbb{D}_1} \{\eta_{ijk}\} & \xrightarrow{\mathbb{D}_2} \{\chi_T\}
\end{align*}
\]

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

\[
\begin{align*}
C^0 & \xrightarrow{\mathbb{D}_0} C^1 & \xrightarrow{\mathbb{D}_1} C^2 & \xrightarrow{\mathbb{D}_2} C^3
\end{align*}
\]

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

\[
\begin{align*}
\overline{C}^3 & \xleftarrow{\mathbb{D}_0^T} \overline{C}^2 & \xleftarrow{\mathbb{D}_1^T} \overline{C}^1 & \xleftarrow{\mathbb{D}_2^T} \overline{C}^0
\end{align*}
\]

**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.

$$
\begin{bmatrix}
1 \\
2 \\
4 \\
7 \\
\end{bmatrix} \quad \begin{array}{c}
\Rightarrow \\
\Rightarrow \\
\Rightarrow \\
\Rightarrow \\
\end{array} \quad \begin{array}{c}
1 \\
2 \\
4 \\
7 \\
\end{array}
$$

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

$$
\begin{bmatrix}
4 \\
6 \\
-2 \\
-8 \\
\end{bmatrix} \quad \begin{array}{c}
\Rightarrow \\
\Rightarrow \\
\Rightarrow \\
\Rightarrow \\
\end{array} \quad \begin{array}{c}
1 \\
5+2-1 \\
-3-5 \\
1+3 \\
\end{array}
$$

These cochain vectors and derivative matrices are the building blocks for equation discretization.
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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:
  \[
  \mathcal{D}_2 B = 0, \quad M_2 B = \overline{H}, \quad \mathcal{D}_1^T \overline{H} = \overline{J}.
  \]

- **‘Dual’ Discrete Equations**, with \( b \) as a dual 2-cochain:
  \[
  \mathcal{D}_0^T \overline{B} = 0, \quad M_1^{-1} \overline{B} = H, \quad \mathcal{D}_1 H = J.
  \]

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

\[
\begin{bmatrix}
1 \\
-3 \\
2 \\
5 \\
3
\end{bmatrix}
\xrightarrow{\mathcal{M}_1}
\begin{bmatrix}
1 \\
-3 \\
2 \\
3
\end{bmatrix}
\]
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.

\[
\text{primal mesh simplex } \sigma^k \leftrightarrow \text{dual mesh cell } \ast \sigma^k
\]

<table>
<thead>
<tr>
<th>type</th>
<th>reference</th>
<th>definition</th>
<th>(M_k)</th>
<th>(M_k^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{DIAGONAL}</td>
<td>[Desbrun et al.]</td>
<td>((M_k^{\text{Diag}})_{ij} := \frac{</td>
<td>\ast \sigma_i^k</td>
<td>}{</td>
</tr>
<tr>
<td>\text{WHITNEY}</td>
<td>[Dodziuk],[Bell]</td>
<td>((M_k^{\text{Whit}})<em>{ij} := \int</em>{\mathcal{T}} \eta_{\sigma_i^k} \cdot \eta_{\sigma_j^k})</td>
<td>sparse</td>
<td>(full)</td>
</tr>
<tr>
<td>\text{DUAL}</td>
<td>[G, Bajaj]</td>
<td>((M_k^{\text{Dual}})^{-1})<em>{ij} := \int</em>{\mathcal{T}} \eta_{\ast \sigma_i^k} \cdot \eta_{\ast \sigma_j^k})</td>
<td>(full)</td>
<td>sparse</td>
</tr>
</tbody>
</table>
The condition number of \((M_{k}^{\text{Dual}})^{-1}\) is governed by different mesh criteria than the condition number of \(M_{k}^{\text{Diag}}\) and \(M_{k}^{\text{Whit}}\).

\[
\begin{align*}
\mathbf{v}_1 &= (0, 0) & \mathbf{v}_3 &= (P, \frac{1}{2}) \\
\mathbf{v}_2 &= (0, 1) & \mathbf{v}_4 &= (-P, \frac{1}{2})
\end{align*}
\]

Condition numbers as functions of \(P\):

<table>
<thead>
<tr>
<th>(P)</th>
<th>(M_1^{\text{Diag}})</th>
<th>(M_1^{\text{Whit}})</th>
<th>((M_1^{\text{Dual}})^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6.3</td>
<td>3.2</td>
<td>1.5</td>
</tr>
<tr>
<td>5</td>
<td>17.2</td>
<td>9.9</td>
<td>1.3</td>
</tr>
<tr>
<td>10</td>
<td>34.6</td>
<td>21.6</td>
<td>1.4</td>
</tr>
</tbody>
</table>

order \(O(P)\) \(O(P)\) \(O(1)\)

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 $\rightarrow$ smaller system $\rightarrow$ faster.

**Ex:** Better condition number in dual system $\rightarrow$ more accurate.

### ‘Primal’ Linear System, with $b$ as a primal 2-cochain:

$$D_2 B = 0, \quad M_2 B = \overline{H}, \quad D_1^T \overline{H} = \overline{J}.$$  

$$\begin{pmatrix} -M_2 & D_2^T \\ D_2 & 0 \end{pmatrix} \begin{pmatrix} B \\ P \end{pmatrix} = \begin{pmatrix} -\overline{H_0} \\ 0 \end{pmatrix}.$$  

Here, $\overline{H_0} \in \bar{C}^1$ satisfies $D_1^T \overline{H_0} = \overline{J}$ and $\overline{H}$ is defined by $\overline{H} := \overline{H_0} + D_2^T \overline{P}$.

Thus $D_1^T \overline{H} = D_1^T (\overline{H_0} + D_2^T \overline{P}) = \overline{J}$ is assured.

### ‘Dual’ Linear System, with $b$ as a dual 2-cochain:

$$D_0^T \overline{B} = 0, \quad M_1^{-1} \overline{B} = \overline{H}, \quad D_1 = \overline{J}.$$  

$$\begin{pmatrix} -M_1^{-1} & D_0 \\ D_0 & 0 \end{pmatrix} \begin{pmatrix} \overline{B} \\ \overline{P} \end{pmatrix} = \begin{pmatrix} -\overline{H_0} \\ 0 \end{pmatrix}.$$  

Here, $\overline{H_0} \in C^1$ satisfies $D_1 \overline{H_0} = \overline{J}$ and $\overline{H}$ is defined by $\overline{H} := M_1^{-1} \overline{B}$.

Thus $D_1 \overline{H} = D_1 (\overline{H_0} + D_0 \overline{P}) = \overline{J}$ is assured.
The duality of the systems is easily visualized via the cochain sequences:

\[ \begin{align*}
    C^0 \xrightarrow{\text{grad}} & C^1 \xrightarrow{\text{curl}} C^2 \xrightarrow{\text{div}} C^3 \\
    H \xrightarrow{\mathbb{D}_1} & J \xrightarrow{\mathbb{M}_2} 0 \\
    0 \xleftarrow{\mathbb{D}_0^T} & B \xleftarrow{\mathbb{D}_1^T} \bar{H} \xleftarrow{\mathbb{M}_1^{-1}} \\
    \bar{C}^3 \xleftarrow{\text{div}} & \bar{C}^2 \xleftarrow{\text{curl}} \bar{C}^1 \xleftarrow{\text{grad}} \bar{C}^0
\end{align*} \]
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?
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Scalar Interpolation: Generalized Barycentric Functions

Let $\Omega$ be a convex polygon in $\mathbb{R}^2$ with vertices $v_1, \ldots, v_n$. Functions $\lambda_i : \Omega \to \mathbb{R}$, $i = 1, \ldots, n$ are called **barycentric coordinates** on $\Omega$ if they satisfy two properties:

1. **Non-negative**: $\lambda_i \geq 0$ on $\Omega$.

2. **Linear Completeness**: For any linear function $L : \Omega \to \mathbb{R}$, $L = \sum_{i=1}^{n} L(v_i) \lambda_i$.

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**: $\sum_{i=1}^{n} v_i \lambda_i(x) = x$.

5. **Interpolation**: $\lambda_i(v_j) = \delta_{ij}$.

**Theorem [Warren, 2003]**

If the $\lambda_i$ are rational functions of degree $n - 2$, then they are unique.
Triangulation Coordinates

Let $\mathcal{T}$ be a triangulation of $\Omega$ formed by adding edges between the $v_j$ in some fashion. Define

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

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

Theorem [Floater, Hormann, Kós, 2006]

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

$$0 \leq \lambda_{i,\mathcal{T}_m}(x) \leq \lambda_i(x) \leq \lambda_{i,\mathcal{T}_M}(x) \leq 1, \quad \forall x \in \Omega.$$ (1)
Let $\mathbf{x} \in \Omega$ and define $A_i(\mathbf{x})$ and $B_i$ as the areas shown.

Define the Wachspress weight function as

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

The Wachspress coordinates are then given by the rational functions

$$\lambda_{Wach}^i(\mathbf{x}) = \frac{w_{Wach}^i(\mathbf{x})}{\sum_{j=1}^{n} w_{Wach}^j(\mathbf{x})}$$

(2)
Let $\mathbf{x} = \mathbf{v}_1$.

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

$$w_{1}^{\text{Wach}}(\mathbf{x}) = B_1 A_2(\mathbf{x}) A_3(\mathbf{x}) A_4(\mathbf{x}) = W$$
$$w_{2}^{\text{Wach}}(\mathbf{x}) = B_2 A_3(\mathbf{x}) A_4(\mathbf{x}) A_5(\mathbf{x}) = 0$$
$$w_{3}^{\text{Wach}}(\mathbf{x}) = B_3 A_4(\mathbf{x}) A_5(\mathbf{x}) A_1(\mathbf{x}) = 0$$
$$w_{4}^{\text{Wach}}(\mathbf{x}) = B_4 A_5(\mathbf{x}) A_1(\mathbf{x}) A_2(\mathbf{x}) = 0$$
$$w_{5}^{\text{Wach}}(\mathbf{x}) = B_5 A_1(\mathbf{x}) A_2(\mathbf{x}) A_3(\mathbf{x}) = 0$$

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

$$\lambda_2^{\text{Wach}}(\mathbf{x}) = \frac{w_{2}^{\text{Wach}}(\mathbf{x})}{\sum w_i^{\text{Wach}}(\mathbf{x})} = 0$$

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 $\{v_i\}$ and define $P' = P \cup \{x\}$.

$$C_i := |V_P(v_i)| = |\{y \in \Omega : |y - v_i| < |y - v_j|, \forall j \neq i\}|$$

= area of cell for $v_i$ in Voronoi diagram on the points of $P$,

$$D(x) := |V_{P'}(x)| = |\{y \in \Omega : |y - x| < |y - v_i|, \forall i\}|$$

= area of cell for $x$ in Voronoi diagram on the points of $P'$.

By a slight abuse of notation, we also define

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

The Sibson coordinates are defined to be

$$\lambda^{\text{Sibs}}_i(x) := \frac{D(x) \cap C_i}{D(x)}$$

or, equivalently,

$$\lambda^{\text{Sibs}}_i(x) = \frac{D(x) \cap C_i}{\sum_{j=1}^{n} D_j(x) \cap C_j}.$$
Let \( g_i : \partial \Omega \to \mathbb{R} \) be the piecewise linear function satisfying
\[
g_i(v_j) = \delta_{ij}, \quad g_i \text{ linear on each edge of } \Omega.
\]

The optimal coordinate function \( \lambda^\text{Opt}_i \) is defined to be the solution of Laplace’s equations with \( g_i \) as boundary data,
\[
\begin{cases}
\Delta (\lambda^\text{Opt}_i) & = 0, \quad \text{on } \Omega, \\
\lambda^\text{Opt}_i & = g_i, \quad \text{on } \partial \Omega.
\end{cases}
\] (3)

These coordinates are optimal in the sense that they minimize the norm of the gradient over all functions satisfying the boundary conditions,
\[
\lambda^\text{Opt}_i = \text{argmin} \left\{ |\lambda|_{H^1(\Omega)} : \lambda = g_i \text{ on } \partial \Omega \right\}.
\]
Polyhedral $H(Curl)$ Vector Interpolation

- Let $\{\lambda_i\}$ denote a set of generalized barycentric coordinates for a polygon (2D) or polyhedra (3D).
- Define for each edge $v_i v_j$:
  \[ \bar{\eta}_{ij} := \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i \]

**Theorem [G,Bajaj]**

Constructing Whitney-like 1-forms analogously to the triangular case produces globally $H(\text{curl})$-conforming vector fields.

**Proof:** Consider edge $v_i v_j$ and $\lambda_k$ associated to a different vertex $v_k$. Then the edge is part of the zero level set of $\lambda_k$. Hence $\nabla \lambda_k$ must be perpendicular to the edge at all points along it and any summand $\lambda_i \nabla \lambda_k$ has no tangential component on the edge. Therefore, the tangential components only depend on $\lambda_i$ and $\lambda_j$. Hence the $H(\text{curl})$ conformity constraints are satisfied.

To decide which definition of $\{\lambda_i\}$ is suitable, we need error estimates.
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 $u$:

$$
\| u - \overline{I}_0 u \|_{H^1(\Omega)} \leq C \text{diam}(\Omega) |u|_{H^2(\Omega)}, \quad \forall u \in H^2(\Omega).
$$

(Note that $\overline{I}_0 u$ 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.


Example showing necessity of geometric criteria for Wachspress coordinates.
Future Work

- Efficient computation of $\lambda_i$ 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