Discrete Exterior Calculus and Polygonal Finite Elements

Andrew Gillette

joint work with Chandrajit Bajaj and Alexander Rand

Department of Mathematics
University of California, San Diego

http://ccom.ucsd.edu/∼agillette/

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

Duality arises from physics

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	$\underbrace{\text{div } b = 0}_{\text{Gauss' law}} \quad \underbrace{\mu b = h}_{\text{constitutive relation}} \quad \underbrace{\text{curl } h = j}_{\text{Ampère's law}}$
BOUNDARY	$\Gamma = \Gamma^e \cup \Gamma^h$, $\hat{n} \cdot b = 0$ on Γ^e, $\hat{n} \times h = 0$ on Γ^h.

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

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

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

Exterior calculus characterizes the problem

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

$$\begin{array}{ccccccc} & & h & & b & & \\ & & \Downarrow & & \Downarrow & & \\ H^1 & \xrightarrow[\text{grad}]{} & H(\text{curl}) & \xrightarrow[\text{curl}]{} & H(\text{div}) & \xrightarrow[\text{div}]{} & L^2 \end{array}$$

- The exterior derivative operator generalizes curl and div .

$$\begin{array}{ccccccc} & & h & & b & & \\ & & \Downarrow & & \Downarrow & & \\ \Lambda^0 & \xrightarrow{d_0} & \Lambda^1 & \xrightarrow{d_1} & \Lambda^2 & \xrightarrow{d_2} & \Lambda^3 \end{array}$$

- The Hodge star operation generalizes the duality relation $*b = h$

$$\begin{array}{ccc} h & & b \\ \Downarrow & & \Downarrow \\ \Lambda^{3-2} & \xleftarrow[*]{\mu} & \Lambda^2 \end{array}$$

Exterior calculus describes duality

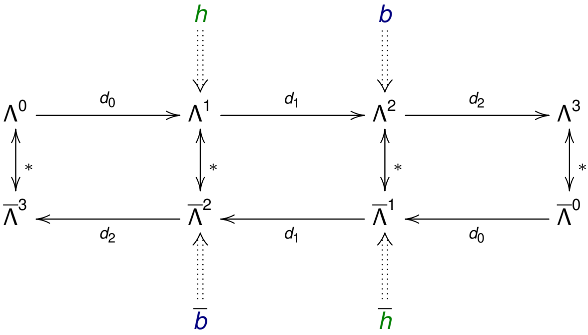
- The Hodge star is an isometry

$$*\Lambda^k \cong \Lambda^{n-k}$$

For instance, when $n = 3$,

$$dydz \xleftrightarrow{\;*\;} dx$$

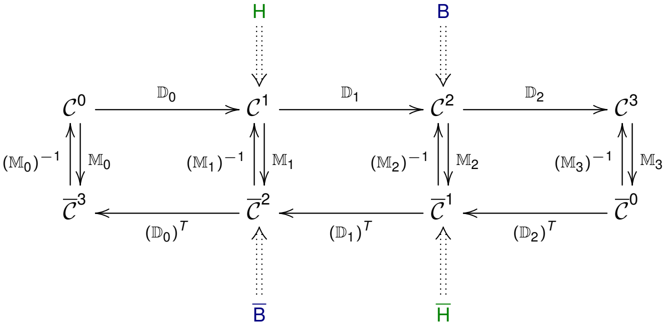
- This suggests **two** canonical treatments from exterior calculus:



DEC describes discrete duality

- The spaces and operators can be discretized by DEC

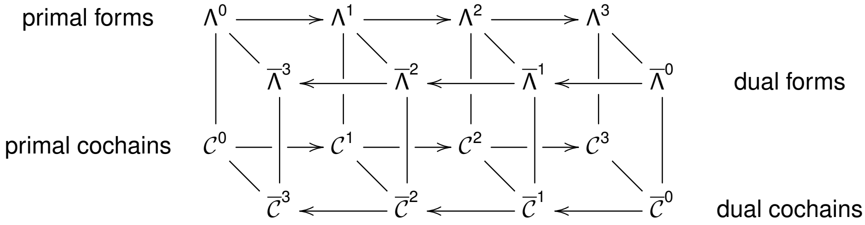
  Desbrun, Hirani, Leok, Marsden; Arnold, Falk, Winther; Bossavit; Shashkov,. . .
- The two treatments are similarly described in the discrete setting:

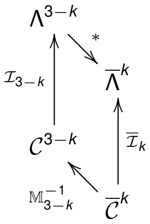


- $\mathcal{C}^k$ and $\overline{\mathcal{C}}^k$ are primal and dual cochain spaces
- $\mathbb{D}_k$ maps are the transposes of adjacency matrices, approximating d
- $\mathbb{M}_k$ maps are square matrices, approximating the local metric (like $*$)

Two ways to recover dual mesh data

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





1. Use primal interpolant: $*\mathcal{I}_{3-k}\mathbb{M}_{3-k}^{-1} : \overline{\mathcal{C}}^k \to \overline{\Lambda}^k$
2. Define dual interpolant: $\overline{\mathcal{I}}_k : \overline{\mathcal{C}}^k \to \overline{\Lambda}^k$

Discretization Stability with $*\mathcal{I}_{3-k}\mathbb{M}_{3-k}^{-1}$

Recall the magnetostatics problem:

$$\underbrace{\text{div } b = 0}_{\text{Gauss' law}} \qquad \underbrace{\mu b = h}_{\text{constitutive relation}} \qquad \underbrace{\text{curl } h = j}_{\text{Ampère's law}}$$

Theorem [Bossavit, 2000]

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

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

There exists a constant C dependent on $||b||_{[H^1]^3}$ but independent of $\mathrm{m_d}$, such that

$$||\mathcal{I}_2\mathrm{B} - b||_{H\Lambda^2} + \left|\left|*\mathcal{I}_2\mathbb{M}_2^{-1}\overline{\mathrm{H}} - h\right|\right|_{H\Lambda^1} \leq C\,\mathrm{m_d}.$$

where $\mathrm{m_d}$ denotes the maximum diameter of a mesh element.

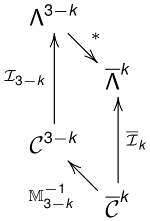
⇒BOSSAVIT *Comp. Electromag. and Geometry*, J. Japan Soc. App. Elec., 2000

Extensions and explanations of this approach in DEC terminology:

⇒G. *Stability of Dual Discretization Methods for PDEs*, Ph.D. Thesis, 2011

Dual mesh interpolation

What about the second approach?



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

For instance:

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

means

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

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

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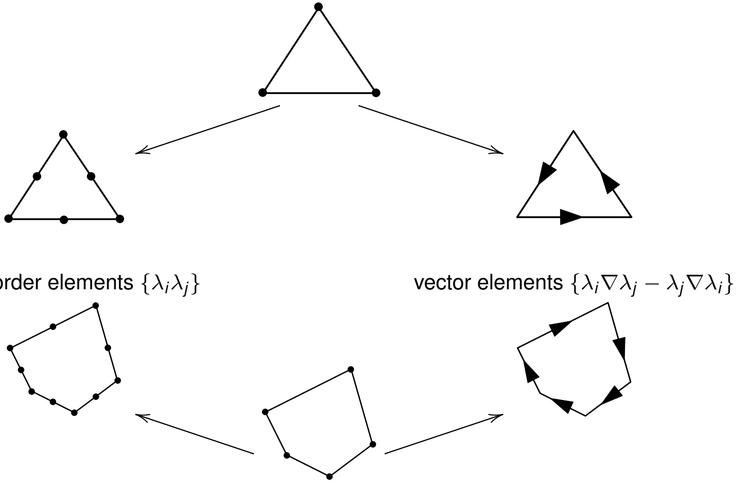
Overview of Approach

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



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

Definition

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

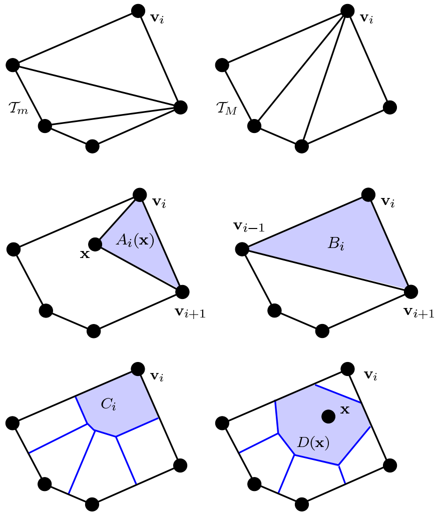
Any set of barycentric coordinates under this definition also satisfies:

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

Many generalizations to choose from . . .



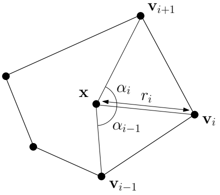
- Triangulation
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

$$0 \leq \lambda_i^{\mathcal{T}_m}(\mathbf{x}) \leq \lambda_i(\mathbf{x}) \leq \lambda_i^{\mathcal{T}_M}(\mathbf{x}) \leq 1$$

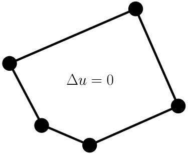
- Wachspress
  ⇒ WACHSPRESS, *A rational finite element basis*, 1975.

- Sibson
  ⇒ SIBSON, *A vector identity for the Dirichlet tessellation*, 1980.

Many generalizations to choose from . . .



- Mean value
  ⇒ FLOATER, *Mean value coordinates*, 2003.
  ⇒ FLOATER, KÓS, REIMERS, *Mean value coordinates in 3D*, 2005.



- Harmonic
  ⇒ WARREN, *Barycentric coordinates for convex polytopes*, 1996.
  ⇒ WARREN, SCHAEFER, HIRANI, DESBRUN, *Barycentric coordinates for convex sets*, 2007.

Many more in graphics contexts...

Outline

Optimal Convergence Estimates on Polygons

Let Ω be a convex polygon with vertices $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

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

$$\underbrace{\left|\left| u - \sum_{i=1}^{n} u(\mathbf{v}_i)\lambda_i \right|\right|_{H^1(\Omega)}}_{\text{approximation error}} \leq \underbrace{C \operatorname{diam}(\Omega) \, |u|_{H^2(\Omega)}}_{\text{optimal error bound}}, \quad \forall u \in H^2(\Omega). \tag{1}$$

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.

VERFÜRTH, *A note on polynomial approximation in Sobolev spaces*, Math. Mod. Num. An., 2008.
DEKEL, LEVIATAN, *The Bramble-Hilbert lemma for convex domains*, SIAM J. Math. An., 2004.

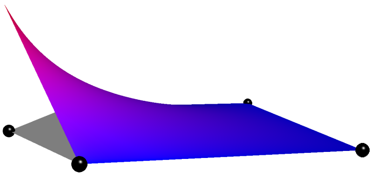
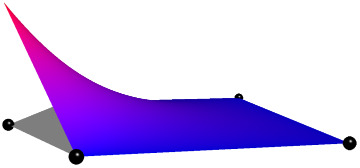
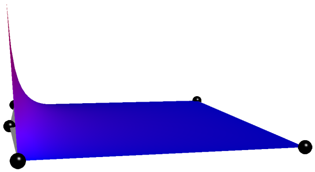
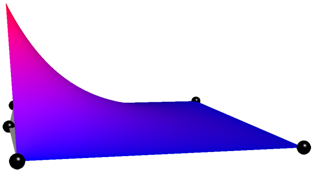
For (1), it suffices to prove an ***H^1*-interpolant estimate** over domains of diameter one:

$$\left|\left| \sum_{i=1}^{n} u(\mathbf{v}_i)\lambda_i \right|\right|_{H^1(\Omega)} \leq C_I \, ||u||_{H^2(\Omega)}, \quad \forall u \in H^1(\Omega). \tag{2}$$

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

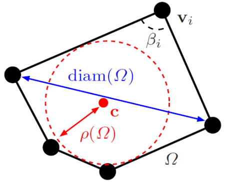
$$||\nabla \lambda_i||_{L^2(\Omega)} \leq C_\lambda. \tag{3}$$

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!

Geometric hypotheses for convergence estimates



Let $\rho(\Omega)$ denote the radius of the largest inscribed circle.
The **aspect ratio** γ 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 $|\mathbf{v}_i - \mathbf{v}_{i-1}| > d_*$

G3. Maximum interior angle: $\exists\ \beta^* < \pi$ such that $\beta_i < \beta^*$

Summary of convergence results

Theorem

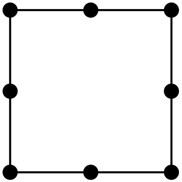
In the table below, any necessary geometric criteria to achieve the optimal convergence estimate are denoted by N. The collective set of geometric criteria denoted by S in each row are sufficient to guarantee the estimate.

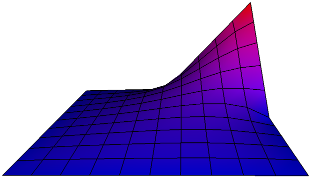
G., RAND, BAJAJ *Error Estimates for Generalized Barycentric Interpolation*, Advances in Computational Mathematics, in press, 2011.

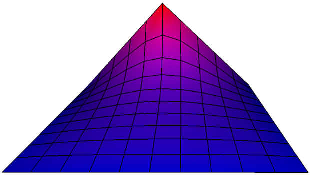
RAND, G., BAJAJ *Interpolation Error Estimates for Mean Value Coordinates*, in preparation, 2011.

		G1 aspect ratio	G2 min. edge	G3 max angle
Triangulated	λ^{Tri}	-	-	S,N
Wachspress	λ^{Wach}	S	S	S,N
Sibson	λ^{Sibs}	S	S	-
Harmonic	λ^{Har}	S	-	-
Mean Value	λ^{MV}	*S*	*S*	-

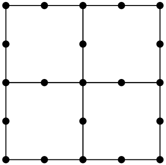
Numerical results confirm theoretical results



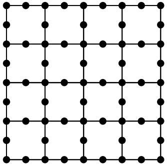




- Mesh of ‘degenerate octagons’ with mean value coordinate basis functions
- Poisson problem, Dirichlet BCs for exact solution $u(x,y) = \sin(x)e^y$



$n = 2$

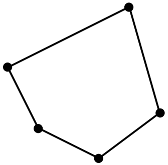


$n = 4$

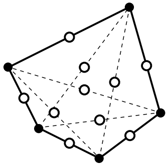
	$\|\|u - u_h\|\|_{L^2}$		$\|\|\nabla(u - u_h)\|\|_{L^2}$	
n	error	rate	error	rate
2	3.35e-3		7.56e-2	
4	8.67e-4	2.03	3.60e-2	1.07
8	2.18e-4	1.99	1.76e-2	1.03
16	5.50e-5	1.99	8.73e-3	1.01
32	1.38e-5	1.99	4.35e-3	1.00
64	3.47e-6	1.99	2.17e-3	1.00
128	8.69e-7	2.00	1.09e-3	1.00

From linear to quadratic elements

A naïve quadratic element is formed by products of linear element basis functions:



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



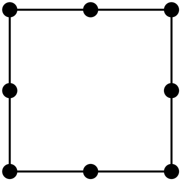
Why is this naïve?

- 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.

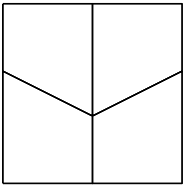
Prior work - Quadrilateral serendipity elements



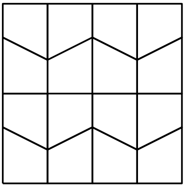
For quadrilaterals, the 'serendipity' element for **rectangles** has long been known to provide quadratic convergence.

STRANG, FIX, *An analysis of the finite element method*, 1973.
HUGHES, *The finite element method*, 1987.

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



$n = 2$



$n = 4$

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

ARNOLD, BOFFI, FALK, *Approximation by Quadrilateral Finite Elements*, Mathematics of Computation, 2002.

Failure for non-affine reference element mappings

Mapped biquadratic elements

	square meshes						trapezoidal meshes					
	$\|u-u_h\|_{L^2}$			$\|\nabla(u-u_h)\|_{L^2}$			$\|u-u_h\|_{L^2}$			$\|\nabla(u-u_h)\|_{L^2}$		
n	err.	%	rate	err.	%	rate	err.	%	rate	err.	%	rate
2	3.5e−02	2.877		4.5e−01	37.253		4.8e−02	3.951		5.9e−01	48.576	
4	4.4e−03	0.360	3.0	1.1e−01	9.333	2.0	5.8e−03	0.475	3.1	1.5e−01	12.082	2.0
8	5.5e−04	0.045	3.0	2.8e−02	2.329	2.0	7.1e−04	0.058	3.0	3.7e−02	3.017	2.0
16	6.9e−05	0.006	3.0	7.1e−03	0.583	2.0	8.7e−05	0.007	3.0	9.2e−03	0.753	2.0
32	8.6e−06	0.001	3.0	1.8e−03	0.146	2.0	1.1e−05	0.001	3.0	2.3e−03	0.188	2.0
64	1.1e−06	0.000	3.0	4.4e−04	0.036	2.0	1.3e−06	0.000	3.0	5.7e−04	0.047	2.0

Serendipity elements

	square meshes						trapezoidal meshes					
	$\|u-u_h\|_{L^2}$			$\|\nabla(u-u_h)\|_{L^2}$			$\|u-u_h\|_{L^2}$			$\|\nabla(u-u_h)\|_{L^2}$		
n	err.	%	rate	err.	%	rate	err.	%	rate	err.	%	rate
2	3.5e−02	2.877		4.5e−01	37.252		5.0e−02	4.066		6.2e−01	51.214	
4	4.4e−03	0.360	3.0	1.1e−01	9.333	2.0	6.7e−03	0.548	2.9	1.8e−01	14.718	1.8
8	5.5e−04	0.045	3.0	2.8e−02	2.329	2.0	9.7e−04	0.080	2.8	5.9e−02	4.836	1.6
16	6.9e−05	0.006	3.0	7.1e−03	0.583	2.0	1.6e−04	0.013	2.6	2.3e−02	1.890	1.4
32	8.6e−06	0.001	3.0	1.8e−03	0.146	2.0	3.3e−05	0.003	2.3	1.0e−02	0.842	1.2
64	1.1e−06	0.000	3.0	4.4e−04	0.036	2.0	7.4e−06	0.001	2.1	4.9e−03	0.401	1.1

ARNOLD, BOFFI, FALK, *Approximation by Quadrilateral Finite Elements*, 2002.

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.

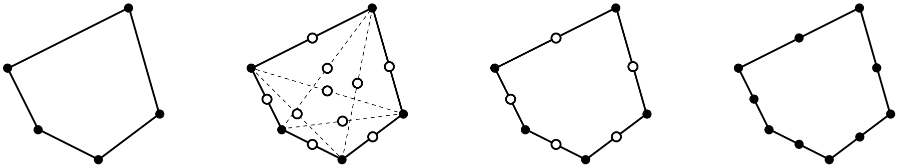
	$\|\|u - u_h\|\|_{L^2}$		$\|\|\nabla(u - u_h)\|\|_{L^2}$	
n	error	rate	error	rate
2	2.34e-3		2.22e-2	
4	3.03e-4	2.95	6.10e-3	1.87
8	3.87e-5	2.97	1.59e-3	1.94
16	4.88e-6	2.99	4.04e-4	1.97
32	6.13e-7	3.00	1.02e-4	1.99
64	7.67e-8	3.00	2.56e-5	1.99
128	9.59e-9	3.00	6.40e-6	2.00
256	1.20e-9	3.00	1.64e-6	1.96

RAND, G., BAJAJ *Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates*, Submitted, 2011

Polygonal Quadratic Serendipity Elements

We define matrices $\mathbb{A}$ and $\mathbb{B}$ to reduce the naïve quadratic basis.

$$\begin{aligned}
\textbf{filled dot} &= \text{Lagrangian domain point} \\
&= \text{all functions in the set evaluate to 0} \\
&\quad\ \text{except the associated function which evaluates to 1} \\
\textbf{open dot} &= \text{non-Lagrangian domain point} \\
&= \text{partition of unity satisfied, but not Lagrange property}
\end{aligned}$$



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

n	$n + \binom{n}{2}$	$2n$	$2n$
Linear	Quadratic	Serendipity	Lagrange

From quadratic to serendipity

Serendipity basis functions ξ_{ij} are constructed as a linear combination of pairwise product functions μ_{ab}:

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

The quadratic basis is ordered as follows:

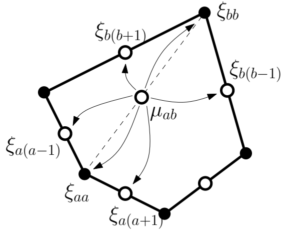
$$\begin{aligned} \mu_{aa} &= \text{basis functions associated with vertices} \\ \mu_{a(a+1)} &= \text{basis functions associated with edge midpoints} \\ \mu_{ab} &= \text{basis functions associated with interior diagonals,} \\ &\qquad \text{i.e. } b \notin \{a-1, a, a+1\} \end{aligned}$$

- The first two types are left alone, resulting in the identify matrix above.
- The c_{ab}^{ij} 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)**: $\sum_i \mathbf{v}_i \xi_{ii} + 2\mathbf{v}_{i(i+1)}\xi_{i(i+1)} = \mathbf{x}.$
- **Quadratic precision (QP)**: $\sum_i \mathbf{v}_i\mathbf{v}_i^T \xi_{ii} + (\mathbf{v}_i\mathbf{v}_{i+1}^T + \mathbf{v}_{i+1}\mathbf{v}_i^T)\xi_{i(i+1)} = \mathbf{x}\mathbf{x}^T.$



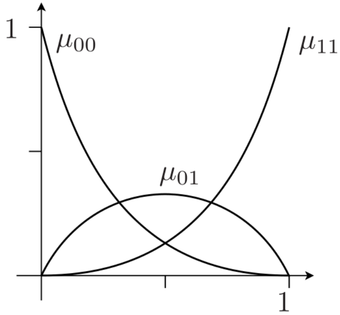
- Six constraints (CP, LP, QP) $\Rightarrow$ six non-zero c_{ab}^{ij} per column.
- We select (arbitrarily) that μ_{ab} contributes to $\xi_{a,a}$, $\xi_{b,b}$, and their neighbors.

Theorem

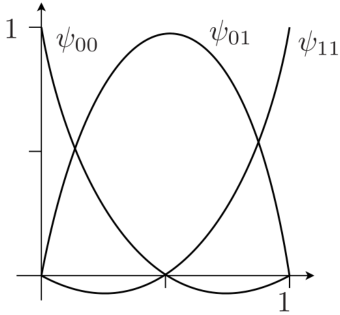
Constants $\{c_{ij}^{ab}\}$ exist for any convex polygon such that the resulting basis $\{\xi_{ij}\}$ satisfies the CP, LP, and QP requirements.

Pairwise products vs. Lagrange basis

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



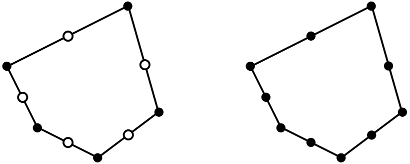
Pairwise products of barycentric functions



Lagrange basis

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

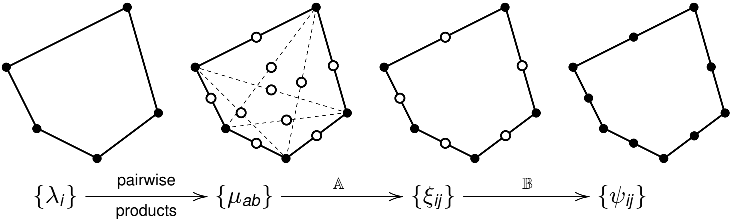
From serendipity to Lagrange



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

$$[\psi_{ij}] = \begin{bmatrix} \psi_{11} \\ \psi_{22} \\ \vdots \\ \psi_{nn} \\ \psi_{12} \\ \psi_{23} \\ \vdots \\ \psi_{1n} \end{bmatrix} = \left[\begin{array}{ccccc|ccccc} 1 & & & & & -1 & & \cdots & & -1 \\ & 1 & & & & -1 & -1 & \cdots & & \\ & & \ddots & & & & \ddots & \ddots & & \\ & & & \ddots & & & & \ddots & \ddots & \\ & & & & 1 & & & & -1 & -1 \\ \hline & & & & & 4 & & & & \\ & & & & & & 4 & & & \\ & & 0 & & & & & \ddots & & \\ & & & & & & & & \ddots & \\ & & & & & & & & & 4 \end{array}\right] \begin{bmatrix} \xi_{11} \\ \xi_{22} \\ \vdots \\ \xi_{nn} \\ \xi_{12} \\ \xi_{23} \\ \vdots \\ \xi_{1n} \end{bmatrix} = \mathbb{B}[\xi_{ij}].$$

Serendipity Theorem



Theorem

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

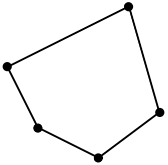
- $||\mathbb{A}||$ is uniformly bounded,
- $||\mathbb{B}||$ is uniformly bounded, and
- The basis $\{\psi_{ij}\}$ interpolates smooth data with $O(h^2)$ error.

RAND, G., BAJAJ *Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates*, Submitted, 2011

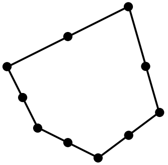
Outline

What DEC has and what it needs

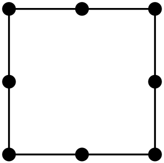
Discrete Exterior Calculus can now make use of these types of elements. . .



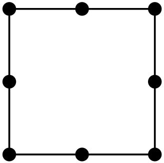
linear



quadratic

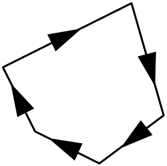


linear

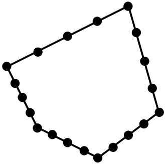


quadratic

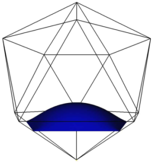
. . . but it still needs . . .



vector



higher order



3D

$\mathbb{D}_k^{\text{higher order}}$

$\mathbb{M}_k^{\text{higher order}}$

analogous operators

Questions?

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