Analysis and Applications of Polygonal and Serendipity Finite Element Methods

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What are *a priori* FEM error estimates?

Poisson's equation in 2D: Given a domain $\mathcal{D} \subset \mathbb{R}^2$ and $f : \mathcal{D} \to \mathbb{R}$, find u such that

$$\begin{array}{lrcll} \text{strong form} & -\Delta u & = & f & u \in H^2(\mathcal{D}) \\ \text{weak form} & \displaystyle\int_{\mathcal{D}} \nabla u \cdot \nabla \phi & = & \displaystyle\int_{\mathcal{D}} f\,\phi & \forall \phi \in H^1(\mathcal{D}) \\ \text{discrete form} & \displaystyle\int_{\mathcal{D}} \nabla u_h \cdot \nabla \phi_h & = & \displaystyle\int_{\mathcal{D}} f\,\phi_h & \forall \phi_h \in V_h \leftarrow \textit{finite dimen.} \subset H^1(\mathcal{D}) \end{array}$$

Typical **finite element method:**

$\to$ Mesh $\mathcal{D}$ by polygons $\{\Omega\}$ with vertices $\{\mathbf{v}_i\}$; define $h := \max \operatorname{diam}(\Omega)$.

$\to$ Fix $\boxed{\text{basis functions } \lambda_i}$ with local piecewise support, e.g. barycentric functions.

$\to$ Define u_h such that it uses the λ_i to approximate u, e.g. $\boxed{u_h := \sum_i u(\mathbf{v}_i)\lambda_i}$

A linear system for u_h can then be derived, admitting an ***a priori* error estimate:**

$$\underbrace{||u - u_h||_{H^1(\Omega)}}_{\text{approximation error}} \leq \underbrace{C\, h^{\,p}\, |u|_{H^2(\Omega)}}_{\text{optimal error bound}}, \quad \forall u \in H^{p+1}(\Omega),$$

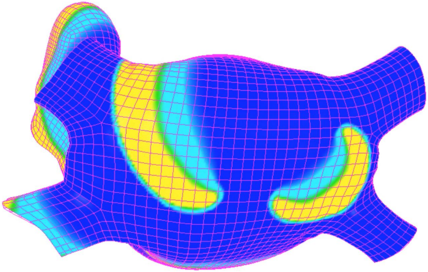
provided that the λ_i span all degree p polynomials on each polygon Ω.

Modern applications require new theory

$$||u - u_h||_{H^1(\Omega)} \leq C\, h^{\,p}\, |u|_{H^2(\Omega)}\,, \quad \forall u \in H^2(\Omega)$$

$\rightarrow$ Modern applications such as patient-specific cardiac electrophysiology need efficient, stable, error-bounded 'real-time' methods.

$\rightarrow$ These methods require both accurate geometry approximation (small h) and accurate function approximation (large p), but both are computationally expensive.



Two trends in Finite Element Methods research can help:

1 Polygonal & polyhedral generalized barycentric coordinate FEM

$\rightarrow$ Greater geometric flexibility from polygonal meshing can alleviate known difficulties with simplicial and cubical elements.

2 Serendipity finite element methods

$\rightarrow$ Long observed but only recently formalized theory ensuring order p function approximation with many fewer basis functions than 'expected.'

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The generalized barycentric coordinate approach

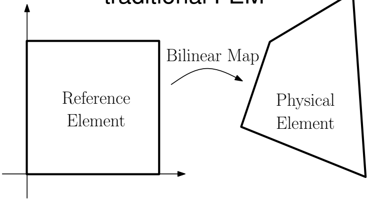
Fix $\Omega \subset \mathbb{R}^2$ a convex polygon with vertices $\mathbf{v}_1, \ldots, \mathbf{v}_n$. We call functions $\lambda_i : \Omega \to \mathbb{R}$ **generalized barycentric coordinates (GBCs)** if they satisfy:

$$\lambda_i \geq 0 \text{ on } \Omega \qquad\qquad L = \sum_{i=1}^{n} L(\mathbf{v}_i)\lambda_i, \quad \forall\, L : \Omega \to \mathbb{R} \text{ linear}$$

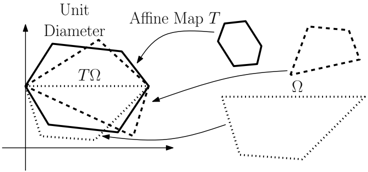
$\to$ Familiar properties are implied by this definition:

$$\underbrace{\sum_{i=1}^{n} \lambda_i \equiv 1}_{\text{partition of unity}} \qquad \underbrace{\sum_{i=1}^{n} \mathbf{v}_i \lambda_i(\mathbf{x}) = \mathbf{x}}_{\text{linear precision}} \qquad \underbrace{\lambda_i(\mathbf{v}_j) = \delta_{ij}}_{\text{interpolation}}$$

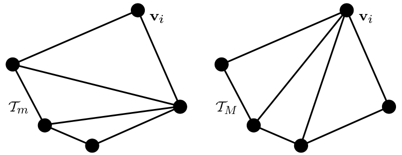
traditional FEM



family of **GBC** reference elements

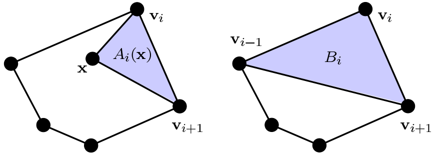


Many generalizations to choose from . . .

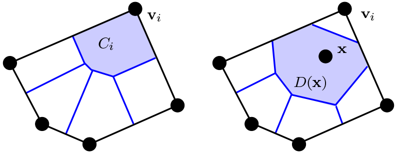


- Triangulation
  $\Rightarrow$ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

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

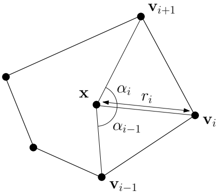


- Wachspress
  $\Rightarrow$ WACHSPRESS, *A Rational Finite Element Basis*, 1975.

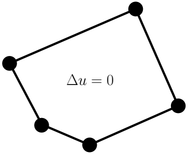


- Sibson / Laplace
  $\Rightarrow$ SIBSON, *A vector identity for the Dirichlet tessellation*, 1980.
  $\Rightarrow$ HIYOSHI, SUGIHARA, *Voronoi-based interpolation with higher continuity*, 2000.

Many generalizations to choose from ...



- Mean value
  $\Rightarrow$ FLOATER, *Mean value coordinates*, 2003.
  $\Rightarrow$ FLOATER, KÓS, REIMERS, *Mean value coordinates in 3D*, 2005.

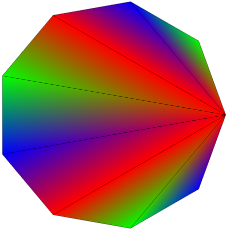


- Harmonic
  $\Rightarrow$ WARREN, *Barycentric coordinates for convex polytopes*, 1996.
  $\Rightarrow$ WARREN, SCHAEFER, HIRANI, DESBRUN, *Barycentric coordinates for convex sets*, 2007.
  $\Rightarrow$ CHRISTIANSEN, *A construction of spaces of compatible differential forms on cellular complexes*, 2008.

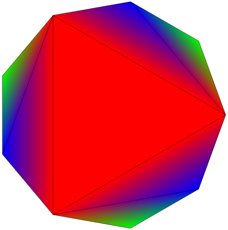
Many more papers could be cited (maximum entropy coordinates, moving least squares coordinates, surface barycentric coordinates, etc...)

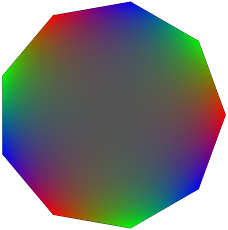
Comparison via ‘eyeball’ norm

Triangulated

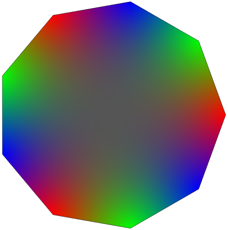


Triangulated





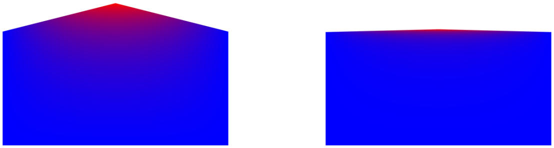
Wachspress



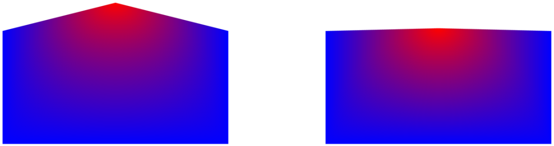
Mean Value

Comparison via ‘eyeball’ norm

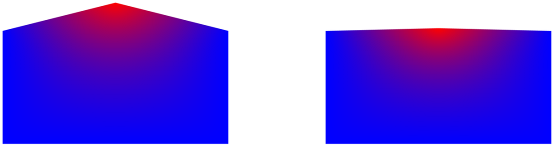
Wachspress



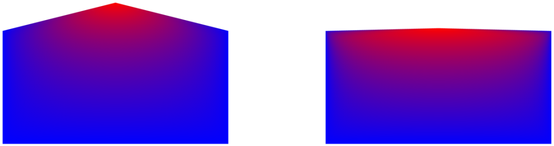
Sibson



Mean Value



Discrete Harmonic



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

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

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:

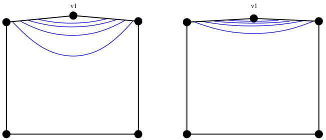
$$\left|\left| \sum_{i=1}^{n} u(\mathbf{v}_i)\lambda_i \right|\right|_{H^1(\Omega)} \leq C_I \,||u||_{H^2(\Omega)}, \quad \forall u \in H^1(\Omega). \tag{2}$$

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

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

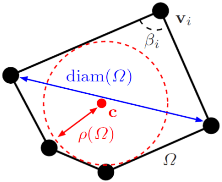
Geometric Hypotheses for Convergence Estimates

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



Let $\rho(\Omega)$ denote the radius of the largest inscribed circle. The **aspect ratio** γ is defined by

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



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	$\lvert\mathbf{v}_i - \mathbf{v}_{i-1}\rvert > d_*$
G3.	MAXIMUM INTERIOR ANGLE:	$\exists\ \beta^* < \pi$	such that	$\beta_i < \beta^*$

A key geometric proposition

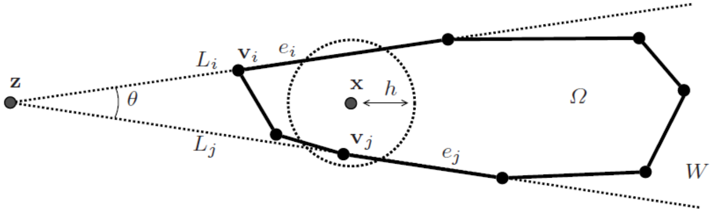
Proposition

Suppose **G1** (max aspect ratio γ^*) and **G2** (min edge length d_*) hold. Define

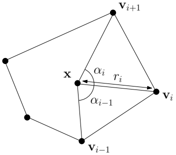
$$h_* := \frac{d_*}{2\gamma^*(1+d_*)} > 0$$

Then for all $\mathbf{x} \in \Omega$, $B(\mathbf{x}, h_*)$ does not intersect any two non-adjacent edges of Ω.

Proof: Suppose $B(\mathbf{x}, h)$ intersects two non-adjacent edges for some $h > 0$. The wedge W formed by these edges can be used to show that either **G1** fails (contradiction) or $h > h_*$.



Gradient bound for mean value coordinates



The **mean value coordinates** are defined by

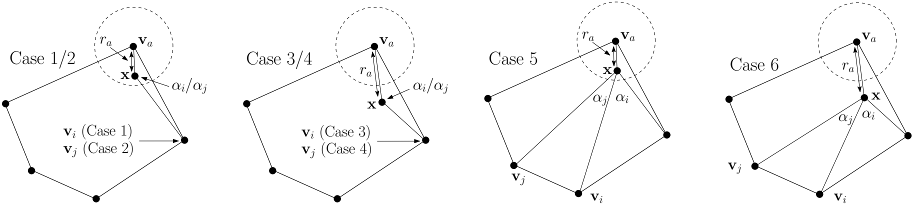
$$\lambda_i^{\mathrm{MV}}(\mathbf{x}) := \frac{w_i(\mathbf{x})}{\sum_{j=1}^{n} w_j(\mathbf{x})} \qquad w_i(\mathbf{x}) := \frac{\tan\left(\frac{\alpha_i(\mathbf{x})}{2}\right) + \tan\left(\frac{\alpha_{i-1}(\mathbf{x})}{2}\right)}{||\mathbf{v}_i - \mathbf{x}||}$$

Theorem

Suppose **G1** (max aspect ratio γ^*) and **G2** (min edge length d_*) hold. Let λ_i be the **mean value** coordinates. Then there exists $C_\lambda > 0$ such that

$$||\lambda_i||_{H^1(\Omega)} \leq C_\lambda$$

Proof: Divide analysis into six cases based on proximity to $\mathbf{v}_a$ and size of α_i and α_j



Polygonal Finite Element Optimal Convergence

Theorem

In the table, any necessary geometric criteria to achieve the ***a priori* linear error estimate** are denoted by N. The set of geometric criteria denoted by S in each row ***taken together*** are sufficient to guarantee the estimate.

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

G., Rand, Bajaj *Error Estimates for Generalized Barycentric Interpolation*
Advances in Computational Mathematics, 37:3, 417-439, 2012

Rand, G., Bajaj *Interpolation Error Estimates for Mean Value Coordinates*,
Advances in Computational Mathematics, in press, 2013.

Outline

1. Linear Polygonal Elements with GBCs
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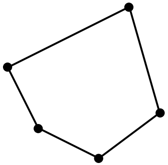
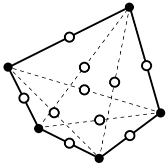
From linear to quadratic elements

A naïve quadratic element is formed by products of linear **GBCs**:



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



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

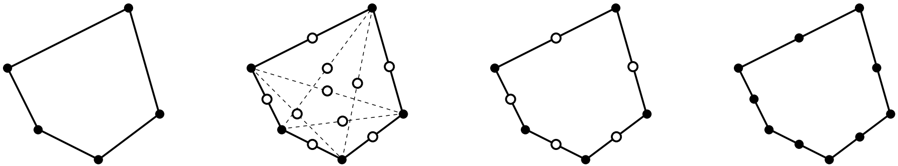
Construct $2n$ basis functions associated to the vertices and edge midpoints of an arbitrary n-gon such that a quadratic convergence estimate is obtained.

Polygonal Quadratic Serendipity Elements

We define matrices $\mathbb{A}$ and $\mathbb{B}$ 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



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

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

From quadratic to serendipity

The bases are ordered as follows:

ξ_{ii}	and	$\lambda_a\lambda_a$	= basis functions associated with vertices
$\xi_{i(i+1)}$	and	$\lambda_a\lambda_{a+1}$	= basis functions associated with edge midpoints
		$\lambda_a\lambda_b$	= basis functions associated with interior diagonals, i.e. $b \notin \{a-1, a, a+1\}$

Serendipity basis functions ξ_{ij} are a linear combination of pairwise products $\lambda_a\lambda_b$:

$$\begin{bmatrix} \xi_{ii} \\ \vdots \\ \xi_{i(i+1)} \end{bmatrix} = \mathbb{A} \begin{bmatrix} \lambda_a\lambda_a \\ \vdots \\ \lambda_a\lambda_{a+1} \\ \vdots \\ \lambda_a\lambda_b \end{bmatrix} = \begin{bmatrix} c_{11}^{11} & \cdots & c_{ab}^{11} & \cdots & c_{(n-2)n}^{11} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{ij} & \cdots & c_{ab}^{ij} & \cdots & c_{(n-2)n}^{ij} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{n(n+1)} & \cdots & c_{ab}^{n(n+1)} & \cdots & c_{(n-2)n}^{n(n+1)} \end{bmatrix} \begin{bmatrix} \lambda_a\lambda_a \\ \vdots \\ \lambda_a\lambda_{a+1} \\ \vdots \\ \lambda_a\lambda_b \end{bmatrix}$$

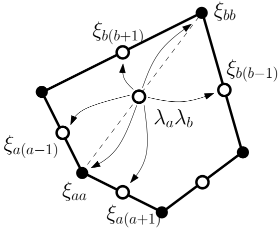
From quadratic to serendipity

We ***require*** the serendipity basis to have quadratic approximation power:

Constant precision: $1 = \sum_i \xi_{ii} + 2\xi_{i(i+1)}$

Linear precision: $\mathbf{x} = \sum_i \mathbf{v}_i\xi_{ii} + 2\mathbf{v}_{i(i+1)}\xi_{i(i+1)}$

Quadratic precision: $\mathbf{x}\mathbf{x}^T = \sum_i \mathbf{v}_i\mathbf{v}_i^T\xi_{ii} + (\mathbf{v}_i\mathbf{v}_{i+1}^T + \mathbf{v}_{i+1}\mathbf{v}_i^T)\xi_{i(i+1)}$



Theorem

Constants $\{c_{ij}^{ab}\}$ exist for **any** convex polygon such that the resulting basis $\{\xi_{ij}\}$ satisfies constant, linear, and quadratic precision requirements.

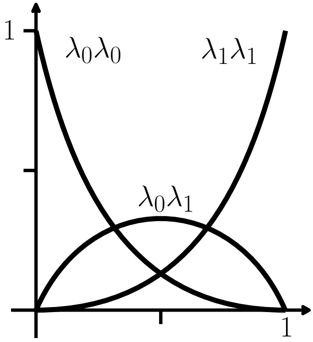
Proof: We produce a coefficient matrix $\mathbb{A}$ with the structure

$$\mathbb{A} := \left[\ \mathbb{I}\ \middle|\ \mathbb{A}'\ \right]$$

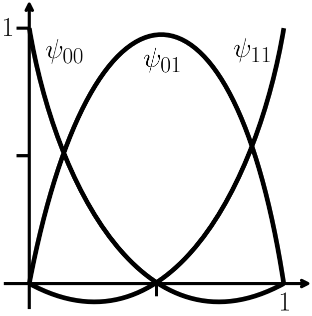
where $\mathbb{A}'$ has only six non-zero entries per column and show that the resulting functions satisfy the six precision equations.

Pairwise products vs. Lagrange basis

Even in 1D, pairwise products of barycentric functions do not form a Lagrange basis at interior degrees of freedom:



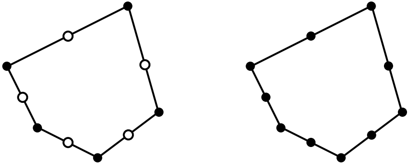
Pairwise products



Lagrange basis

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

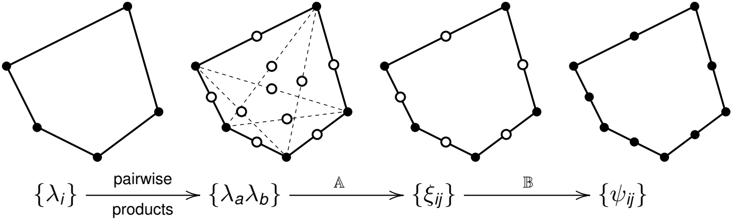
From serendipity to Lagrange



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

$$[\psi_{ij}] = \begin{bmatrix} \psi_{11} \\ \psi_{22} \\ \vdots \\ \psi_{nn} \\ \psi_{12} \\ \psi_{23} \\ \vdots \\ \psi_{n1} \end{bmatrix} = \left[\begin{array}{ccccc|ccccc}
1 & & & & & -1 & & \cdots & & -1 \\
& 1 & & & & -1 & -1 & \cdots & & \\
& & \ddots & & & & \ddots & \ddots & & \\
& & & \ddots & & & & \ddots & \ddots & \\
& & & & 1 & & & & -1 & -1 \\ \hline
& & & & & 4 & & & & \\
& & & & & & 4 & & & \\
& & 0 & & & & & \ddots & & \\
& & & & & & & & \ddots & \\
& & & & & & & & & 4
\end{array}\right] \begin{bmatrix} \xi_{11} \\ \xi_{22} \\ \vdots \\ \xi_{nn} \\ \xi_{12} \\ \xi_{23} \\ \vdots \\ \xi_{n1} \end{bmatrix} = \mathbb{B}[\xi_{ij}].$$

Serendipity Theorem



Theorem

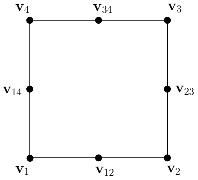
Given bounds on polygon aspect ratio (**G1**), minimum edge length (**G2**), and maximum interior angles (**G3**):

- $||\mathbb{A}||$ is uniformly bounded,
- $||\mathbb{B}||$ is uniformly bounded, and
- $\text{span}\{\psi_{ij}\} \supset \mathcal{P}_2(\mathbb{R}^2)$ = quadratic polynomials in x and y

We obtain the quadratic *a priori* error estimate: $\boxed{||u - u_h||_{H^1(\Omega)} \leq C\, h^{\mathbf{2}}\, |u|_{H^3(\Omega)}}$

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

Special case of a square



Bilinear functions are barycentric coordinates:

$$\begin{aligned}\lambda_1 &= (1-x)(1-y)\\ \lambda_2 &= x(1-y)\\ \lambda_3 &= xy\\ \lambda_4 &= (1-x)y\end{aligned}$$

Compute $[\xi_{ij}] := \left[\ \mathbb{I}\ \middle|\ \mathbb{A}'\ \right][\lambda_a\lambda_b]$

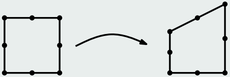
$$\begin{bmatrix}\xi_{11}\\ \xi_{22}\\ \xi_{33}\\ \xi_{44}\\ \xi_{12}\\ \xi_{23}\\ \xi_{34}\\ \xi_{14}\end{bmatrix} = \begin{bmatrix}1 & & 0 & -1 & 0\\ 0 & & 0 & 0 & -1\\ 0 & & 0 & -1 & 0\\ 0 & \cdots & 0 & 0 & -1\\ 0 & \cdots & 0 & 1/2 & 1/2\\ 0 & & 0 & 1/2 & 1/2\\ 0 & & 0 & 1/2 & 1/2\\ 0 & & 1 & 1/2 & 1/2\end{bmatrix}\begin{bmatrix}\lambda_1\lambda_1\\ \lambda_2\lambda_2\\ \lambda_3\lambda_3\\ \lambda_4\lambda_4\\ \lambda_1\lambda_2\\ \lambda_2\lambda_3\\ \lambda_3\lambda_4\\ \lambda_1\lambda_4\end{bmatrix} = \begin{bmatrix}(1-x)(1-y)(1-x-y)\\ x(1-y)(x-y)\\ xy(-1+x+y)\\ (1-x)y(y-x)\\ (1-x)x(1-y)\\ x(1-y)y\\ (1-x)xy\\ (1-x)(1-y)y\end{bmatrix}$$

$$\text{span}\left\{\xi_{ii},\xi_{i(i+1)}\right\} = \text{span}\left\{1,x,y,x^2,y^2,xy,x^2y,xy^2\right\} =: \mathcal{S}_2(I^2)$$

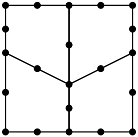
Hence, this provides a computational basis for the serendipity space $\mathcal{S}_2(I^2)$ defined in

ARNOLD, AWANOU *The serendipity family of finite elements*, Found. Comp. Math, 2011.

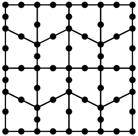
Numerical evidence for non-affine image of a square

Instead of mapping  ,
use quadratic serendipity **GBC** interpolation with mean value coordinates:

$$u_h = I_q u := \sum_{i=1}^{n} u(\mathbf{v}_i)\psi_{ii} + u\left(\frac{\mathbf{v}_i + \mathbf{v}_{i+1}}{2}\right)\psi_{i(i+1)}$$



$n = 2$



$n = 4$

Non-affine bilinear mapping

	$\|\|u - u_h\|\|_{L^2}$		$\|\|\nabla(u - u_h)\|\|_{L^2}$	
n	error	rate	error	rate
2	5.0e-2		6.2e-1	
4	6.7e-3	2.9	1.8e-1	1.8
8	9.7e-4	2.8	5.9e-2	1.6
16	1.6e-4	2.6	2.3e-2	1.4
32	3.3e-5	2.3	1.0e-2	1.2
64	7.4e-6	2.1	4.96e-3	1.1

ARNOLD, BOFFI, FALK, Math. Comp., 2002

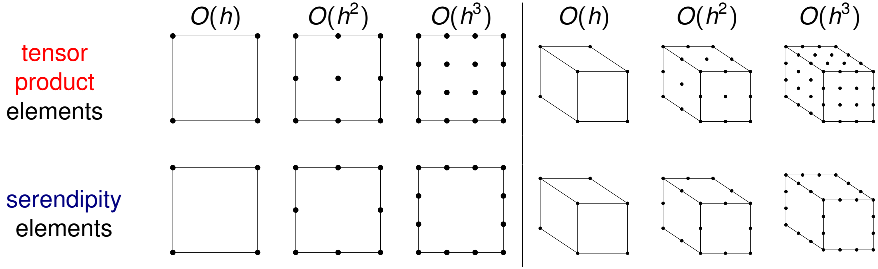
Quadratic serendipity **GBC** method

	$\|\|u - u_h\|\|_{L^2}$		$\|\|\nabla(u - u_h)\|\|_{L^2}$	
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

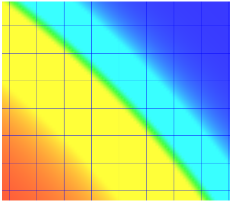
Outline

Serendipity Spaces on Cubes in $\mathbb{R}^d$

Tensor product methods on cubical meshes in $\mathbb{R}^d$ are well known, but serendipity methods will converge at the *same rate* with *fewer basis functions* per element:



Example: For $O(h^3)$, $d = 3$, 50% fewer functions $\rightarrow$ $\boxed{\approx 50\% \text{ smaller linear system}}$



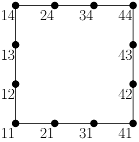
$\rightarrow$ Many modern applications use tensor product elements, often due to ease of implementation.

$\rightarrow$ Serendipity elements can reduce computation time, but implementation requires a geometric decomposition.

What is a geometric decomposition?

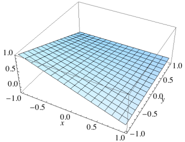
A **geometric decomposition** for a finite element space is an explicit correspondence:

$$\left\{\begin{matrix} 1, x, y, x^2, y^2, xy, \\ x^3, y^3, x^2y, xy^2, \\ x^3y, xy^3 \end{matrix}\right\} \longleftrightarrow \left\{\begin{matrix} \vartheta_{11}, \vartheta_{14}, \vartheta_{41}, \vartheta_{44}, \\ \vartheta_{12}, \vartheta_{13}, \vartheta_{42}, \vartheta_{43}, \\ \vartheta_{21}, \vartheta_{31}, \vartheta_{24}, \vartheta_{34} \end{matrix}\right\} \longleftrightarrow$$

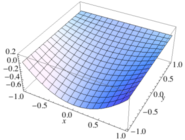


monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

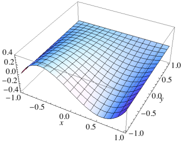
$\rightarrow$ Previously known basis functions employ Legendre polynomials
$\rightarrow$ These functions bear no symmetrical correspondence to the domain points



$\frac{1}{4}(x-1)(y-1)$
vertex



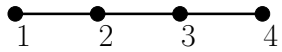
$-\frac{1}{4}\sqrt{\frac{3}{2}}\left(x^2-1\right)(y-1)$
edge (quadratic)



$-\frac{1}{4}\sqrt{\frac{5}{2}}x\left(x^2-1\right)(y-1)$
edge (cubic)

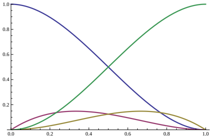
SZABÓ AND I. BABUŠKA *Finite element analysis*, Wiley Interscience, 1991.

Cubic Hermite Geometric Decomposition: 1D

$\{1, x, x^2, x^3\}$	$\longleftrightarrow$	$\{\psi_1, \psi_2, \psi_3, \psi_4\}$	$\longleftrightarrow$	
	approxim.		*geometry*	
monomials	$\longleftrightarrow$	**basis functions**	$\longleftrightarrow$	**domain points**

Cubic Hermite Basis on $[0, 1]$

$$\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} := \begin{bmatrix} 1 - 3x^2 + 2x^3 \\ x - 2x^2 + x^3 \\ x^2 - x^3 \\ 3x^2 - 2x^3 \end{bmatrix}$$

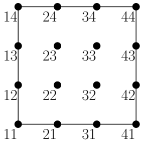


Approximation: $x^r = \sum_{i=1}^{4} \varepsilon_{r,i}\psi_i$, for $r = 0, 1, 2, 3$, where $[\varepsilon_{r,i}] = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & -2 & 1 \\ 0 & 0 & -3 & 1 \end{pmatrix}$

Geometry: $u = u(0)\psi_1 + u'(0)\psi_2 - u'(1)\psi_3 + u(1)\psi_4, \qquad \forall u \in \underbrace{\mathcal{P}_3([0,1])}_{\text{cubic polynomials}}$

Cubic Hermite Geometric Decomposition: 2D

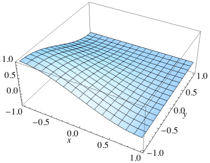
$$\underbrace{\left\{\begin{array}{c} x^r y^s \\ 0 \le r,s \le 3 \end{array}\right\}}_{\mathcal{Q}_3([0,1]^2)} \quad \longleftrightarrow \quad \left\{\begin{array}{c} \psi_i(x)\psi_j(y) \\ 1 \le i,j \le 4 \end{array}\right\} \quad \longleftrightarrow$$



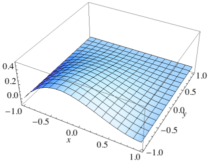
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s = \sum_{i=1}^{4} \sum_{j=1}^{4} \varepsilon_{r,i}\varepsilon_{s,j}\psi_{ij}$, for $0 \le r,s \le 3$, $\varepsilon_{r,i}$ as in 1D.

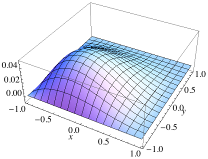
Geometry:



ψ_{11}



ψ_{21}

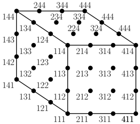


ψ_{22}

$$u = u|_{(0,0)}\psi_{11} + \partial_x u|_{(0,0)}\psi_{21} + \partial_y u|_{(0,0)}\psi_{12} + \partial_x\partial_y u|_{(0,0)}\psi_{22} + \cdots, \qquad \forall u \in \mathcal{Q}_3([0,1]^2)$$

Cubic Hermite Geometric Decomposition: 3D

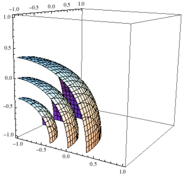
$$\underbrace{\left\{ \begin{array}{c} x^r y^s z^t \\ 0 \leq r, s, t \leq 3 \end{array} \right\}}_{\mathcal{Q}_3([0,1]^3)} \quad \longleftrightarrow \quad \begin{array}{c} \psi_i(x)\psi_j(y)\psi_k(z) \\ 1 \leq i, j, k \leq 4 \end{array} \quad \longleftrightarrow$$



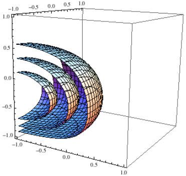
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s z^t = \sum_{i=1}^{4} \sum_{j=1}^{4} \sum_{k=1}^{4} \varepsilon_{r,i}\varepsilon_{s,j}\varepsilon_{t,k}\psi_{ijk}$, for $0 \leq r, s, t \leq 3$, $\varepsilon_{r,i}$ as in 1D.

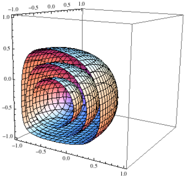
Geometry: Contours of level sets of the basis functions:



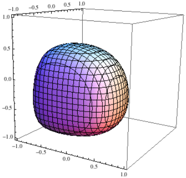
ψ_{111}



ψ_{112}



ψ_{212}



ψ_{222}

Two families of finite elements on cubical meshes

$\mathcal{Q}_r\Lambda^k([0,1]^n) \longrightarrow$ standard tensor product spaces ($\leq$ degree r in each variable)

early work: Raviart, Thomas 1976, Nedelec 1980
more recently: Arnold, Boffi, Bonizzoni arXiv:1212.6559, 2012

$\mathcal{S}_r\Lambda^k([0,1]^n) \longrightarrow$ serendipity finite element spaces (superlinear degree r)

early work: Strang, Fix *An analysis of the finite element method* 1973
more recently: Arnold, Awanou FoCM 11:3, 2011, and arXiv:1204.2595, 2012.

The **superlinear** degree of a polynomial ignores linearly-appearing variables.

$$n=2: \quad \{\overbrace{\underbrace{1,x,y,x^2,y^2,xy,x^3,y^3,x^2y,xy^2,x^3y,xy^3}_{\mathcal{S}_3\Lambda^0([0,1]^2)\ \text{(dim=12)}},x^2y^2,x^3y^2,x^2y^3,x^3y^3}^{\mathcal{Q}_3\Lambda^0([0,1]^2)\ \text{(dim=16)}}\}$$

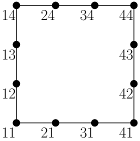
$$n=3: \quad \{\overbrace{\underbrace{1,\ldots,xyz,\ \ x^3y,x^3z,y^3z,\ldots,x^3yz,xy^3z,xyz^3}_{\mathcal{S}_3\Lambda^0([0,1]^3)\ \text{(dim=32)}},x^3y^2,\ldots,x^3y^3z^3}^{\mathcal{Q}_3\Lambda^0([0,1]^3)\ \text{(dim=64)}}\}$$

$\mathcal{Q}_r\Lambda^k$ and $\mathcal{S}_r\Lambda^k$ and have the **same** key mathematical properties needed for stability (degree, inclusion, trace, subcomplex, unisolvence, commuting projections)
but for fixed $k \geq 0$, $r, n \geq 2$ the serendipity spaces have **fewer** degrees of freedom

Cubic Hermite Serendipity Geom. Decomp: 2D

Theorem [G, 2012]: A Hermite-like geometric decomposition of $\mathcal{S}_3([0,1]^2)$ exists.

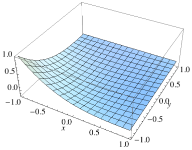
$$\underbrace{\left\{ \begin{array}{c} x^r y^s \\ \text{sldeg} \leq 3 \end{array} \right\}}_{\mathcal{S}_3([0,1]^2)} \quad \longleftrightarrow \quad \left\{ \begin{array}{c} \vartheta_{\ell m} \\ \text{(to be defined)} \end{array} \right\} \quad \longleftrightarrow$$



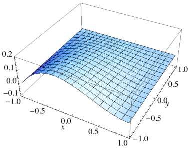
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s = \sum_{\ell m} \varepsilon_{r,i} \varepsilon_{s,j} \vartheta_{\ell m}$, for superlinear degree$(x^r y^s) \leq 3$

Geometry:



ϑ_{11}



ϑ_{21}

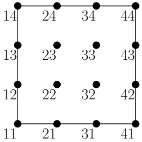
$$\begin{aligned} u &= u|_{(0,0)} \vartheta_{11} \\ &\quad + \partial_x u|_{(0,0)} \vartheta_{21} \\ &\quad + \partial_y u|_{(0,0)} \vartheta_{12} \\ &\quad + \cdots \end{aligned}$$

$\forall u \in \mathcal{S}_3([0,1]^2)$

Proof Overview: *(akin to quadratic approach on polygons)*

1 Fix index sets and basis orderings based on domain points:

$$\begin{aligned} V &= \text{vertices } (11, 14, \ldots) \\ E &= \text{edges } (12, 13, \ldots) \\ D &= \text{interior } (22, 23, \ldots) \end{aligned} \quad \longleftrightarrow$$



$$[\vartheta_{\ell m}] := [\ \vartheta_{11}, \vartheta_{14}, \vartheta_{41}, \vartheta_{44},\quad \vartheta_{12}, \vartheta_{13}, \vartheta_{42}, \vartheta_{43}, \vartheta_{21}, \vartheta_{31}, \vartheta_{24}, \vartheta_{34}\ ],$$

$$[\psi_{ij}] := [\ \underbrace{\psi_{11}, \psi_{14}, \psi_{41}, \psi_{44}}_{\text{indices in } V},\ \underbrace{\psi_{12}, \psi_{13}, \psi_{42}, \psi_{43}, \psi_{21}, \psi_{31}, \psi_{24}, \psi_{34}}_{\text{indices in } E},\ \underbrace{\psi_{22}, \psi_{23}, \psi_{32}, \psi_{33}}_{\text{indices in } D}\ ]$$

2 Define a 12×16 matrix $\mathbb{H}$ with entries $h_{ij}^{\ell m}$ so that $\ell m \in V \cup E$, $ij \in V \cup E \cup D$.

3 Define the serendipity basis functions $\vartheta_{\ell m}$ via

$$\boxed{[\vartheta_{\ell m}] := \mathbb{H}[\psi_{ij}]}$$

and show that the approximation and geometry properties hold.

Cubic Hermite Serendipity Geom. Decomp: 2D

Proof Details:

$\boxed{\textbf{2}}$ Define a 12×16 matrix $\mathbb{H}$ with entries $h_{ij}^{\ell m}$ so that $\ell m \in V \cup E$, $ij \in V \cup E \cup D$.

$$\mathbb{H} := \left[\begin{array}{c|cccc} & -1 & 1 & 1 & -1 \\ & 1 & -1 & -1 & 1 \\ & 1 & -1 & -1 & 1 \\ & -1 & 1 & 1 & -1 \\ & -1 & 0 & 1 & 0 \\ \mathbb{I} & 0 & -1 & 0 & 1 \\ \text{(12x12 identity matrix)} & 1 & 0 & -1 & 0 \\ & 0 & 1 & 0 & -1 \\ & -1 & 1 & 0 & 0 \\ & 0 & 0 & -1 & 1 \\ & 1 & -1 & 0 & 0 \\ & 0 & 0 & 1 & -1 \end{array}\right]$$

$\boxed{\textbf{3}}$ Define $[\vartheta_{\ell m}] := \mathbb{H}[\psi_{ij}]$. The geometry property holds since for $\ell m \in V \cup E$,

$$\vartheta_{\ell m} = \underbrace{\psi_{\ell m}}_{\text{bicubic Hermite}} + \underbrace{\sum_{ij \in D} h_{ij}^{\ell m} \psi_{ij}}_{\text{zero on boundary}} \implies \vartheta_{\ell m} \equiv \psi_{\ell m} \ \text{ on edges}$$

Cubic Hermite Serendipity Geom. Decomp: 2D

Proof Details:

To prove that the approximation property holds, observe:

$$[\vartheta_{\ell m}] := \mathbb{H}[\psi_{ij}] \quad \text{implies} \quad \sum_{ij} h_{ij}^{\ell m}\psi_{ij} = \vartheta_{\ell m}$$

For all (r, s) pairs such that $\text{sldeg}(x^r y^s) \leq 3$, the matrix entries in column ij satisfy

$$\varepsilon_{r,i}\varepsilon_{s,j} = \sum_{\ell m \in V \cup E} \varepsilon_{r,\ell}\varepsilon_{s,m} h_{ij}^{\ell m}$$

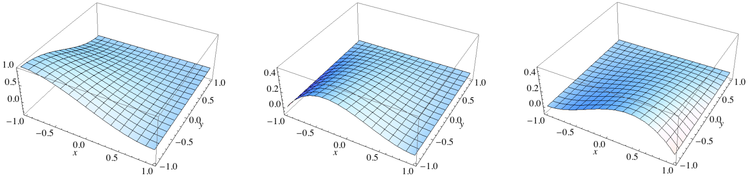
Substitute these into the Hermite 2D approximation property:

$$\begin{aligned} x^r y^s &= \sum_{ij \in V \cup E \cup D} \varepsilon_{r,i}\varepsilon_{s,j}\psi_{ij} = \sum_{ij}\sum_{\ell m} \varepsilon_{r,\ell}\varepsilon_{s,m} h_{ij}^{\ell m}\psi_{ij} \\ &= \sum_{\ell m} \varepsilon_{r,\ell}\varepsilon_{s,m} \sum_{ij} h_{ij}^{\ell m}\psi_{ij} = \sum_{\ell m} \varepsilon_{r,\ell}\varepsilon_{s,m}\vartheta_{\ell m} \end{aligned}$$

Hence $[\vartheta_{\ell m}]$ is a basis for $\mathcal{S}_2([0,1]^2)$, completing the geometric decomposition. $\square$

Hermite Style Serendipity Functions (2D)

$$
[\vartheta_{\ell m}] = \begin{bmatrix} \vartheta_{11} \\ \vartheta_{14} \\ \vartheta_{41} \\ \vartheta_{44} \\ \vartheta_{12} \\ \vartheta_{13} \\ \vartheta_{42} \\ \vartheta_{43} \\ \vartheta_{21} \\ \vartheta_{31} \\ \vartheta_{24} \\ \vartheta_{34} \end{bmatrix} = \begin{bmatrix} -(x-1)(y-1)(-2+x+x^2+y+y^2) \\ (x-1)(y+1)(-2+x+x^2-y+y^2) \\ (x+1)(y-1)(-2-x+x^2+y+y^2) \\ -(x+1)(y+1)(-2-x+x^2-y+y^2) \\ -(x-1)(y-1)^2(y+1) \\ (x-1)(y-1)(y+1)^2 \\ (x+1)(y-1)^2(y+1) \\ -(x+1)(y-1)(y+1)^2 \\ -(x-1)^2(x+1)(y-1) \\ (x-1)(x+1)^2(y-1) \\ (x-1)^2(x+1)(y+1) \\ -(x-1)(x+1)^2(y+1) \end{bmatrix} \cdot \frac{1}{8}
$$

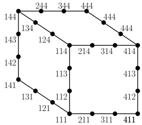


ϑ_{11} ϑ_{21} ϑ_{31}

Cubic Hermite Serendipity Geom. Decomp: 3D

Theorem [G, 2012]: A Hermite-like geometric decomposition of $\mathcal{S}_3([0,1]^3)$ exists.

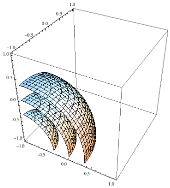
$$\underbrace{\left\{ \begin{array}{c} x^r y^s z^t \\ \text{sldeg} \leq 3 \end{array} \right\}}_{\mathcal{S}_3([0,1]^3)} \longleftrightarrow \left\{ \begin{array}{c} \vartheta_{\ell mn} \\ \text{(to be defined)} \end{array} \right\} \longleftrightarrow$$



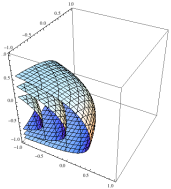
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s z^t = \sum_{\ell mn} \varepsilon_{r,i}\varepsilon_{s,j}\varepsilon_{t,k}\vartheta_{\ell mn}$, for superlinear degree$(x^r y^s z^t) \leq 3$

Geometry:



ϑ_{111}



ϑ_{112}

$$\begin{aligned} u &= u|_{(0,0,0)}\vartheta_{111} \\ &\quad + \partial_x u|_{(0,0,0)}\vartheta_{211} \\ &\quad + \partial_y u|_{(0,0,0)}\vartheta_{121} \\ &\quad + \partial_z u|_{(0,0,0)}\vartheta_{112} \\ &\quad + \cdots \end{aligned}$$

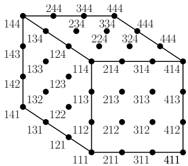
$\forall u \in \mathcal{S}_3([0,1]^3)$

Cubic Hermite Serendipity Geom. Decomp: 3D

Proof Overview:

1 Fix index sets and basis orderings based on domain points:

$$
\begin{aligned}
V &= \text{vertices } (111, \ldots) \\
E &= \text{edges } (112, \ldots) \\
F &= \text{face interior } (122, \ldots) \\
M &= \text{volume interior } (222, \ldots)
\end{aligned}
\qquad \longleftrightarrow
$$



$$
[\vartheta_{\ell mn}] := [\ \vartheta_{111}, \ldots, \vartheta_{444}, \ \ \vartheta_{112}, \ldots, \vartheta_{443}\ ],
$$

$$
[\psi_{ijk}] := [\ \underbrace{\psi_{111}, \ldots, \psi_{444},}_{\text{indices in } V} \ \underbrace{\psi_{112}, \ldots, \psi_{443},}_{\text{indices in } E} \ \underbrace{\psi_{122}, \ldots, \psi_{433},}_{\text{indices in } F} \ \underbrace{\psi_{222}, \ldots, \psi_{333}}_{\text{indices in } M}\ ]
$$

2 Define a 32×64 matrix $\mathbb{W}$ with entries $h_{ijk}^{\ell mn}$ (where $\ell mn \in V \cup E$)

3 Define the serendipity basis functions $\vartheta_{\ell mn}$ via

$$
\boxed{[\vartheta_{\ell mn}] := \mathbb{W}[\psi_{ijk}]}
$$

and show that the approximation and geometry properties hold.

Cubic Hermite Serendipity Geom. Decomp: 3D

Proof Details:

2 Define a 32×64 matrix $\mathbb{W}$ with entries $h_{ijk}^{\ell mn}$ so that $\ell mn \in V \cup E$

$$\mathbb{W} := \left[\begin{array}{c|c} \mathbb{I} & \text{specific full rank} \\ \text{(32x32 identity matrix)} & \text{32x32 matrix} \\ & \text{with entries -1, 0, or 1} \end{array} \right]$$

3 Define $[\vartheta_{\ell mn}] := \mathbb{W}[\psi_{ijk}]$.

$\longrightarrow$ Confirm directly that $[\vartheta_{\ell mn}]$ restricts to $[\vartheta_{\ell m}]$ on faces.

$\longrightarrow$ Similar proof technique confirms geometry and approximation properties.

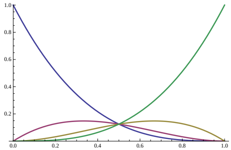
$$[\vartheta_{\ell mn}] = \begin{bmatrix} \vartheta_{111} \\ \vartheta_{114} \\ \vdots \\ \vartheta_{442} \\ \vartheta_{443} \end{bmatrix} = \begin{bmatrix} (x-1)(y-1)(z-1)(-2+x+x^2+y+y^2+z+z^2) \\ -(x-1)(y-1)(z+1)(-2+x+x^2+y+y^2-z+z^2) \\ \vdots \\ (x+1)(y+1)(z-1)^2(z+1) \\ -(x+1)(y+1)(z-1)(z+1)^2 \end{bmatrix} \cdot \frac{1}{16}$$

Complete list and more details in my paper:

GILLETTE *Hermite and Bernstein Style Basis Functions for Cubic Serendipity Spaces on Squares and Cubes*, arXiv:1208.5973, 2012

Cubic Bernstein Basis on $[0,1]$

$$\begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{bmatrix} := \begin{bmatrix}(1-x)^3\\ (1-x)^2x\\ (1-x)x^2\\ x^3\end{bmatrix}$$

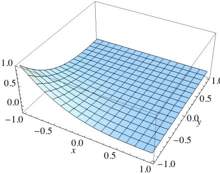


Theorem [G, 2012]: Bernstein-like geometric decompositions of $\mathcal{S}_3([0,1]^2)$ and $\mathcal{S}_3([0,1]^3)$ exist.

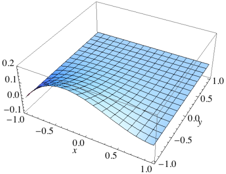
$$[\xi_{\ell m}] = \begin{bmatrix}\xi_{11}\\ \xi_{14}\\ \vdots\\ \xi_{24}\\ \xi_{34}\end{bmatrix} = \begin{bmatrix}(x-1)(y-1)(-2-2x+x^2-2y+y^2)\\ -(x-1)(y+1)(-2-2x+x^2+2y+y^2)\\ \vdots\\ (x-1)^2(x+1)(y+1)\\ -(x-1)(x+1)^2(y+1)\end{bmatrix}\cdot\frac{1}{16}$$

$$[\xi_{\ell mn}] = \begin{bmatrix}\xi_{111}\\ \xi_{114}\\ \vdots\\ \xi_{442}\\ \xi_{443}\end{bmatrix} = \begin{bmatrix}-(x-1)(y-1)(z-1)(-5-2x+x^2-2y+y^2-2z+z^2)\\ (x-1)(y-1)(z+1)(-5-2x+x^2-2y+y^2+2z+z^2)\\ \vdots\\ (x+1)(y+1)(z-1)^2(z+1)\\ -(x+1)(y+1)(z-1)(z+1)^2\end{bmatrix}\cdot\frac{1}{32}$$

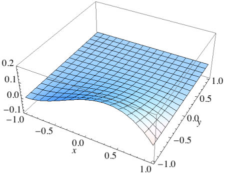
Bernstein Style Serendipity Functions (2D)



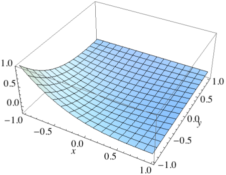
β_{11}



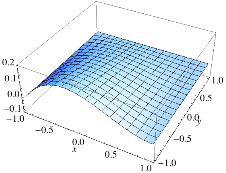
β_{21}



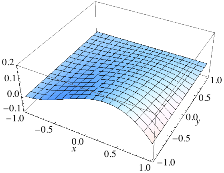
β_{31}



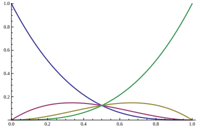
ξ_{11}



ξ_{21}



ξ_{31}

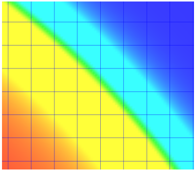


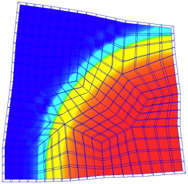
Bicubic Bernstein functions (top) and Bernstein-style serendipity functions (bottom).

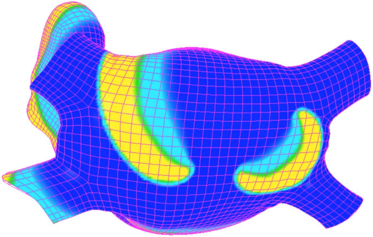
$\rightarrow$ Note boundary agreement with Bernstein functions.

Outline

Application: Cardiac Electrophysiology







$\rightarrow$ Cubic Hermite serendipity functions recently incorporated into Continuity software package for cardiac electrophysiology models.

$\rightarrow$ Used to solve the *monodomain* equations, a type of reaction-diffusion equations

$\rightarrow$ Initial results show agreement of serendipity and standard bicubics on a benchmark problem with a **4x computational speedup** in 3D.

$\rightarrow$ Fast computation essential to clinical applications and 'real time' simulations

GONZALEZ, VINCENT, G., MCCULLOCH *High Order Interpolation Methods in Cardiac Electrophysiology Simulation*, in preparation, 2013.

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Thanks for the opportunity to speak!

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