Discrete Exterior Calculus and Polygonal Finite Elements

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joint work with Chandrajit Bajaj and Alexander Rand

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2. Background: What are polygonal finite elements?
3. Results: Linear and quadratic Lagrange-like elements
4. Conclusions and looking ahead
Outline

1. Motivation: Why DEC needs polygonal finite elements
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Duality arises from physics

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**
- $\text{div } b = 0$ (Gauss’ law)
- $\mu b = h$ (constitutive relation)
- $\text{curl } h = j$ (Ampère’s law)

**BOUNDARY**
$\Gamma = \Gamma^e \cup \Gamma^h$, $\hat{n} \cdot b = 0$ on $\Gamma^e$, $\hat{n} \times h = 0$ on $\Gamma^h$.

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

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

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

- Hence $h$ and $b$ fit naturally inside the $L^2$ deRham Diagram:

  $\begin{align*}
  H^1 \xrightarrow{\text{grad}} H(\text{curl}) \xrightarrow{\text{curl}} H(\text{div}) \xrightarrow{\text{div}} L^2
  \end{align*}$

- The exterior derivative operator generalizes curl and div.

  $\begin{align*}
  \Lambda^0 \xrightarrow{d_0} \Lambda^1 \xrightarrow{d_1} \Lambda^2 \xrightarrow{d_2} \Lambda^3
  \end{align*}$

- The Hodge star operation generalizes the duality relation $\ast b = h$
Exterior calculus describes duality

- The Hodge star is an isometry

\[ *\Lambda^k \cong \Lambda^{n-k} \]

For instance, when \( n = 3 \),

\[ dydz \quad * \quad dx \]

- This suggests two canonical treatments from exterior calculus:
DEC describes discrete duality

- The spaces and operators can be discretized by DEC
  Desbrun, Hirani, Leok, Marsden; Arnold, Falk, Winther; Bossavit; Shashkov, . . .
- The two treatments are similarly described in the discrete setting:

\[ \begin{array}{cccc}
C^0 & \rightarrow & D_0 & \rightarrow & C^1 \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\
M_0 & \rightarrow & (M_0)^{-1} & \rightarrow & M_1 \\
\uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\
C^3 & \leftarrow & D_0^T & \leftarrow & C^2 \\
\end{array} \]

\[ \begin{array}{cccc}
C^2 & \rightarrow & D_2 & \rightarrow & C^3 \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\
M_2 & \rightarrow & (M_2)^{-1} & \rightarrow & M_3 \\
\uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\
C^1 & \leftarrow & D_2^T & \leftarrow & C^0 \\
\end{array} \]

- \( C^k \) and \( \overline{C}^k \) are primal and dual cochain spaces
- \( D_k \) maps are the transposes of adjacency matrices, approximating \( d \)
- \( M_k \) maps are square matrices, approximating the local metric (like \( \ast \))
Two ways to recover dual mesh data

How can we interpolate piecewise functions from data on dual meshes?

1. Use primal interpolant: \( *I_{3-k}M^{-1}_{3-k} : \overline{C}^k \rightarrow \Lambda^k \)
2. Define dual interpolant: \( \overline{I}_k : \overline{C}^k \rightarrow \Lambda^k \)
Recall the magnetostatics problem:

\[
\begin{aligned}
\text{div } b &= 0 \\
\mu b &= h \\
\text{curl } h &= j
\end{aligned}
\]

Gauss’ law 
constitutive relation 
Ampère’s law

**Theorem [Bossavit, 2000]**

Let \( \Omega \) be a contractible, compact domain in \( \mathbb{R}^3 \), meshed by tetrahedra of bounded aspect ratio. Let \((B, \overline{H})\) be a solution pair to the discrete magnetostatics problem

\[
\begin{aligned}
\mathcal{D}_2 B &= 0, \\
\mathcal{M}_2 B &= \overline{H}, \\
\mathcal{D}_1 \overline{H} &= \overline{J}
\end{aligned}
\]

There exists a constant \( C \) dependent on \( \|b\|_{[H^1]_3} \) but independent of \( m_d \), such that

\[
\|I_2 B - b\|_{H^2} + \|*I_2 \mathcal{M}_2^{-1} \overline{H} - h\|_{H^1} \leq C m_d.
\]

where \( m_d \) denotes the maximum diameter of a mesh element.


Extensions and explanations of this approach in DEC terminology:

Dual mesh interpolation

What about the second approach?

Define dual interpolant: $\overline{I}_k : \overline{C}^k \to \overline{\Lambda}^k$

For instance:

$\overline{I}_0 : \overline{C}^0 \to \overline{\Lambda}^0$

means

$\overline{I}_0 : \left\{ \begin{array}{c}
\text{values at} \\
\text{nodes of} \\
\text{dual mesh}
\end{array} \right\} \to \left\{ \begin{array}{c}
\text{piecewise-defined} \\
\text{function in } H^1
\end{array} \right\}$

This is asking for a finite element theory for polygonal / polyhedral meshes.
Outline

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Overview of Approach

linear elements: $\{\lambda_i\} = \text{(triangular) barycentric coordinates}$

higher order elements $\{\lambda_i \lambda_j\}$

vector elements $\{\lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i\}$

linear elements: $\{\lambda_i\} = \text{generalized barycentric coordinates}$
Definition

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 $L : \Omega \to \mathbb{R}$, $L = \sum_{i=1}^{n} L(v_i) \lambda_i$.

Any set of barycentric coordinates under this definition also satisfies:

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.
Many generalizations to choose from . . .

- **Triangulation**
  \[ 0 \leq \lambda_i^{T_m}(x) \leq \lambda_i(x) \leq \lambda_i^{T_M}(x) \leq 1 \]

- **Wachspress**
  \[ \Rightarrow WACHSPRESS, A \text{ rational finite element basis}, 1975. \]

- **Sibson**
  \[ \Rightarrow \text{SIBSON, A vector identity for the Dirichlet tessellation}, 1980. \]
Many generalizations to choose from . . .

- Mean value
  \[ \Delta u = 0 \]
  \[ \Rightarrow \text{FLOATER}, \text{ Mean value coordinates}, 2003. \]
  \[ \Rightarrow \text{FLOATER, Kós, Reimers, Mean value coordinates in 3D}, 2005. \]

- Harmonic
  \[ \Rightarrow \text{Warren, Barycentric coordinates for convex polytopes}, 1996. \]
  \[ \Rightarrow \text{Warren, Schaefer, Hirani, Desbrun, Barycentric coordinates for convex sets}, 2007. \]

Many more in graphics contexts...
Outline

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Optimal Convergence Estimates on Polygons

Let $\Omega$ be a convex polygon with vertices $v_1, \ldots, v_n$.

For linear elements, an **optimal convergence estimate** has the form

$$
\| u - \sum_{i=1}^{n} u(v_i) \lambda_i \|_{H^1(\Omega)} \leq C \text{diam}(\Omega) \| u \|_{H^2(\Omega)}, \quad \forall u \in H^2(\Omega). \quad (1)
$$

The **Bramble-Hilbert lemma** in this context says that any $u \in H^2(\Omega)$ is close to a first order polynomial in $H^1$ norm.


For (1), it suffices to prove an **$H^1$-interpolant estimate** over domains of diameter one:

$$
\left\| \sum_{i=1}^{n} u(v_i) \lambda_i \right\|_{H^1(\Omega)} \leq C_i \| u \|_{H^2(\Omega)}, \quad \forall u \in H^1(\Omega). \quad (2)
$$

For (2), it suffices to **bound the gradients** of the $\{\lambda_i\}$, i.e. prove $\exists C_\lambda \in \mathbb{R}$ such that

$$
\| \nabla \lambda_i \|_{L^2(\Omega)} \leq C_\lambda. \quad (3)
$$
Polygonal geometry is crucial

To bound the gradients of the coordinates, we need control of the geometry.

Wachspress | Mean Value
---|---

(0,1.5)

(0,1.05)

The Wachspress coordinates blow up as interior angles get large, but the Mean Value coordinates do not!
Let $\rho(\Omega)$ denote the radius of the largest inscribed circle. The **aspect ratio** $\gamma$ is defined by

$$\gamma = \frac{\text{diam}(\Omega)}{\rho(\Omega)} \in (2, \infty)$$

Three possible geometric conditions on a polygonal mesh:

**G1. Bounded Aspect Ratio:** $\exists \gamma^* < \infty$ such that $\gamma < \gamma^*$

**G2. Minimum Edge Length:** $\exists d_* > 0$ such that $|v_i - v_{i-1}| > d_*$

**G3. Maximum Interior Angle:** $\exists \beta^* < \pi$ such that $\beta_i < \beta^*$
Summary of convergence results

**Theorem**

In the table below, any necessary geometric criteria to achieve the optimal convergence estimate are denoted by N. The collective set of geometric criteria denoted by S in each row are sufficient to guarantee the estimate.


<table>
<thead>
<tr>
<th>Geometric Criteria</th>
<th>G1 aspect ratio</th>
<th>G2 min. edge</th>
<th>G3 max angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangulated</td>
<td>$\lambda^{\text{Tri}}$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Wachspress</td>
<td>$\lambda^{\text{Wach}}$</td>
<td>S</td>
<td>S</td>
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<td>Sibson</td>
<td>$\lambda^{\text{Sibs}}$</td>
<td>S</td>
<td>S</td>
</tr>
<tr>
<td>Harmonic</td>
<td>$\lambda^{\text{Har}}$</td>
<td>S</td>
<td>-</td>
</tr>
<tr>
<td>Mean Value</td>
<td>$\lambda^{\text{MV}}$</td>
<td>S</td>
<td>S</td>
</tr>
</tbody>
</table>
Numerical results confirm theoretical results

Mesh of ‘degenerate octagons’ with mean value coordinate basis functions

Poisson problem, Dirichlet BCs for exact solution $u(x, y) = \sin(x)e^y$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$|u - u_h|_{L^2}$</th>
<th>$|\nabla (u - u_h)|_{L^2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.35e-3</td>
<td>7.56e-2</td>
</tr>
<tr>
<td>4</td>
<td>8.67e-4</td>
<td>3.60e-2, 1.07</td>
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<tr>
<td>8</td>
<td>2.18e-4</td>
<td>1.76e-2, 1.03</td>
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<tr>
<td>16</td>
<td>5.50e-5</td>
<td>8.73e-3, 1.01</td>
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<td>1.38e-5</td>
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<td>3.47e-6</td>
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<tr>
<td>128</td>
<td>8.69e-7</td>
<td>1.09e-3, 1.00</td>
</tr>
</tbody>
</table>
A naïve quadratic element is formed by products of linear element basis functions:

\[ \{ \lambda_i \} \xrightarrow{\text{pairwise products}} \{ \lambda_a \lambda_b \} \]

Why is this naïve?

- For an \( n \)-gon, this construction gives \( n + \binom{n}{2} \) basis functions \( \lambda_a \lambda_b \)
- The space of quadratic polynomials is only dimension 6: \( \{1, x, y, xy, x^2, y^2\} \)
- Conforming to a linear function on the boundary requires 2 degrees of freedom per edge \( \Rightarrow \) only 2n functions needed!

Problem Statement

Construct 2n basis functions associated to the vertices and edge midpoints of an arbitrary \( n \)-gon such that a quadratic convergence estimate is obtained.
For quadrilaterals, the ‘serendipity’ element for rectangles has long been known to provide quadratic convergence.


The technique works more generally for affine mappings of the reference element to a physical element (‘affine’ = preserves collinearity and ratios of distances)

For non-affine meshes of quadrilaterals, however, the serendipity construction is known to provide sub-optimal convergence.

### Mapped bi-quadratic elements

<table>
<thead>
<tr>
<th>$n$</th>
<th>$|u - u_h|_{L^2}$ err.</th>
<th>$%$</th>
<th>Rate</th>
</tr>
</thead>
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<tr>
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<td>2.877</td>
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<td>4</td>
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<td>64</td>
<td>1.1e-06</td>
<td>0.000</td>
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<td>4.5e-01</td>
<td>37.253</td>
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<tr>
<td>1.1e-01</td>
<td>9.333</td>
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<tr>
<td>2.8e-02</td>
<td>2.329</td>
<td>2.0</td>
</tr>
<tr>
<td>7.1e-03</td>
<td>0.583</td>
<td>2.0</td>
</tr>
<tr>
<td>1.8e-03</td>
<td>0.146</td>
<td>2.0</td>
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<td>4.4e-04</td>
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<td>8.7e-05</td>
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<td>3.0</td>
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<td>1.1e-05</td>
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<tr>
<td>5.7e-04</td>
<td>0.047</td>
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### Serendipity elements

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<tr>
<td>5.0e-02</td>
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<tr>
<td>4.9e-03</td>
<td>0.401</td>
<td>1.1</td>
</tr>
</tbody>
</table>

Generalized barycentric quadrilateral elements

- Generalized barycentric coordinates allow for a quadratic serendipity construction on any quadrilateral.
- Since the analysis holds for affine mappings, these serve as reference elements for a wider range of quadrilaterals.
- The trapezoidal meshes satisfy the geometry bounds and hence we can recover the optimal convergence rate.

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<td>256</td>
<td>1.20e-9 3.00</td>
<td>1.64e-6 1.96</td>
</tr>
</tbody>
</table>

**Rand, G., Bajaj** *Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates*, Submitted, 2011
We define matrices $A$ and $B$ to reduce the naïve quadratic basis.

**filled dot** = Lagrangian domain point

= all functions in the set evaluate to 0

except the associated function which evaluates to 1

**open dot** = non-Lagrangian domain point

= partition of unity satisfied, but not Lagrange property

\[
\{\lambda_i\} \xrightarrow{\text{pairwise products}} \{\mu_{ab}\} \xrightarrow{A} \{\xi_{ij}\} \xrightarrow{B} \{\psi_{ij}\}
\]

- Linear
- Quadratic
- Serendipity
- Lagrange

\[
n \quad n + \binom{n}{2} \quad 2n \quad 2n
\]
Serendipity basis functions $\xi_{ij}$ are constructed as a linear combination of pairwise product functions $\mu_{ab}$:

$$[\xi_{ij}] = A \begin{bmatrix} \mu_{aa} \\ \mu_{a(a+1)} \\ \mu_{ab} \end{bmatrix} = \begin{bmatrix} 1 & c_{ij}^{ab} \end{bmatrix} \begin{bmatrix} \mu_{aa} \\ \mu_{a(a+1)} \\ \mu_{ab} \end{bmatrix}$$

The quadratic basis is ordered as follows:

- $\mu_{aa}$ = basis functions associated with vertices
- $\mu_{a(a+1)}$ = basis functions associated with edge midpoints
- $\mu_{ab}$ = basis functions associated with interior diagonals, i.e. $b \notin \{a - 1, a, a + 1\}$

- The first two types are left alone, resulting in the identity matrix above.
- The $c_{ij}^{ab}$ values define how the interior basis functions are added into the boundary basis functions.
From quadratic to serendipity

We require the serendipity basis to have quadratic approximation power:

- **Constant precision (CP):** \[ \sum_i \xi_{ii} + 2\xi_{i(i+1)} = 1. \]

- **Linear precision (LP):** \[ \sum_i v_i \xi_{ii} + 2v_{i(i+1)}\xi_{i(i+1)} = x. \]

- **Quadratic precision (QP):** \[ \sum_i v_i v_i^T \xi_{ii} + (v_i v_{i+1}^T + v_{i+1} v_i^T)\xi_{i(i+1)} = xx^T. \]

- Six constraints (CP, LP, QP) \(\Rightarrow\) six non-zero \(c_{ab}^{ij}\) per column.

- We select (arbitrarily) that \(\mu_{ab}\) contributes to \(\xi_{a,a}\), \(\xi_{b,b}\), and their neighbors.

**Theorem**

Constants \(\{c_{ij}^{ab}\}\) exist for any convex polygon such that the resulting basis \(\{\xi_{ij}\}\) satisfies the CP, LP, and QP requirements.
Pairwise products vs. Lagrange basis

Pairwise products of barycentric functions do not form a Lagrange basis at interior degrees of freedom:

Translation between these two bases is straightforward and generalizes to the higher dimensional case...
From serendipity to Lagrange

$$\{\xi_{ij}\} \xrightarrow{B} \{\psi_{ij}\}$$

$$\begin{bmatrix} \psi_{11} \\ \psi_{22} \\ \vdots \\ \psi_{nn} \\ \psi_{12} \\ \vdots \\ \psi_{1n} \end{bmatrix} = B \begin{bmatrix} \xi_{11} \\ \xi_{22} \\ \vdots \\ \xi_{nn} \\ \xi_{12} \\ \vdots \\ \xi_{1n} \end{bmatrix}.$$
Serendipity Theorem

Given bounds on polygon aspect ratio (G1), minimum edge length (G2), and maximum interior angles (G3):

- \( \|A\| \) is uniformly bounded,
- \( \|B\| \) is uniformly bounded, and
- The basis \( \{\psi_{ij}\} \) interpolates smooth data with \( O(h^2) \) error.

Rand, G., Bajaj *Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates*, Submitted, 2011
Outline

1. Motivation: Why DEC needs polygonal finite elements
2. Background: What are polygonal finite elements?
3. Results: Linear and quadratic Lagrange-like elements
4. Conclusions and looking ahead
What DEC has and what it needs

Discrete Exterior Calculus can now make use of these types of elements...

... but it still needs ...

linear  quadratic

vector  higher order

3D    analogous operators
Questions?

- Slides and pre-prints available at http://ccom.ucsd.edu/~agillette